Weierstraß–Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Micro-macro transition by interpolation, smoothing/averaging and scaling of particle trajectories

Wolfgang Dreyer, Ralf Guckel

submitted: 15th March 2002

Weierstrass Institute for Applied Analysis and Stochastics
Mohrenstr. 39, D-10117 Berlin, Germany
e-mail: dreyer@wias-berlin.de

Preprint No. 725
Berlin 2002

Edited by
Weierstraß–Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
D — 10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail (X.400): c=de;a=d400-gw;p=WIAS-BERLIN;s=preprint
E-Mail (Internet): preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

We consider a Newtonian system of many diatomic molecules, each of which consisting of two atoms of equal mass, which are separated by a fixed distance. The barycenters are allowed to move along some fixed straight line. Moreover, each molecule has an additional rotational degree of freedom. The atoms of neighbouring molecules interact to each other by a generic pair potential. By means of this example we propose a new method for deriving macroscopic models from microscopic ones. The method is based on the definition of macroscopic observables and the derivation of corresponding balance laws by interpolation, smoothing/averaging and subsequent scaling of particle trajectories.

1 Introduction

The subject of micro-macro transitions can be outlined as follows. Assume we will describe some physical system on the microscopic or atomic scale. This involves a set of microscopic observables and parameters, measured in microscopic time and space units, along with an evolution equation, which determines the values of the observables from given initial and/or boundary values. The aim is to derive consequences that this microscopic system imposes on some larger, macroscopic scales. In particular, one wish to identify macroscopic observables and parameters as well as macroscopic governing equations which allow one to determine the macroscopic observables from given initial or/and boundary values by techniques from modern analysis. On the other hand, given any macroscopic law, one might as well ask, whether the expected solutions can in some sense be approximated and analyzed by particle solutions, that is by some microscopic law. Typically, the microscopic setting consists of a finite or infinite system of particles being governed by Newton's law, and the macroscopic setting consists of a closed system of partial differential equations, equipped with appropriate initial and boundary conditions.

In [3] macroscopic observables have been defined by means of what is called window function there. This means that macroscopic observables were defined by time and space averages in phase space of the microscopic solutions. There results an infinite sequence of coupled balance laws, and the so-called closure problem is to cut off this infinite sequence to get a finite system of equations, which one is able to handle. A remarkable feature of a wide class of particle solutions observed in [3] turned out to be their scale invariance.

The present paper is devoted to a seemingly new way to derive macroscopic models from microscopic ones. The key idea is to interpolate and/or smooth and/or average and scale the trajectories of the microscopic motion appropriately. The paper is organized as follows. In the next section we introduce the microscopic model. In section 3 we define observables by applying successively a linear interpolation and a smoothing/averaging operator to the particle trajectories. In contrast to [3], the smoothing/averaging is about particle indices, not about phase space. The same point of view is considered in [4] and recently in [1] and [2]. In fact, this idea results from the paper [4] which proves its usefullness for rigorous transitions between various scales. Furthermore, the averaging is spacelike only. In section 4 we present a few numerical results. In section 5 we introduce and investigate properties of sequences of macroscopic observables depending on two parameters, one of which representing a lattice parameter, the other one describing the amount of smoothing/averaging introduced. In section 6 we introduce the concept of Young measure valued solutions, [5], and illustrate this introduction with a simple explicit example.

2 The microscopic model

Let $M \in \mathbb{N}$. We consider a system of $N = 2M$ particles. These particles are arranged to form a set of diatomic molecules. Each molecule consists of two atoms of equal mass. We denote by $m > 0$ the molecular mass, and by $d > 0$ the molecular diameter, and we write

$$z_j = (x_j, y_j) , \quad j = 1, 2, \ldots, N , \tag{2.1}$$

for the cartesian coordinates of the particles. We introduce new coordinates $s_j \in \mathbb{R}$ (barycenter), $\alpha_j \in [0, 2\pi)$ (angle), $j = 1, 2, \ldots, M$ as follows:

$$x_j = s_j + \frac{1}{2} d \cos \alpha_j , \tag{2.2}$$

$$x_{j+M} = s_j - \frac{1}{2} d \cos \alpha_j , \tag{2.3}$$

$$y_j = \frac{1}{2} d \sin \alpha_j , \tag{2.4}$$

$$y_{j+M} = -\frac{1}{2} d \sin \alpha_j . \tag{2.5}$$

The physical system is assumed to be completely determined by a Hamiltonian

$$H = K + \Phi \tag{2.6}$$

with kinetic energy

$$\begin{aligned} K &= \sum_{j=1}^{N} \frac{1}{4} m |\dot{z}_j|^2 && (2.7) \\ &= \frac{1}{4} m \sum_{j=1}^{M} \left(|\dot{z}_j|^2 + |\dot{z}_{j+M}|^2 \right) && (2.8) \\ &= \frac{1}{2} m \sum_{j=1}^{M} \left(\dot{s}_j^2 + \frac{1}{4} d^2 \dot{\alpha}_j^2 \right) && (2.9) \end{aligned}$$

and potential energy

$$\begin{aligned} \Phi &= \frac{1}{4} \sum_{j=1}^{M-1} \Big(\varphi\big(|z_j - z_{j+1}|\big) + \varphi\big(|z_j - z_{j+M+1}|\big) + && (2.10) \\ &\qquad + \varphi\big(|z_{j+1} - z_{j+M}|\big) + \varphi\big(|z_{j+M} - z_{j+M+1}|\big) \Big) && (2.11) \\ &= \frac{1}{4} \sum_{j=1}^{M-1} \Big(\varphi\big(|z_j - z_{j+1}|\big) + \varphi\big(|z_j - z_{j+1} + d\zeta_{j+1}|\big) + && (2.12) \\ &\qquad + \varphi\big(|z_j - z_{j+1} - d\zeta_j|\big) + \varphi\big(|z_j - z_{j+1} + d(\zeta_{j+1} - \zeta_j)|\big) \Big) , && (2.13) \end{aligned}$$

where

$$\zeta_j = (\cos \alpha_j, \sin \alpha_j) \ . \qquad (2.14)$$

The function $\varphi : (0, \infty) \longrightarrow \mathbb{R}$ is a generic pair potential satisfying

$$\lim_{r \to 0} \varphi(r) = +\infty \ . \qquad (2.15)$$

The microscopic governing equations are

$$\begin{aligned} m \ddot{s}_j &= -\frac{\partial \Phi}{\partial s_j} , && (2.16) \\ \frac{1}{4} m d^2 \ddot{\alpha}_j &= -\frac{\partial \Phi}{\partial \alpha_j} . && (2.17) \end{aligned}$$

After a straightforward computation and some rearrangements we arrive at the system of equations depicted on pages 4, 5. From now on we shall assume that the system consists of infinitely many particles, $j \in \mathbb{Z}$. Moreover, we confine ourselves to the case of non-diffusive motion, that is

$$\max \left\{ s_j(t) \pm \frac{1}{2} d \cos \alpha_j(t) \right\} < \min \left\{ s_{j+1}(t) \pm \frac{1}{2} d \cos \alpha_{j+1}(t) \right\} \ , \quad j \in \mathbb{Z} \ , \quad t \geqslant 0 \ . \qquad (2.18)$$

$$
\begin{aligned}
m\ddot{s}_j = \ & \frac{1}{4}\Bigg\{ \frac{\varphi'(|z_{j+1}-z_j|)}{|z_{j+1}-z_j|}(x_{j+1}-x_j) - \frac{\varphi'(|z_j-z_{j-1}|)}{|z_j-z_{j-1}|}(x_j-x_{j-1}) + \\
& + \frac{\varphi'(|z_{j+1}-z_j-d\zeta_{j+1}|)}{|z_{j+1}-z_j-d\zeta_{j+1}|}(x_{j+1}-x_j-d\cos\alpha_{j+1}) - \frac{\varphi'(|z_j-z_{j-1}-d\zeta_j|)}{|z_j-z_{j-1}-d\zeta_j|}(x_j-x_{j-1}-d\cos\alpha_j) + \\
& + \frac{\varphi'(|z_{j+1}-z_j+d\zeta_j|)}{|z_{j+1}-z_j+d\zeta_j|}(x_{j+1}-x_j+d\cos\alpha_j) - \frac{\varphi'(|z_j-z_{j-1}+d\zeta_{j-1}|)}{|z_j-z_{j-1}+d\zeta_{j-1}|}(x_j-x_{j-1}+d\cos\alpha_{j-1}) + \\
& + \frac{\varphi'(|z_{j+1}-z_j-d(\zeta_{j+1}-\zeta_j)|)}{|z_{j+1}-z_j-d(\zeta_{j+1}-\zeta_j)|}\big(x_{j+1}-x_j-d(\cos\alpha_{j+1}-\cos\alpha_j)\big) - \\
& - \frac{\varphi'(|z_j-z_{j-1}-d(\zeta_j-\zeta_{j-1})|)}{|z_j-z_{j-1}-d(\zeta_j-\zeta_{j-1})|}\big(x_j-x_{j-1}-d(\cos\alpha_j-\cos\alpha_{j-1})\big)\Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
m\ddot{\alpha}_j = \ & \frac{1}{d^2}\Bigg\{ \left(\frac{\varphi'(|z_j-z_{j-1}|)}{|z_j-z_{j-1}|} - \frac{\varphi'(|z_j-z_{j-1}-d\zeta_j|)}{|z_j-z_{j-1}-d\zeta_j|}\right)\big((x_j-x_{j-1})\sin\alpha_j-(y_j-y_{j-1})\cos\alpha_j\big) + \\
& + \left(\frac{\varphi'(|z_{j+1}-z_j+d\zeta_j|)}{|z_{j+1}-z_j+d\zeta_j|} - \frac{\varphi'(|z_{j+1}-z_j|)}{|z_{j+1}-z_j|}\right)\big((x_{j+1}-x_j)\sin\alpha_j-(y_{j+1}-y_j)\cos\alpha_j\big) + \\
& + \left(\frac{\varphi'(|z_j-z_{j-1}+d\zeta_{j-1}|)}{|z_j-z_{j-1}+d\zeta_{j-1}|} - \frac{\varphi'(|z_j-z_{j-1}-d(\zeta_j-\zeta_{j-1})|)}{|z_j-z_{j-1}-d(\zeta_j-\zeta_{j-1})|}\right)\big((x_j-x_{j-1})\sin\alpha_j-(y_j-y_{j-1})\cos\alpha_j+d\sin(\alpha_j-\alpha_{j-1})\big) + \\
& + \left(\frac{\varphi'(|z_{j+1}-z_j-d(\zeta_{j+1}-\zeta_j)|)}{|z_{j+1}-z_j-d(\zeta_{j+1}-\zeta_j)|} - \frac{\varphi'(|z_{j+1}-z_j-d\zeta_{j+1}|)}{|z_{j+1}-z_j-d\zeta_{j+1}|}\right)\big((x_{j+1}-x_j)\sin\alpha_j-(y_{j+1}-y_j)\cos\alpha_j+d\sin(\alpha_{j+1}-\alpha_j)\big)\Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
|z_{j+1} - z_j|^2 &= (s_{j+1} - s_j)^2 + d(s_{j+1} - s_j)(\cos\alpha_{j+1} - \cos\alpha_j) + \frac{1}{2}d^2\big(1 - \cos(\alpha_{j+1} - \alpha_j)\big) \\
|z_{j+1} - z_j - d\zeta_{j+1}|^2 &= (s_{j+1} - s_j)^2 - d(s_{j+1} - s_j)(\cos\alpha_j + \cos\alpha_{j+1}) + \frac{1}{2}d^2\big(1 + \cos(\alpha_{j+1} - \alpha_j)\big) \\
|z_{j+1} - z_j + d\zeta_j|^2 &= (s_{j+1} - s_j)^2 + d(s_{j+1} - s_j)(\cos\alpha_j + \cos\alpha_{j+1}) + \frac{1}{2}d^2\big(1 + \cos(\alpha_{j+1} - \alpha_j)\big) \\
|z_{j+1} - z_j - d(\zeta_{j+1} - \zeta_j)|^2 &= (s_{j+1} - s_j)^2 - d(s_{j+1} - s_j)(\cos\alpha_{j+1} - \cos\alpha_j) + \frac{1}{2}d^2\big(1 - \cos(\alpha_{j+1} - \alpha_j)\big)
\end{aligned}
$$

$$
\begin{aligned}
x_{j+1} - x_j &= s_{j+1} - s_j + \frac{1}{2}d(\cos\alpha_{j+1} - \cos\alpha_j) \\
x_{j+1} - x_j - d\cos\alpha_{j+1} &= s_{j+1} - s_j - \frac{1}{2}d(\cos\alpha_{j+1} + \cos\alpha_j) \\
x_{j+1} - x_j + d\cos\alpha_j &= s_{j+1} - s_j + \frac{1}{2}d(\cos\alpha_{j+1} + \cos\alpha_j) \\
x_{j+1} - x_j - d(\cos\alpha_{j+1} - \cos\alpha_j) &= s_{j+1} - s_j - \frac{1}{2}d(\cos\alpha_{j+1} - \cos\alpha_j)
\end{aligned}
$$

$$
\begin{aligned}
(x_j - x_{j-1})\sin\alpha_j - (y_j - y_{j-1})\cos\alpha_j &= (s_j - s_{j-1})\sin\alpha_j - \frac{1}{2}d\sin(\alpha_j - \alpha_{j-1}) \\
(x_{j+1} - x_j)\sin\alpha_j - (y_{j+1} - y_j)\cos\alpha_j &= (s_{j+1} - s_j)\sin\alpha_j - \frac{1}{2}d\sin(\alpha_{j+1} - \alpha_j) \\
(x_j - x_{j-1})\sin\alpha_j - (y_j - y_{j-1})\cos\alpha_j + d\sin(\alpha_j - \alpha_{j-1}) &= (s_j - s_{j-1})\sin\alpha_j + \frac{1}{2}d\sin(\alpha_j - \alpha_{j-1}) \\
(x_{j+1} - x_j)\sin\alpha_j - (y_{j+1} - y_j)\cos\alpha_j + d\sin(\alpha_{j+1} - \alpha_j) &= (s_{j+1} - s_j)\sin\alpha_j + \frac{1}{2}d\sin(\alpha_{j+1} - \alpha_j)
\end{aligned}
$$

Suppose φ is an analytic mapping and d is in some sense small. Then we have an expansion

$$\Phi = \sum_{l=0}^{\infty} d^{2l} \Phi^{(l)} \ , \tag{2.19}$$

where the first two coefficients are

$$\begin{aligned}
\Phi^{(0)} &= \sum_j \varphi\left(s_{j+1} - s_j\right) \ , \\
\Phi^{(1)} &= \sum_j \frac{1}{2} \left(\frac{\varphi'\left(s_{j+1} - s_j\right)}{s_{j+1} - s_j} \left(\sin^2 \alpha_j + \sin^2 \alpha_{j+1}\right) + \right. \\
&\qquad \left. + \varphi''\left(s_{j+1} - s_j\right) \left(\cos^2 \alpha_j + \cos^2 \alpha_{j+1}\right) \right) \ .
\end{aligned}$$

The resulting simplified equations of motion read

$$\begin{aligned}
m \ddot{s}_j &= \varphi'\left(s_{j+1} - s_j\right) - \varphi'\left(s_j - s_{j-1}\right) + && (2.20) \\
&+ \frac{1}{8} d^2 \left\{ \left(\frac{\varphi'(s_{j+1} - s_j)}{s_{j+1} - s_j} \right)' \left(\sin^2 \alpha_{j+1} + \sin^2 \alpha_j\right) - \right. && (2.21) \\
&\qquad - \left(\frac{\varphi'(s_j - s_{j-1})}{s_j - s_{j-1}} \right)' \left(\sin^2 \alpha_j + \sin^2 \alpha_{j-1}\right) + && (2.22) \\
&\qquad + \varphi'''\left(s_{j+1} - s_j\right) \left(\cos^2 \alpha_{j+1} + \cos^2 \alpha_j\right) - && (2.23) \\
&\qquad \left. - \varphi'''\left(s_j - s_{j-1}\right) \left(\cos^2 \alpha_j + \cos^2 \alpha_{j-1}\right) \right\} \ , && (2.24) \\
m \ddot{\alpha}_j &= \frac{1}{2} \left\{ \varphi''\left(s_{j+1} - s_j\right) - \frac{\varphi'\left(s_{j+1} - s_j\right)}{s_{j+1} - s_j} + \right. && (2.25) \\
&\qquad \left. + \varphi''\left(s_j - s_{j-1}\right) - \frac{\varphi'\left(s_j - s_{j-1}\right)}{s_j - s_{j-1}} \right\} \sin 2\alpha_j \ . && (2.26)
\end{aligned}$$

Here the prime $'$ denotes differentiation with respect to $s_{j+1} - s_j$ or $s_j - s_{j-1}$, respectively.

If we replace Φ by $\Phi^{(0)} + d^2 \Phi^{(1)}$ we will speak of the approximated model, otherwise we speak of the full model. In case $d = 0$ we meet the simple atomic chain (without spin), which has been considered in [3]. If $d > 0$ we speak of the atomic spin chain.

As an indispensable part of a micro-macro transition, it is necessary to establish a link between microscopic and macroscopic initial or/and boundary data. Let $\rho_0, v_0, \dot{\psi}_0 : \mathbb{R} \longrightarrow \mathbb{R}$ and $\psi_0 : \mathbb{R} \longrightarrow \widetilde{\mathbb{R}}$ be given measurable functions, where

$$\widetilde{\mathbb{R}} := \mathbb{R}/[0, 2\pi) \ . \tag{2.27}$$

We assume that ρ_0 is uniformly bounded from below and from above in the sense that $0 < \rho_* \leqslant \rho_0(x) \leqslant \rho^*$, uniformly in $x \in \mathbb{R}$. We now introduce a small lattice parameter $\varepsilon > 0$, which will be related to the particle number in the chain by $\varepsilon =$

$1/N$. Having prescribed ε, we define corresponding sequences $\{s^\varepsilon_{j,0}\}_{j\in\mathbb{Z}}$, $\{\dot{s}^\varepsilon_{j,0}\}_{j\in\mathbb{Z}}$, $\{\alpha^\varepsilon_{j,0}\}_{j\in\mathbb{Z}}$ and $\{\dot{\alpha}^\varepsilon_{j,0}\}_{j\in\mathbb{Z}}$ as follows. Set

$$s^\varepsilon_{0,0} := 0 \ , \tag{2.28}$$

and, given $j \in \mathbb{N}_0$,

$$s^\varepsilon_{j+1,0} := s^\varepsilon_{j,0} + \frac{1}{\rho_0(\varepsilon s_{j,0})} \tag{2.29}$$

$$s^\varepsilon_{-(j+1),0} := \sup\left\{ s \in \mathbb{R} : s < s^\varepsilon_{-j,0} \ , \ \ s^\varepsilon_{-j,0} = s + \frac{1}{\rho_0(\varepsilon s)} \right\} \ . \tag{2.30}$$

Moreover, given $j \in \mathbb{Z}$,

$$\dot{s}^\varepsilon_{j,0} := v_0(\varepsilon s^\varepsilon_{j,0}) \ , \tag{2.31}$$

$$\alpha^\varepsilon_{j,0} := \psi_0(\varepsilon s^\varepsilon_{j,0}) \ , \tag{2.32}$$

$$\dot{\alpha}^\varepsilon_{j,0} := \dot{\psi}_0(\varepsilon s^\varepsilon_{j,0}) \ . \tag{2.33}$$

The quantities m, d and φ do not depend on ε, they are kept fixed.

In what follows, we denote by $s^\varepsilon_j = s^\varepsilon_j(t)$, $\alpha^\varepsilon_j = \alpha^\varepsilon_j(t)$, $j \in \mathbb{Z}$, $t \geqslant 0$, the solution of the initial value problem according to the initial data just constructed. Moreover, we shall use the terms $z^\varepsilon_j(t)$, $x^\varepsilon_j(t)$, $y^\varepsilon_j(t)$ and $\zeta^\varepsilon_j(t)$, which are connected to $s^\varepsilon_j(t)$ and $\alpha^\varepsilon_j(t)$ through (2.1), (2.2), (2.4) and (2.14).

3 Balance laws

3.1 Interpolation

As a first step towards the derivation of macroscopic observables and corresponding governing equations we shall now derive balance laws. Although the equations we shall derive are not balance laws in the strong sense, we will use this term for convenience.

In a first step we wish to interpolate the trajectories. To this end we introduce continuous mappings $s^\varepsilon : \mathbb{R}^2_+ \longrightarrow \mathbb{R}$ and $\alpha^\varepsilon : \mathbb{R}^2_+ \longrightarrow \widetilde{\mathbb{R}}$, such that

$$s^\varepsilon(t,j) = s^\varepsilon_j(t) \quad \text{and} \quad \alpha^\varepsilon(t,j) = \alpha^\varepsilon_j(t) \ , \quad \text{if } j \in \mathbb{Z} \ . \tag{3.1}$$

This can be achieved as follows. We denote by $\mathcal{S}$ the set of sequences of real numbers, labelled by integers, that is $\mathcal{S} := \mathbb{R}^{\mathbb{Z}}$. As usual, given $s \in \mathcal{S}$ and $j \in \mathbb{Z}$ we shall write $s(j) = s_j$. Next, let

$$I : \mathcal{S} \longrightarrow C([0,1]) \tag{3.2}$$

be a mapping such that the following properties are satisfied:

(i) $(Is)(j) = s_j,\ j = 0,1,$

(ii) $(Is)(j) < (Is)(k)$, if $j < k$.

Moreover, we introduce shift operators $S_k : \mathcal{S} \longrightarrow \mathcal{S}$ by setting

$$(S_k s)_j := s_{j+k} \tag{3.3}$$

and for given $j \in \mathbb{R}$ we define

$$\begin{aligned} j^- &:= \sup\{l \in \mathbb{Z}; l \leqslant j\}\ , && (3.4)\\ j^+ &:= j^- + 1\ . && (3.5) \end{aligned}$$

Then we set

$$\begin{aligned} s^\varepsilon(t,j) &:= \left[IS_j^{-1} s^\varepsilon(t)\right](j - j^-)\ , && (3.6)\\ \alpha^\varepsilon(t,j) &:= \left[IS_j^{-1} \alpha^\varepsilon(t)\right](j - j^-)\ . && (3.7) \end{aligned}$$

Obviously, by (i) the relation (3.1) is satisfied. Moreover, in view of (ii) there exists a mapping $\imath^\varepsilon : \mathbb{R}_+^2 \longrightarrow \mathbb{R}$ such that

$$\begin{aligned} x &= s^\varepsilon\big(t, \imath^\varepsilon(t,x)\big)\ , && (3.8)\\ j &= \imath^\varepsilon\big(t, s^\varepsilon(t,j)\big)\ . && (3.9) \end{aligned}$$

From (3.8), (3.9) it follows that

$$\begin{aligned} \frac{\partial s^\varepsilon}{\partial t} + \frac{\partial s^\varepsilon}{\partial j}\frac{\partial \imath^\varepsilon}{\partial x} &= 0\ , && (3.10)\\ \frac{\partial \imath^\varepsilon}{\partial t} + \frac{\partial \imath^\varepsilon}{\partial x}\frac{\partial s^\varepsilon}{\partial t} &= 0\ , && (3.11)\\ \frac{\partial s^\varepsilon}{\partial j}\frac{\partial \imath^\varepsilon}{\partial x} &= 1\ , && (3.12) \end{aligned}$$

whenever the respective expressions exist.

In what follows, we shall confine ourselves to a special case, namely on piecewise linear interpolation:

$$(Is)(j) := (1-j)s_0 + js_1\ . \tag{3.13}$$

The corresponding interpolated particle trajectories read

$$\begin{aligned} s^\varepsilon(t,j) &= (j^+ - j)s^\varepsilon_{j^-}(t) + (j - j^-)s^\varepsilon_{j^+}(t) && (3.14)\\ \alpha^\varepsilon(t,j) &= (j^+ - j)\alpha^\varepsilon_{j^-}(t) + (j - j^-)\alpha^\varepsilon_{j^+}(t)\ . && (3.15) \end{aligned}$$

$$
\begin{aligned}
\rho^\varepsilon(t,x) &:= \left[\frac{\partial s^\varepsilon}{\partial j}\big(t,\imath^\varepsilon(t,x)\big)\right]^{-1}, && (3.16)\\
v^\varepsilon(t,x) &:= \frac{\partial s^\varepsilon}{\partial t}\big(t,\imath^\varepsilon(t,x)\big)\,, && (3.17)\\
\psi^\varepsilon(t,x) &:= \alpha^\varepsilon\big(t,\imath^\varepsilon(t,x)\big)\,, && (3.18)\\
\dot\psi^\varepsilon(t,x) &:= \frac{\partial \alpha^\varepsilon}{\partial t}\big(t,\imath^\varepsilon(t,x)\big)\,. && (3.19)
\end{aligned}
$$

Proposition 3.1. *The microscopic particle density, velocity, angle and spin distributions defined above, cf.* (3.16)–(3.19)*, satisfy*

$$
\begin{aligned}
\frac{\partial\rho^\varepsilon}{\partial t}(t,x)+\frac{\partial(\rho^\varepsilon v^\varepsilon)}{\partial x}(t,x) &= 0\,, && (3.20)\\
\frac{\partial(\rho^\varepsilon v^\varepsilon)}{\partial t}(t,x)+\frac{\partial(\rho^\varepsilon (v^\varepsilon)^2)}{\partial x}(t,x) &= \rho^\varepsilon(t,x)\frac{\partial^2 s^\varepsilon}{\partial t^2}\big(t,\imath^\varepsilon(t,x)\big)\,, && (3.21)\\
\frac{\partial(\rho^\varepsilon \psi^\varepsilon)}{\partial t}(t,x)+\frac{\partial(\rho^\varepsilon v^\varepsilon\psi^\varepsilon)}{\partial x}(t,x) &= \rho^\varepsilon(t,x)\dot\psi^\varepsilon(t,x)\,, && (3.22)\\
\frac{\partial(\rho^\varepsilon \dot\psi^\varepsilon)}{\partial t}(t,x)+\frac{\partial(\rho^\varepsilon v^\varepsilon\dot\psi^\varepsilon)}{\partial x}(t,x) &= \rho^\varepsilon(t,x)\frac{\partial^2 \alpha^\varepsilon}{\partial t^2}\big(t,\imath^\varepsilon(t,x)\big)\,, && (3.23)
\end{aligned}
$$

whenever the respective derivatives are defined.

Proof. This is just a straightforward computation. Indeed, by applying the chain rule we infer from (3.16)–(3.19) and (3.8), (3.9):

$$
\begin{aligned}
\frac{\partial\rho^\varepsilon}{\partial x}(t,x) &= -\big(\rho^\varepsilon(t,x)\big)^2\frac{\partial^2 a^\varepsilon}{\partial j^2}\big(t,\imath^\varepsilon(t,x)\big)\frac{\partial \imath^\varepsilon}{\partial x}(t,x)\,,\\
\frac{\partial v^\varepsilon}{\partial x}(t,x) &= \frac{\partial^2 a^\varepsilon}{\partial t\partial j}\big(t,\imath^\varepsilon(t,x)\big)\frac{\partial \imath^\varepsilon}{\partial x}(t,x)\\
\frac{\partial\rho^\varepsilon}{\partial t}(t,x) &= -\big(\rho^\varepsilon(t,x)\big)^2\left[\frac{\partial^2 a^\varepsilon}{\partial t\partial j}\big(t,\imath^\varepsilon(t,x)\big)+\frac{\partial^2 a^\varepsilon}{\partial j^2}\big(t,\imath^\varepsilon(t,x)\big)\frac{\partial \imath^\varepsilon}{\partial t}(t,x)\right]\\
&= -\big(\rho^\varepsilon(t,x)\big)^2\left[\frac{1}{\rho^\varepsilon(t,x)}\frac{\partial v^\varepsilon}{\partial x}(t,x)-\frac{1}{\big(\rho^\varepsilon(t,x)\big)^2}\frac{\frac{\partial \imath^\varepsilon}{\partial t}(t,x)}{\frac{\partial \imath^\varepsilon}{\partial x}(t,x)}\frac{\partial \rho^\varepsilon}{\partial x}(t,x)\right]\\
&= -\rho^\varepsilon(t,x)\frac{\partial v^\varepsilon}{\partial x}(t,x)-v^\varepsilon(t,x)\frac{\partial\rho^\varepsilon}{\partial x}(t,x)\,,\\
\frac{\partial v^\varepsilon}{\partial t}(t,x) &= \frac{\partial^2 a^\varepsilon}{\partial t^2}\big(t,\imath^\varepsilon(t,x)\big)+\frac{\partial^2 a^\varepsilon}{\partial t\partial j}\big(t,\imath^\varepsilon(t,x)\big)\frac{\partial \imath^\varepsilon}{\partial t}(t,x)\\
&= \frac{\partial^2 a^\varepsilon}{\partial t^2}\big(t,\imath^\varepsilon(t,x)\big)+\frac{1}{\rho^\varepsilon(t,x)}\frac{\partial v^\varepsilon}{\partial x}(t,x)\left(-\frac{\partial \imath^\varepsilon}{\partial x}(t,x)\frac{\partial a^\varepsilon}{\partial t}\big(t,\imath^\varepsilon(t,x)\big)\right)\\
&= \frac{\partial^2 a^\varepsilon}{\partial t^2}\big(t,\imath^\varepsilon(t,x)\big)-v^\varepsilon(t,x)\frac{\partial v^\varepsilon}{\partial x}(t,x)\,,\\
\frac{\partial\dot\psi^\varepsilon}{\partial t}(t,x) &= \frac{\partial^2 \alpha^\varepsilon}{\partial t^2}\big(t,\imath^\varepsilon(t,x)\big)-v^\varepsilon(t,x)\frac{\partial\dot\psi^\varepsilon}{\partial x}(t,x)\,.
\end{aligned}
$$

Note that $\rho^\varepsilon(\partial_t + v^\varepsilon \partial_x) = \partial_t(\rho^\varepsilon .) + \partial_x(\rho^\varepsilon v^\varepsilon .)$. When putting these relations together, the result follows. □

Note that, in case ρ_0 is continuous, it holds

$$\forall x \in \mathbb{R} : \rho_0^\varepsilon(x) := \rho^\varepsilon(0,x) \longrightarrow \rho_0(x) \quad \text{as } \varepsilon \to 0 \,, \tag{3.24}$$

and corresponding relations are of course valid for the fields v, ψ and $\dot\psi$ too.

We now have to evaluate the right hand sides of (3.21) and (3.23). We have

$$\begin{aligned} \rho^\varepsilon(t,x) &= \Big(s^\varepsilon_{\imath^{\varepsilon,+}(t,x)}(t) - s^\varepsilon_{\imath^{\varepsilon,-}(t,x)}(t)\Big)^{-1} \,, \\ v^\varepsilon(t,x) &= \big(\imath^{\varepsilon,+}(t,x) - \imath^\varepsilon(t,x)\big)\dot s^\varepsilon_{\imath^{\varepsilon,-}(t,x)}(t) + \big(\imath^\varepsilon(t,x) - \imath^{\varepsilon,-}(t,x)\big)\dot s^\varepsilon_{\imath^{\varepsilon,+}(t,x)}(t) \,, \end{aligned}$$

where

$$\imath^{\varepsilon,-}(t,x) = \sup\big\{j \in \mathbb{Z}; s^\varepsilon_j(t) \leqslant x\big\} \,, \tag{3.25}$$

$$\imath^{\varepsilon,+}(t,x) = \imath^{\varepsilon,-}(t,x) + 1 \,, \tag{3.26}$$

$$\imath^\varepsilon(t,x) = \rho^\varepsilon(t,x)\Big(x - \big(\imath^{\varepsilon,+}(t,x)s^\varepsilon(t,\imath^{\varepsilon,-}(t,x)) + \imath^{\varepsilon,-}(t,x)s^\varepsilon(t,\imath^{\varepsilon,+}(t,x))\big)\Big) . \tag{3.27}$$

Similar expression can be written down for ψ^ε and $\dot\psi^\varepsilon$, respectively. We observe that

$$\imath^\varepsilon(t,x) - \frac{\imath^{\varepsilon,-}(t,x) + \imath^{\varepsilon,+}(t,x)}{2} = \rho^\varepsilon(t,x)\Big(x - s^\varepsilon\big(t,\imath^{\varepsilon,\pm}(t,x)\big)\Big) \pm \frac{1}{2} \,. \tag{3.28}$$

In order to be able to rewrite the resulting balance laws in a more compact form, we introduce

$$\rho^\varepsilon_\pm(t,x) := \left[\frac{\partial s^\varepsilon}{\partial j}\big(t,\imath^\varepsilon(t,x) \pm 1\big)\right]^{-1} \,, \tag{3.29}$$

$$v^\varepsilon_\pm(t,x) := \frac{\partial s^\varepsilon}{\partial t}\big(t,\imath^\varepsilon(t,x) \pm 1\big) \,, \tag{3.30}$$

$$\psi^\varepsilon_\pm(t,x) := \alpha^\varepsilon\big(t,\imath^\varepsilon(t,x) \pm 1\big) \,, \tag{3.31}$$

$$\dot\psi^\varepsilon_\pm(t,x) := \frac{\partial \alpha^\varepsilon}{\partial t}\big(t,\imath^\varepsilon(t,x) \pm 1\big) \,. \tag{3.32}$$

By definition we have

$$\frac{\partial^2 s^\varepsilon}{\partial t^2}(t,j) = (j^+ - j)\ddot s^\varepsilon_{j^-} + (j - j^-)\ddot s^\varepsilon_{j^+} \tag{3.33}$$

$$= \ddot s^\varepsilon_{j^-} + (j - j^-)(\ddot s^\varepsilon_{j^+} - \ddot s^\varepsilon_{j^-}) \tag{3.34}$$

$$= \ddot s^\varepsilon_{j^+} + (j - j^+)(\ddot s^\varepsilon_{j^+} - \ddot s^\varepsilon_{j^-}) \tag{3.35}$$

$$= \frac{1}{2}(\ddot s^\varepsilon_{j^+} + \ddot s^\varepsilon_{j^-}) + \left(j - \frac{j^- + j^+}{2}\right)(\ddot s^\varepsilon_{j^+} - \ddot s^\varepsilon_{j^-}) \,, \tag{3.36}$$

and in case $d=0$ the right hand side of (3.21) can therefore be written

$$\frac{\partial^2 s^\varepsilon}{\partial t^2}\big(t,\imath^\varepsilon(t,x)\big) = (\imath^{\varepsilon,+}-\imath^\varepsilon)\left(\varphi'\left(\frac{1}{\rho^\varepsilon}\right)-\varphi'\left(\frac{1}{\rho^\varepsilon_-}\right)\right)+ \tag{3.37}$$

$$+(\imath^\varepsilon-\imath^{\varepsilon,-})\left(\varphi'\left(\frac{1}{\rho^\varepsilon_+}\right)-\varphi'\left(\frac{1}{\rho^\varepsilon}\right)\right) \tag{3.38}$$

$$=\frac{1}{2}\left(\varphi'\left(\frac{1}{\rho^\varepsilon_+}\right)-\varphi'\left(\frac{1}{\rho^\varepsilon_-}\right)\right)+ \tag{3.39}$$

$$+\left(\imath^\varepsilon-\frac{\imath^{\varepsilon,-}+\imath^{\varepsilon,+}}{2}\right)\left(\varphi'\left(\frac{1}{\rho^\varepsilon_+}\right)+\varphi'\left(\frac{1}{\rho^\varepsilon_-}\right)-2\varphi'\left(\frac{1}{\rho^\varepsilon}\right)\right) \tag{3.40}$$

The basic idea is to introduce scaled fields $\overline{\rho}^\varepsilon$ and $\overline{v}^\varepsilon$, say, by $\overline{\rho}^\varepsilon(t,x):=\rho^\varepsilon(\varepsilon^{-1}t,\varepsilon^{-1}x)$ and by $\overline{v}^\varepsilon(t,x):=v^\varepsilon(\varepsilon^{-1}t,\varepsilon^{-1}x)$. From (3.20), (3.21) and the above relation we get

$$\frac{\partial\overline{\rho}^\varepsilon}{\partial t}+\frac{\partial(\overline{\rho}^\varepsilon\overline{v}^\varepsilon)}{\partial x}=0\ , \tag{3.41}$$

$$\frac{\partial(\overline{\rho}^\varepsilon\overline{v}^\varepsilon)}{\partial t}+\frac{\partial(\overline{\rho}^\varepsilon(\overline{v}^\varepsilon)^2)}{\partial x}=\overline{\rho}^\varepsilon\cdot\left\{\frac{1}{2\varepsilon}\left(\varphi'\left(\frac{1}{\overline{\rho}^\varepsilon_+}\right)-\varphi'\left(\frac{1}{\overline{\rho}^\varepsilon_-}\right)\right)+\right. \tag{3.42}$$

$$\left.+\left(\overline{\imath}^\varepsilon-\frac{\overline{\imath}^{\varepsilon,-}+\overline{\imath}^{\varepsilon,+}}{2}\right)\frac{1}{\varepsilon^2}\left(\varphi'\left(\frac{1}{\overline{\rho}^\varepsilon_+}\right)+\varphi'\left(\frac{1}{\overline{\rho}^\varepsilon_-}\right)-2\varphi'\left(\frac{1}{\overline{\rho}^\varepsilon}\right)\right)\right\}\ , \tag{3.43}$$

where $\overline{\rho}^\varepsilon_\pm(t,x) = \left[\frac{\partial\overline{s}^\varepsilon}{\partial j}\big(t,\overline{\imath}^\varepsilon(t,x)\pm\varepsilon\big)\right]^{-1}$, $\overline{s}^\varepsilon(t,j) = \varepsilon s^\varepsilon(\varepsilon^{-1}t,\varepsilon^{-1}j)$, $\overline{\imath}^\varepsilon(t,x) = \varepsilon\imath^\varepsilon(\varepsilon^{-1}t,\varepsilon^{-1}x)$. Now, letting ε tend to 0, and assuming that $\overline{\rho}^\varepsilon$ tends to a smooth limiting field ρ, the first expression on the right hand side of (3.42) looks like $\partial_x\varphi'(1/\rho)$., and the second tends to 0. We arrive at the the so called cold closure micro-macro transition [3].

3.2 Smoothing of discontinuous sequences

The procedure carried out so far is easy to handle. Note, however, that the approximating sequences are discontinuous. In order to get smooth approximating sequences, we will apply a smoothing operator. Let $\delta>0$ be an additional real parameter, and let J^δ be a mollifier, that is

$$J^\delta\in C^\infty(\mathbb{R})\ ,\quad J^\delta\geqslant 0\ ,\quad \int_{-\infty}^{\infty}J^\delta(x)\,\mathrm{d}x=1\ . \tag{3.44}$$

Furthermore, given any $\beta>0$, we assume that

$$\left\{J^\delta\geqslant\beta\right\}\longrightarrow\{0\}\quad\text{as }\delta\to 0\ . \tag{3.45}$$

A particular choice is

$$J^\delta(x):=\delta^{-1}J^1(\delta^{-1}x)\ , \tag{3.46}$$

where we assume that (3.44) is satisfied for $\delta = 1$, and where $\lim_{x\to\infty} xJ^1(x) = 0$. Additionally we assume here that J^δ is even, $J^\delta(x) = J^\delta(-x)$, $x \in \mathbb{R}$.

$$\begin{aligned} s^{\varepsilon,\delta}(t,j) &:= \left(J^\delta * s^\varepsilon(t,.)\right)(j)\ , && (3.47)\\ \alpha^{\varepsilon,\delta}(t,j) &:= \left(J^\delta * \alpha^\varepsilon(t,.)\right)(j)\ . && (3.48)\end{aligned}$$

Then $s^{\varepsilon,\delta}$ and $\alpha^{\varepsilon,\delta}$ are smooth mappings, and $s^{\varepsilon,\delta}$ is still invertible in view of

$$\frac{\partial s^{\varepsilon,\delta}}{\partial j}(t,j) = \int_{-\infty}^{\infty} \frac{\partial}{\partial j}\left(J^\delta(j-k)\right)s^\varepsilon(t,k)\,\mathrm{d}k = \int_{-\infty}^{\infty} J^\delta(j-k)\frac{\partial}{\partial k}\left(s^\varepsilon(t,k)\right)\mathrm{d}k > 0\ . \quad (3.49)$$

Denoting by $\imath^{\varepsilon,\delta}$ the inverse mapping we define corresponding functions $\rho^{\varepsilon,\delta}$, $\upsilon^{\varepsilon,\delta}$, $\psi^{\varepsilon,\delta}$, $\dot{\psi}^{\varepsilon,\delta}$ along the same lines as before, cf. (3.16)–(3.19), with $\imath^\varepsilon$ replaced by $\imath^{\varepsilon,\delta}$. The relations (3.8), (3.9) remain valid by definiton, and so these fields are smooth and satisfy the equations (3.20)–(3.23).

In order to be able to write subsequent formulae in a more compact form, we need to introduce some more notation:

$$\begin{aligned} Z_{j,1} &:= 0, && (3.50)\\ Z_{j,2} &:= -\zeta_{j+1}, && (3.51)\\ Z_{j,3} &:= \zeta_j, && (3.52)\\ Z_{j,4} &:= Z_{j,2} + Z_{j,3}. && (3.53)\end{aligned}$$

We find

$$\begin{aligned} \frac{\partial^2 s^{\varepsilon,\delta}}{\partial t^2}(t,j) &= \int_{-\infty}^{\infty} J^\delta(j-k)\frac{\partial^2 s^\varepsilon}{\partial t^2}(t,k)\,\mathrm{d}k && (3.54)\\ &= \int_{-\infty}^{\infty} J^\delta(j-k)\left((k-k^-)\ddot{s}^\varepsilon_{k^+}(t) + (k^+-k)\ddot{s}^\varepsilon_{k^-}(t)\right)\mathrm{d}k\ , && (3.55)\end{aligned}$$

and, as the right hand side of the first equation on page 4 has the structure $a(z_{j+1}, z_j) - a(z_j, z_{j-1})$, where

$$a(z_{j+1}, z_j) = \sum_{l=0}^{3} \frac{\varphi'\left(|z_{j+1} - z_j + dZ_{j,l}|\right)}{|z_{j+1} - z_j + dZ_{j,l}|}\left(x_{j+1} - x_j + dZ^1_{j,l}\right)\ , \quad (3.56)$$

we get

$$\int_{-\infty}^{\infty} J^\delta(j-k)(k-k^-)\ddot{s}^\varepsilon_{k^+}(t)\,\mathrm{d}k = \tag{3.57}$$

$$= \int_{-\infty}^{\infty} J^\delta(j-k)(k-k^-)\big(a(z^\varepsilon_{k^++1}(t), z^\varepsilon_{k^+}(t)) - a(z^\varepsilon_{k^+}(t), z^\varepsilon_{k^-}(t))\big)\,\mathrm{d}k \tag{3.58}$$

$$= \int_{-\infty}^{\infty} \big(J^\delta(j-k) - J^\delta(j-1-k)\big)(k-k^-)a(z^\varepsilon_{k^++1}(t), z^\varepsilon_{k^+}(t))\,\mathrm{d}k \tag{3.59}$$

Analogous

$$\int_{-\infty}^{\infty} J^\delta(j-k)(k^+-k)\ddot{s}^\varepsilon_{k^-}(t)\,\mathrm{d}k = \tag{3.60}$$

$$= \int_{-\infty}^{\infty} \big(J^\delta(j-k) - J^\delta(j-1-k)\big)(k^+-k)a(z^\varepsilon_{k^+}(t), z^\varepsilon_{k^-}(t))\,\mathrm{d}k\ . \tag{3.61}$$

In view of

$$J^\delta\big(\imath^{\varepsilon,\delta}(t,x)-k\big) - J^\delta\big(\imath^{\varepsilon,\delta}(t,x)-1-k\big) = \tag{3.62}$$

$$= -\int_0^1 \frac{d}{ds} J^\delta\big(\imath^{\varepsilon,\delta}(t,x)-k-s\big)\,\mathrm{d}s \tag{3.63}$$

$$= \frac{1}{\frac{\partial \imath^{\varepsilon,\delta}}{\partial x}(t,x)} \frac{\partial}{\partial x} \int_0^1 J^\delta\big(\imath^{\varepsilon,\delta}(t,x)-k-s\big)\,\mathrm{d}s \tag{3.64}$$

we have thus proved that

$$\rho^{\varepsilon,\delta}(t,x)\frac{\partial^2 s^{\varepsilon,\delta}}{\partial t^2}\big(t,\imath^{\varepsilon,\delta}(t,x)\big) = \frac{\partial p^{\varepsilon,\delta}}{\partial x}(t,x)\ , \tag{3.65}$$

where

$$p^{\varepsilon,\delta}(t,x) = \int_{-\infty}^{\infty}\int_0^1 J^\delta\big(\imath^{\varepsilon,\delta}(t,x)-k-s\big)\big)P^{\varepsilon,\delta}(t,k)\,\mathrm{d}s\,\mathrm{d}k\ , \tag{3.66}$$

$$P^{\varepsilon,\delta}(t,k) = (k-k^-)a(z^\varepsilon_{k^++1}(t), z^\varepsilon_{k^+}(t)) + (k^+-k)a(z^\varepsilon_{k^+}(t), z^\varepsilon_{k^-}(t))\ . \tag{3.67}$$

$$
\begin{aligned}
p^{\varepsilon,\delta}(t,x) &= \int_{-\infty}^{\infty}\int_{0}^{1}\Big((k-k^{-})J^{\delta}\left(\imath^{\varepsilon,\delta}(t,x)-k-s+1\right)\big)+(k^{+}-k)J^{\delta}\left(\imath^{\varepsilon,\delta}(t,x)-k-s\right)\Big)\, a(k^{\varepsilon}_{j^{+}}(t), z^{\varepsilon}_{k^{-}}(t))\,\mathrm{d}s\,\mathrm{d}k \\
&= \int_{-\infty}^{\infty}\int_{0}^{1} J^{\delta}\left(\imath^{\varepsilon,\delta}(t,x)-k-s\right)\big)a(z^{\varepsilon}_{k^{+}}(t), z^{\varepsilon}_{k^{-}}(t))\,\mathrm{d}s\,\mathrm{d}k\,+ \\
&\quad + \int_{-\infty}^{\infty}\int_{0}^{1}(k-k^{\pm})\Big[J^{\delta}\left(\imath^{\varepsilon,\delta}(t,x)-k-s+1\right)\big)-J^{\delta}\left(\imath^{\varepsilon,\delta}(t,x)-k-s\right)\Big)\Big]\, a(z^{\varepsilon}_{k^{+}}(t), z^{\varepsilon}_{k^{-}}(t))\,\mathrm{d}s\,\mathrm{d}k \\
&= \int_{-\infty}^{\infty}\int_{0}^{1} J^{\delta}\big(\imath^{\varepsilon,\delta}(t,x)-k-s\big)\big)a(z^{\varepsilon}_{k^{+}}(t), z^{\varepsilon}_{k^{-}}(t))\,\mathrm{d}s\,\mathrm{d}k\,+ \\
&\quad + \frac{1}{\rho^{\varepsilon,\delta}(t,x)}\frac{\partial}{\partial x}\int_{-\infty}^{\infty}\int_{0}^{1}\int_{0}^{1}(k-k^{\pm})\Big[J^{\delta}\left(\imath^{\varepsilon,\delta}(t,x)-k-s+\sigma\right)\big)\Big]\, a(z^{\varepsilon}_{k^{+}}(t), z^{\varepsilon}_{k^{-}}(t))\,\mathrm{d}s\,\mathrm{d}\sigma\,\mathrm{d}k \\
&= p_1^{\varepsilon,\delta}(t,x) + \frac{1}{\rho^{\varepsilon,\delta}(t,x)}\frac{\partial p_2^{\varepsilon,\delta}}{\partial x}(t,x)\ .
\end{aligned}
$$

Now, the right hand side of the second relation on page 4 can be written in the form

$$
\begin{aligned}
& b(z_{j+1}, z_j) - b(z_j, z_{j-1}) && (3.68)\\
& + \sin\alpha_j\left(c(z_{j+1}, z_j) - c(z_j, z_{j-1})\right) && (3.69)\\
& + \sin\alpha_j\left(d(z_{j+1}, z_j) + d(z_j, z_{j-1})\right)\ . && (3.70)
\end{aligned}
$$

Here

$$
b(z_{j+1}, z_j) = \frac{1}{2} d\sum_{l=1}^{4}(-1)^{\left[\frac{l}{2}\right]}\frac{\varphi'\left(|z_{j+1}-z_j+dZ^1_{j,l}|\right)}{|z_{j+1}-z_j+dZ^1_{j,l}|}\sin\left(\alpha_{j+1}-\alpha_j\right)\ , \tag{3.71}
$$

and

$$
c = c_1 + c_2\ , \quad d = d_1 + d_2\ , \tag{3.72}
$$

where

$$
\begin{aligned}
c_1(z_{j+1}, z_j) &= -\frac{\varphi'\left(|z_{j+1}-z_j|\right)}{|z_{j+1}-z_j|}(s_{j+1}-s_j) && (3.73)\\
c_2(z_{j+1}, z_j) &= \frac{\varphi'\left(|z_{j+1}-z_j-d(\zeta_{j+1}-\zeta_j)|\right)}{|z_{j+1}-z_j-d(\zeta_{j+1}-\zeta_j)|}(s_{j+1}-s_j) && (3.74)\\
d_1(z_{j+1}, z_j) &= -\frac{\varphi'\left(|z_{j+1}-z_j-d\zeta_{j+1}|\right)}{|z_{j+1}-z_j-d\zeta_{j+1}|}(s_{j+1}-s_j) && (3.75)\\
d_2(z_{j+1}, z_j) &= \frac{\varphi'\left(|z_{j+1}-z_j+d\zeta_j|\right)}{|z_{j+1}-z_j+d\zeta_j|}(s_{j+1}-s_j) && (3.76)
\end{aligned}
$$

Following the same argumentation as above we deduce that

$$\rho^{\varepsilon,\delta}(t,x)\frac{\partial^2\alpha^{\varepsilon,\delta}}{\partial t^2}\big(t,\imath^{\varepsilon,\delta}(t,x)\big) = \frac{\partial}{\partial x}\left\{p_3^{\varepsilon,\delta}(t,x)+\frac{1}{\rho^{\varepsilon,\delta}(t,x)}\frac{\partial p_4^{\varepsilon,\delta}}{\partial x}(t,x)\right\}+ +p_5^{\varepsilon,\delta}(t,x)+p_6^{\varepsilon,\delta}(t,x)\ , \tag{3.77}$$

where

$$p_3^{\varepsilon,\delta}(t,x)=\int_{-\infty}^{\infty}\int_0^1 J^\delta\big(\imath^{\varepsilon,\delta}(t,x)-k-s\big)b(z^\varepsilon_{k^+}(t),z^\varepsilon_{k^-}(t))\,\mathrm{d}s\,\mathrm{d}k \tag{3.78}$$

$$p_4^{\varepsilon,\delta}(t,x)=\int_{-\infty}^{\infty}\int_0^1\int_0^1 (k-k^\pm)\left[J^\delta\big(\imath^{\varepsilon,\delta}(t,x)-k-s+\sigma\big)\right]b(z^\varepsilon_{k^+}(t),z^\varepsilon_{k^-}(t))\,\mathrm{d}s\,\mathrm{d}\sigma\,\mathrm{d}k \tag{3.79}$$

$$p_5^{\varepsilon,\delta}(t,x)=\int_{-\infty}^{\infty}[(k-k^-)J^\delta(\imath^{\varepsilon,\delta}(t,x)-k+1)+(k^+-k)J^\delta(\imath^{\varepsilon,\delta}(t,x)-k)]\times \times\sin\alpha_{k^-}(c(z_{k^+}(t),z_{k^-}(t))-c(z_{k^-}(t),z_{k^--1}(t)))\mathrm{d}k \tag{3.80}$$

$$p_6^{\varepsilon,\delta}(t,x)=\int_{-\infty}^{\infty}[(k-k^-)J^\delta(\imath^{\varepsilon,\delta}(t,x)-k+1)+(k^+-k)J^\delta(\imath^{\varepsilon,\delta}(t,x)-k)]\times \times\sin\alpha_{k^-}(d(z_{k^+}(t),z_{k^-}(t))-d(z_{k^-}(t),z_{k^--1}(t)))\mathrm{d}k \tag{3.81}$$

There is a relation which might prove to be useful in later applications.

Proposition 3.2. *Let $N\in\mathbb{N}$. Then we have an expansion of the form*

$$p^{\varepsilon,\delta}=p_1^{\varepsilon,\delta}+\frac{1}{\rho^{\varepsilon,\delta}}\frac{\partial}{\partial x}\left\{p_2^{\varepsilon,\delta}+\frac{1}{\rho^{\varepsilon,\delta}}\frac{\partial}{\partial x}\left\{p_3^{\varepsilon,\delta}+\ldots\left\{p_N^{\varepsilon,\delta}+\frac{1}{\rho^{\varepsilon,\delta}}\frac{\partial q_N^{\varepsilon,\delta}}{\partial x}\right\}\ldots\right\}\right\} \tag{3.82}$$

where $p_1^{\varepsilon,\delta}=\int_{-\infty}^{\infty}\int_0^1 J^\delta\left(\imath^{\varepsilon,\delta}-k-s\right)a\left(z^\varepsilon_{k^+},z^\varepsilon_{k^-}\right)\mathrm{d}s\,\mathrm{d}k$ *and*

$$p_N^{\varepsilon,\delta}=\int_{-\infty}^{\infty}\underbrace{\int_0^1\ldots\int_0^1}_{N\ times}(k-k^\pm)J^\delta\left(\imath^{\varepsilon,\delta}-k-s_1-\ldots-s_N\right)a\left(z^\varepsilon_{k^+},z^\varepsilon_{k^-}\right)\mathrm{d}s_1\ldots\mathrm{d}s_N\,\mathrm{d}k\ ,\ N\geqslant 2\ ,$$

$$q_N^{\varepsilon,\delta}=\int_{-\infty}^{\infty}\underbrace{\int_0^1\ldots\int_0^1}_{N+1\ times}(k-k^\pm)J^\delta\left(\imath^{\varepsilon,\delta}-k-s_1-\ldots-s_N+\sigma\right)a\left(z^\varepsilon_{k^+},z^\varepsilon_{k^-}\right)\mathrm{d}s_1\ldots\mathrm{d}s_N\,\mathrm{d}\sigma\,\mathrm{d}k\ .$$

Proof. It suffices to prove that $q_N^{\varepsilon,\delta} = p_{N+1}^{\varepsilon,\delta} + \frac{1}{\rho^{\varepsilon,\delta}} \frac{\partial q_{N+1}^{\varepsilon,\delta}}{\partial x}$. This follows from

$$\begin{aligned}
J^\delta\left(\imath^{\varepsilon,\delta} - k - s_1 - \ldots - s_N + \sigma\right) &= J^\delta\left(\imath^{\varepsilon,\delta} - k - s_1 - \ldots - s_N + \sigma - 1\right) + \\
&\quad + \int_0^1 -\frac{d}{d\tau} J^\delta\left(\imath^{\varepsilon,\delta} - k - s_1 - \ldots - s_N + \sigma - \tau\right) \mathrm{d}\tau \\
&= J^\delta\left(\imath^{\varepsilon,\delta} - k - s_1 - \ldots - s_N + \sigma - 1\right) + \\
&\quad + \frac{1}{\rho^{\varepsilon,\delta}} \frac{\partial}{\partial x} \int_0^1 J^\delta\left(\imath^{\varepsilon,\delta} - k - s_1 - \ldots - s_N - s_{N+1} + \sigma\right) \mathrm{d}s_{N+1}
\end{aligned}$$

by integrating about k, s_1, ..., s_N and σ and substituting $\sigma - 1 = -s_{N+1}$ within the first summand. □

Let $d = 0$. In order to establish a link to [3], we define the specific energy of the j-th particle, e_j, by

$$e_j := \frac{1}{2} m \dot{s}_j^2 + \frac{1}{2}\left(\varphi(s_{j+1} - s_j) + \varphi(s_j - s_{j-1})\right) . \tag{3.83}$$

It follows

$$\begin{aligned}
\dot{e}_j &= m \dot{s}_j \ddot{s}_j + \frac{1}{2}\left(\varphi'(s_{j+1} - s_j)(\dot{s}_{j+1} - \dot{s}_j) + \varphi'(s_j - s_{j-1})(\dot{s}_j - \dot{s}_{j-1})\right) && (3.84) \\
&= \frac{1}{2}\left(\varphi'(s_{j+1} - s_j)(\dot{s}_{j+1} + \dot{s}_j) - \varphi'(s_j - s_{j-1})(\dot{s}_j + \dot{s}_{j-1})\right) . && (3.85)
\end{aligned}$$

Therefore, denoting by $e_j^\varepsilon(t)$ the corresponding value with s_j replaced by $s_j^\varepsilon(t)$, and setting

$$\begin{aligned}
e^\varepsilon(t, j) &:= \left[I S_j^{-1} e^\varepsilon(t)\right](j - j^-) , && (3.86) \\
e^{\varepsilon,\delta}(t, x) &:= \left(J^\delta * e^\varepsilon(t, .)\right)\left(\imath^{\varepsilon,\delta}(t, x)\right) , && (3.87)
\end{aligned}$$

we arrive at

$$\begin{aligned}
\frac{\partial}{\partial t} \rho^{\varepsilon,\delta} + \frac{\partial}{\partial x}\left(\rho^{\varepsilon,\delta} v^{\varepsilon,\delta}\right) &= 0 , && (3.88) \\
\frac{\partial}{\partial t}\left(\rho^{\varepsilon,\delta} v^{\varepsilon,\delta}\right) + \frac{\partial}{\partial x}\left(\rho^{\varepsilon,\delta} (v^{\varepsilon,\delta})^2 + p^{\varepsilon,\delta}\right) &= 0 , && (3.89) \\
\frac{\partial}{\partial t}\left(\rho^{\varepsilon,\delta} e^{\varepsilon,\delta}\right) + \frac{\partial}{\partial x}\left(\rho^{\varepsilon,\delta} v^{\varepsilon,\delta} e^{\varepsilon,\delta} + v^{\varepsilon,\delta} p^{\varepsilon,\delta} + q^{\varepsilon,\delta}\right) &= 0 , && (3.90)
\end{aligned}$$

which is formally the same system of balance laws derived in [3] for the atomic chain (without spin). The representations of pressure p and heat flux q now read

$$p^{\varepsilon,\delta} = -\int_{-\infty}^{\infty}\int_{0}^{1} J^\delta\left(\imath^{\varepsilon,\delta} - k - s\right)\varphi'\left(z^\varepsilon_{k+} - z^\varepsilon_{k-}\right)\mathrm{d}s\,\mathrm{d}k +$$

$$-\frac{1}{\rho^{\varepsilon,\delta}}\frac{\partial}{\partial x}\int_{-\infty}^{\infty}\int_{0}^{1}\int_{0}^{1}(k-k^{\pm})J^\delta\left(\imath^{\varepsilon,\delta} - k - s + \sigma\right)\varphi'\left(z^\varepsilon_{k+} - z^\varepsilon_{k-}\right)\mathrm{d}s\,\mathrm{d}\sigma\,\mathrm{d}k\ ,$$

$$q^{\varepsilon,\delta} = -\int_{-\infty}^{\infty}\int_{0}^{1} J^\delta\left(\imath^{\varepsilon,\delta} - k - s\right)\varphi'\left(s^\varepsilon_{k+} - s^\varepsilon_{k-}\right)\left[\frac{1}{2}\left(\dot{s}^\varepsilon_{k+} + \dot{s}^\varepsilon_{k-}\right) - v^{\varepsilon,\delta}\right]\mathrm{d}s\,\mathrm{d}k +$$

$$-\frac{1}{\rho^{\varepsilon,\delta}}\frac{\partial}{\partial x}\int_{-\infty}^{\infty}\int_{0}^{1}\int_{0}^{1}(k-k^{\pm})J^\delta\left(\imath^{\varepsilon,\delta} - k - s + \sigma\right)\varphi'\left(s^\varepsilon_{k+} - s^\varepsilon_{k-}\right)\left[\frac{1}{2}\left(\dot{s}^\varepsilon_{k+} + \dot{s}^\varepsilon_{k-}\right) - v^{\varepsilon,\delta}\right]\mathrm{d}s\,\mathrm{d}\sigma\,\mathrm{d}k\ .$$

Remark 3.3. As long as we restrict our attention to the case of piecewise linear interpolation, all integrals about the k variable can be evaluated and replaced by sums. Note that, however, that the interpolation of particle trajectories is of interest in itself. But in order to get approximating sequences which are at least continuous, we have to take interpolation formulas into account, which become necessarily nonlinear. While piecewise polynomial interpolation does not seem to yield appropriate results, piecewise spline interpolation is more favourable. The resulting balance laws look much more complicated, so we refrain from carrying out the details here.

4 Numerical experiments

The numerical experiments carried out are based on the so-called velocity Verlet scheme, which is one of the most popular numerical integration methods for systems of ordinary differential equations of the form

$$\dot{q}_j = p_j\ , \tag{4.1}$$
$$\dot{p}_j = F_j\left(q_k\right)\ . \tag{4.2}$$

Denoting by $\Delta t > 0$ the timestep, and by $q_j^{(n)}$ and $p_j^{(n)}$ the approximate (generalized) j-th particle coordinates and velocities, respectively, computed at time $t_n = n\cdot(\Delta t)$, $n \in \mathbb{N}_0$, this algorithm reads as follows:

$$q_j^{(n+1)} = q_j^{(n)} + p_j^{(n)}\cdot(\Delta t) + \frac{1}{2}F_j\left(q_k^{(n)}\right)\cdot(\Delta t)^2\ , \tag{4.3}$$
$$p_j^{(n+1)} = p_j^{(n)} + \frac{1}{2}\left[F_j\left(q_k^{(n)}\right) + F_j\left(q_k^{(n+1)}\right)\right]\cdot(\Delta t)\ . \tag{4.4}$$

Compared to the more basic Verlet-Störmer algorithm used in [3], the scheme (4.3), (4.4) is advantageous in so far as it's accuracy in the p-component is locally and globally better than for Verlet-Störmer. In particular, the (kinetic) energy is better conserved when using (4.3), (4.4). For a numerical analysis of (4.3), (4.4) and related schemes, the reader is referred to [6] and the references cited therein.

All simulations have been carried out under almost equal conditions on several machines, with double precision, and with parameters

$$m = 1.0 \,, \quad d = 0.1 \tag{4.5}$$

and timestep

$$\Delta t = 0.001 \,. \tag{4.6}$$

The pair potential φ is of Lennard-Jones type:

$$\varphi(r) = \frac{1}{8}\left(\frac{1}{r}\right)^4 - \frac{1}{4}\left(\frac{1}{r}\right)^2 \,. \tag{4.7}$$

Falling back on the setting introduced at the very beginning of section 2, we consider initial value problems with an increasing number N of particles and a lattice parameter $\varepsilon \sim \frac{1}{N}$. The particles at the boundary of the chain are kept fixed.

initial data: $\rho_0(x) = \rho_{0,l}$, if $x < 0$, $\rho_0(x) = \rho_{0,r}$, if $x \geqslant 0$

$$\rho_{0,l} = 1.36 \,, \qquad \rho_{0,r} = 1.0 \,, \tag{4.8}$$
$$v_{0,l} = 0.53 \,, \qquad v_{0,r} = 0.0 \,, \tag{4.9}$$
$$\psi_{0,l} = 0.5 \cdot \pi \,, \quad \psi_{0,r} = 0.5 \cdot 3 \,, \tag{4.10}$$
$$\dot{\psi}_{0,l} = 0.0 \,, \qquad \dot{\psi}_{0,r} = 0.0 \,. \tag{4.11}$$

The macroscopic observables are computed with a Gaussian distribution:

$$J^\delta(x) = \frac{1}{\sqrt{\pi}} e^{-x^2} \,. \tag{4.12}$$

The figures depicted on the subsequent pages visualize the observed density, velocity, angle and spin distributions, respectively. One can identify three space-time regions, denoted I, II and III from up to down, in which the solution shows quite different qualitative behavior.

Figures 1–3: The initial conditions ρ_0, v_0 are choosen to ensure the occurence of a single shock wave, if $d = 0$, cf. [3].

Figures 4–6: The discontinuity of ϕ_0 leads to the occurence of some kind of microstructure within the space-time regions I and II. The particular shape of the region II depends on the initial condition ϕ_0.

Figures 7, 8: Given a velocity distribution v and a spin distribution $\dot{\phi}$, we define corresponding temperature and spin-temperature distribution via

$$
\begin{aligned}
T_v(t,x) &:= \int_{-\infty}^{\infty} J(\imath(t,x)-k)\left(\frac{\partial s}{\partial t}(t,k)-v(t,x)\right)^2 \mathrm{d}k, \\
T_{\dot{\psi}}(t,x) &:= \int_{-\infty}^{\infty} J(\imath(t,x)-k)\left(\frac{\partial \alpha}{\partial t}(t,k)-\dot{\psi}(t,x)\right)^2 \mathrm{d}k.
\end{aligned}
$$

Here we have dropped the dependencies on ε, δ. The development of temperature and spin-temperature is restricted to the space-time region II. While the development of temperature is concentrated in the vicinity of the shock front, spin-temperature develops uniformly within the region II. Furthermore, turning to the approximated model, the development of temperature remains unchanged, while the development of spin-tempereture is drastically reduced.

5 Micro-macro transition

Up to now, the microscopic setting has not been left. We shall next introduce macroscopic time and space scales by defining scaled fields as follows. For simplicity, from now on we do not consider the energy balance and the corresponding scalings.

$$
\begin{aligned}
\overline{\rho}^{\varepsilon,\delta}(t,x) &:= \rho^{\varepsilon,\delta}\left(\varepsilon^{-1}t, \varepsilon^{-1}x\right) \ , && (5.1)\\
\overline{v}^{\varepsilon,\delta}(t,x) &:= v^{\varepsilon,\delta}\left(\varepsilon^{-1}t, \varepsilon^{-1}x\right) \ , && (5.2)\\
\overline{\psi}^{\varepsilon,\delta}(t,x) &:= \psi^{\varepsilon,\delta}\left(\varepsilon^{-1}t, \varepsilon^{-1}x\right) \ , && (5.3)\\
\overline{\dot{\psi}}^{\varepsilon,\delta}(t,x) &:= \varepsilon^{-1}\dot{\psi}^{\varepsilon}\left(\varepsilon^{-1}t, \varepsilon^{-1}x\right) \ . && (5.4)
\end{aligned}
$$

If we define

$$
\begin{aligned}
\overline{s}^{\varepsilon,\delta}(t,j) &:= \varepsilon s^{\varepsilon,\delta}(\varepsilon^{-1}t, \varepsilon^{-1}j) \ , && (5.5)\\
\overline{\imath}^{\varepsilon,\delta}(t,x) &:= \varepsilon \imath^{\varepsilon,\delta}(\varepsilon^{-1}t, \varepsilon^{-1}x) && (5.6)
\end{aligned}
$$

there still holds

$$
\begin{aligned}
x &= \overline{s}^{\varepsilon,\delta}\left(t, \overline{\imath}^{\varepsilon,\delta}(t,x)\right) \ , && (5.7)\\
j &= \overline{\imath}^{\varepsilon,\delta}\left(t, \overline{s}^{\varepsilon,\delta}(t,j)\right) \ . && (5.8)
\end{aligned}
$$

Setting

$$
\overline{\alpha}^{\varepsilon,\delta}(t,j) := \alpha^{\varepsilon,\delta}(\varepsilon^{-1}t, \varepsilon^{-1}j) \qquad (5.9)
$$

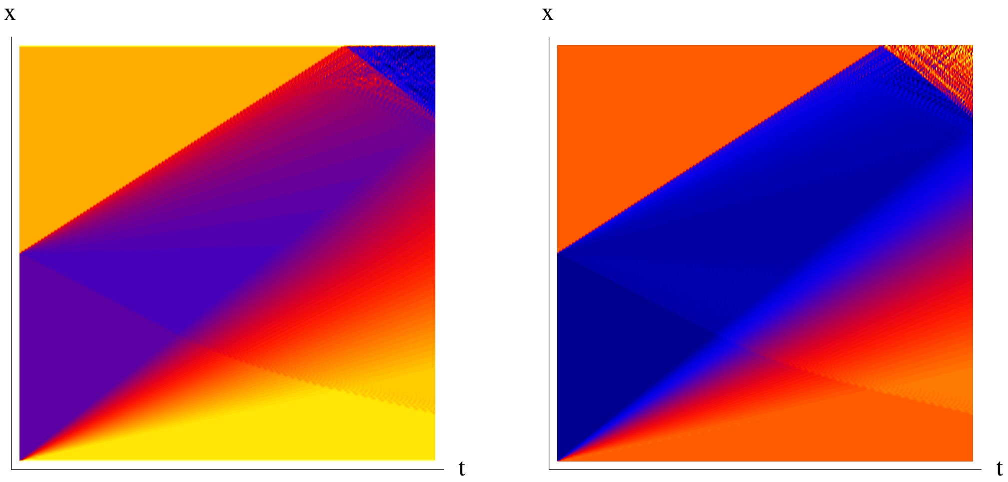


Figure 1: density and velocity for the full model, $N = 2000$

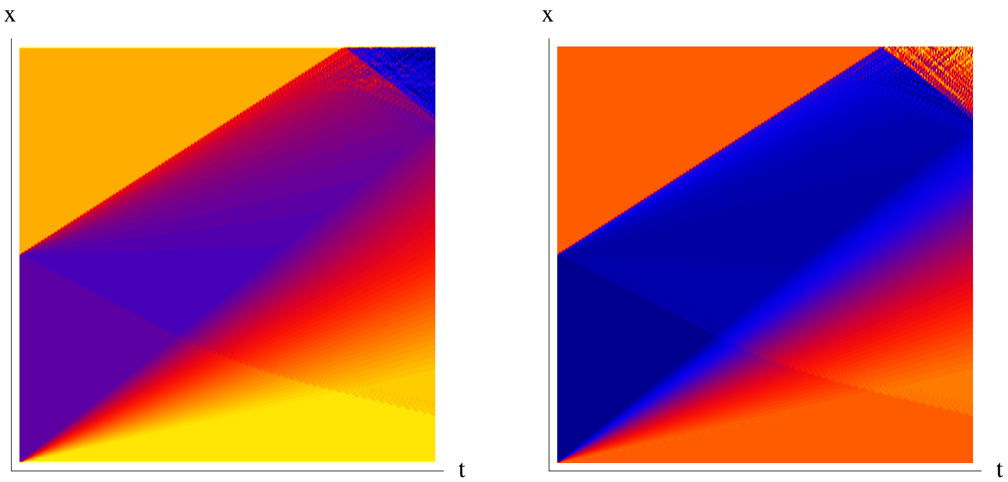


Figure 2: density and velocity for the approximated model, $N = 2000$

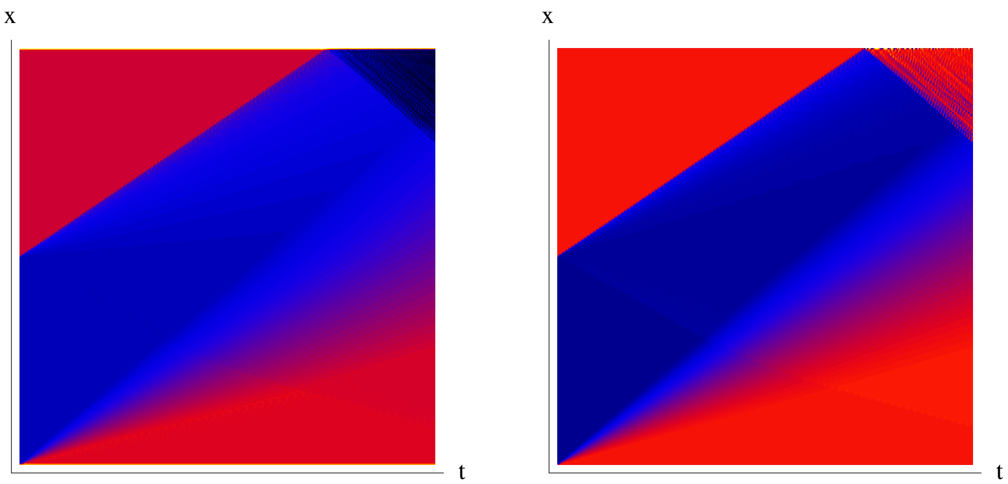


Figure 3: density and velocity in case $d = 0.0$, $N = 2000$

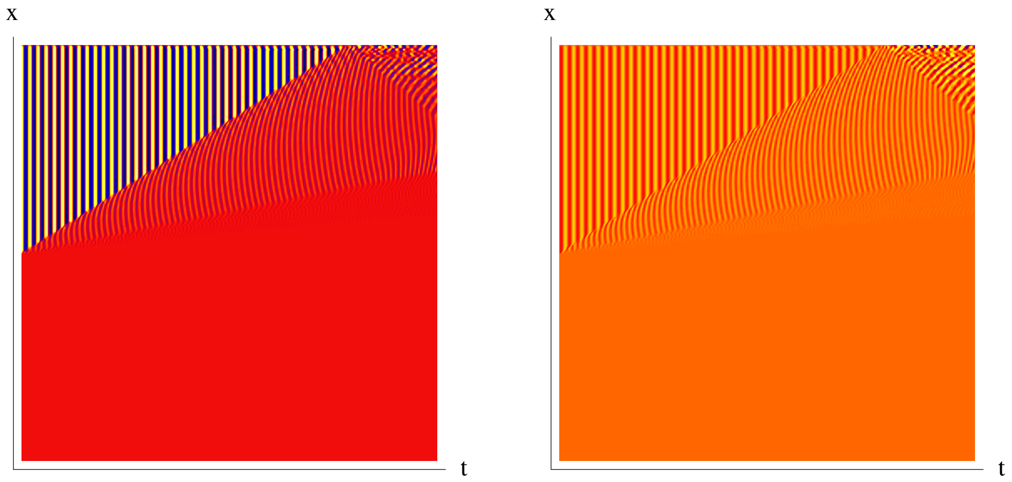


Figure 4: angle and spin for the full model, $N = 1000$

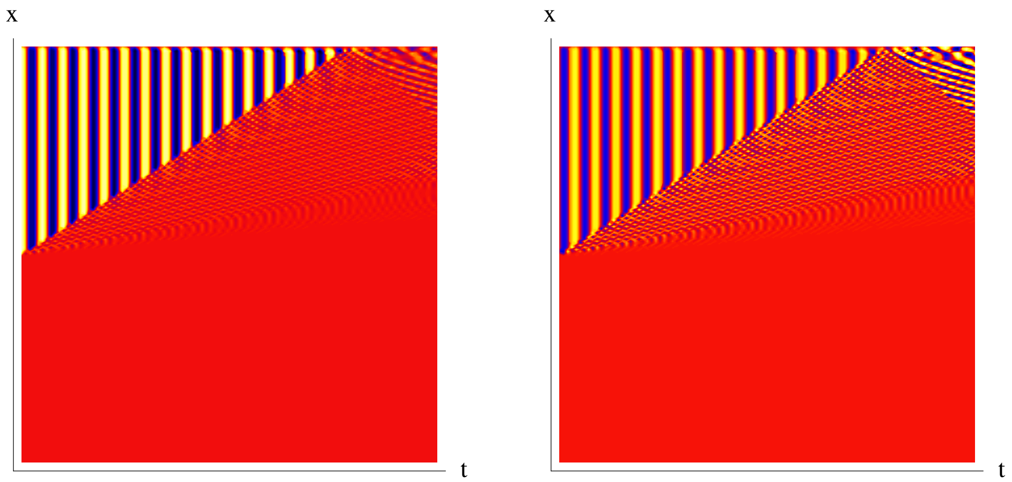


Figure 5: angle and spin for the full model, $N = 2000$

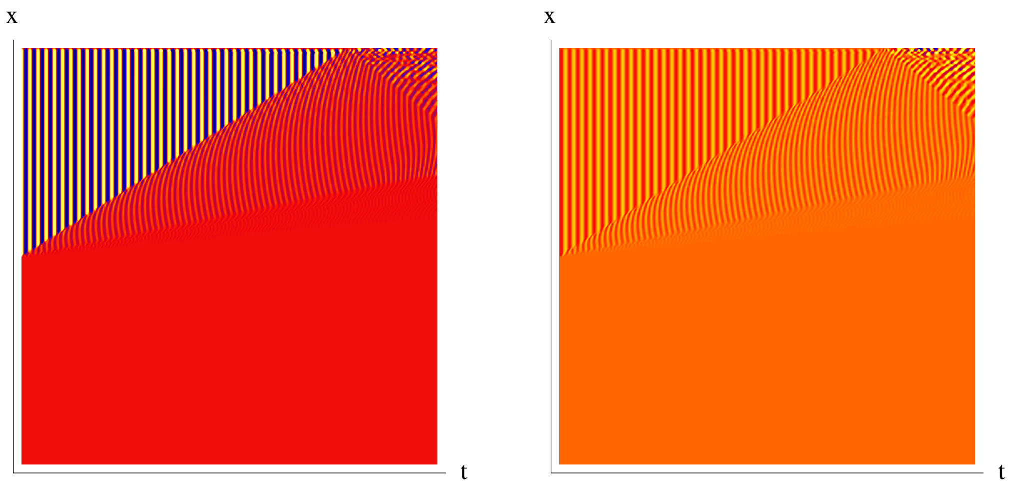


Figure 6: angle and spin for the full model, $N = 4000$

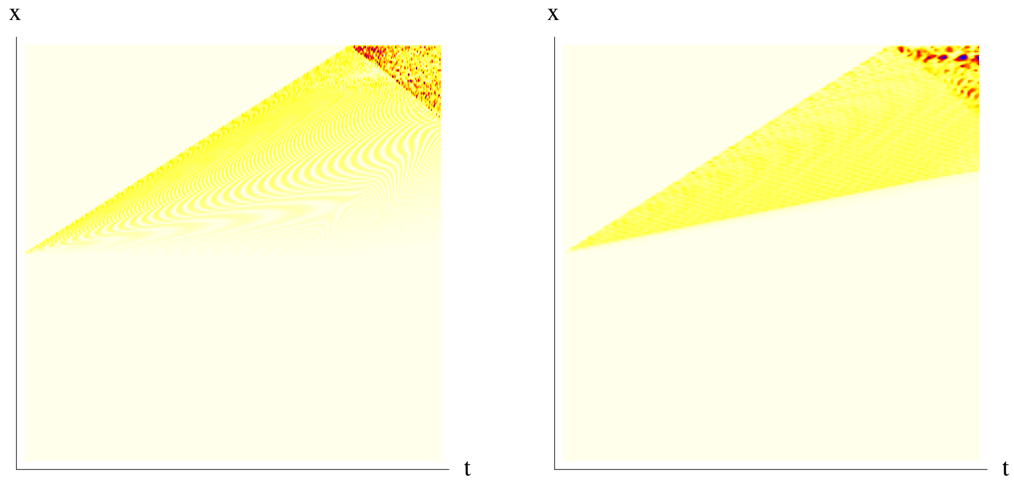


Figure 7: temperature and spin-temperature for the full model, $N = 2000$

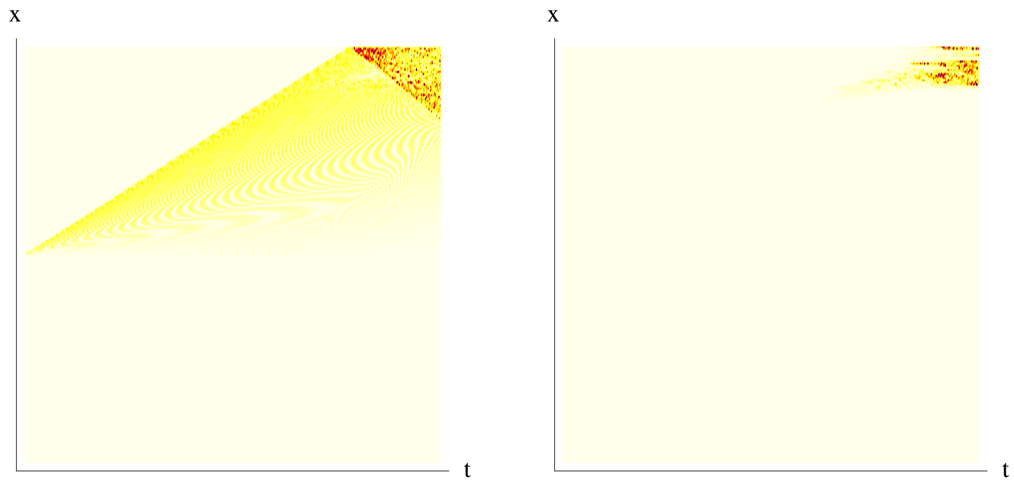


Figure 8: temperature and spin-temperature for the approximated model, $N = 2000$

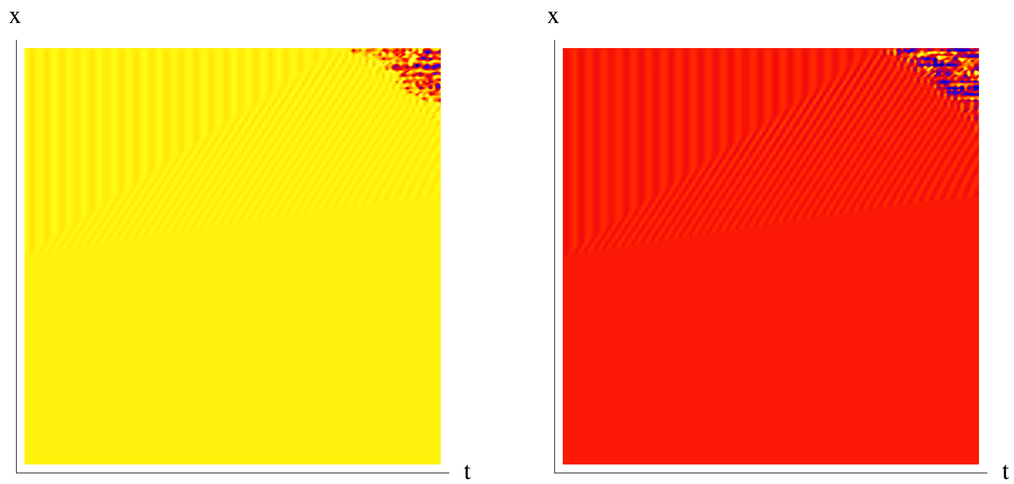


Figure 9: angle and spin for the approximated model, $N = 2000$

one has

$$\frac{\partial\overline{\rho}^{\varepsilon,\delta}}{\partial t}(t,x)+\frac{\partial(\overline{\rho}^{\varepsilon,\delta}\overline{v}^{\varepsilon,\delta})}{\partial x}(t,x) = 0\,, \tag{5.10}$$

$$\frac{\partial(\overline{\rho}^{\varepsilon,\delta}\overline{v}^{\varepsilon,\delta})}{\partial t}(t,x)+\frac{\partial(\overline{\rho}^{\varepsilon,\delta}(\overline{v}^{\varepsilon,\delta})^2)}{\partial t}(t,x) = \overline{\rho}^{\varepsilon,\delta}(t,x)\frac{\partial^2\overline{s}^{\varepsilon,\delta}}{\partial t^2}\big(t,\overline{\imath}^{\varepsilon,\delta}(t,x)\big)\,, \tag{5.11}$$

$$\frac{\partial(\overline{\rho}^{\varepsilon,\delta}\overline{\psi}^{\varepsilon,\delta})}{\partial t}(t,x)+\frac{\partial(\overline{\rho}^{\varepsilon,\delta}\overline{v}^{\varepsilon,\delta}\overline{\psi}^{\varepsilon,\delta})}{\partial x}(t,x) = \overline{\rho}^{\varepsilon,\delta}(t,x)\overline{\dot{\psi}}^{\varepsilon,\delta}(t,x)\,, \tag{5.12}$$

$$\frac{\partial(\overline{\rho}^{\varepsilon,\delta}\overline{\dot{\psi}}^{\varepsilon,\delta})}{\partial t}(t,x)+\varepsilon^{1-\tau}\frac{\partial(\overline{\rho}^{\varepsilon,\delta}\overline{v}^{\varepsilon,\delta}\overline{\dot{\psi}}^{\varepsilon,\delta})}{\partial x}(t,x) = \overline{\rho}^{\varepsilon,\delta}(t,x)\frac{\partial^2\overline{\alpha}^{\varepsilon,\delta}}{\partial t^2}\big(t,\overline{\imath}^{\varepsilon,\delta}(t,x)\big)\,. \tag{5.13}$$

This system can now be reduced to

$$\frac{\partial\bar{\rho}^{\varepsilon,\delta}}{\partial t}+\frac{(\partial\bar{\rho}^{\varepsilon,\delta}\bar{v}^{\varepsilon,\delta})}{\partial x} = 0, \tag{5.14}$$

$$\frac{(\partial\bar{\rho}^{\varepsilon,\delta}\bar{v}^{\varepsilon,\delta})}{\partial t}+\frac{\partial(\bar{\rho}^{\varepsilon,\delta}(\bar{v}^{\varepsilon,\delta})^2)}{\partial x} = \frac{\partial\bar{p}^{\varepsilon,\delta}}{\partial x}, \tag{5.15}$$

where $\bar{p}^{\varepsilon,\delta}=\bar{p}_1^{\varepsilon,\delta}+\frac{1}{\partial(\bar{\rho}^{\varepsilon,\delta}}\frac{\partial\bar{p}_2^{\varepsilon,\delta}}{\partial x}$,

$$\bar{p}_1^{\varepsilon,\delta}=\int_{-\infty}^{\infty}\int_0^1 J^\delta\left(\varepsilon^{-1}\overline{\imath}^{\varepsilon,\delta}(t,x)-k-s\right)\alpha\left(z^\varepsilon_{k^+}(\varepsilon^{-1}t),z^\varepsilon_{k^-}(\varepsilon^{-1}t)\right)\mathrm{d}s\mathrm{d}k, \tag{5.16}$$

$$\bar{p}_2^{\varepsilon,\delta}=\varepsilon\cdot\int_{-\infty}^{\infty}\int_0^1(k-k^\pm)J^\delta\left(\varepsilon^{-1}\overline{\imath}^{\varepsilon,\delta}(t,x)-k-s+\sigma\right)\alpha\big(z^\varepsilon_{k^+}(\varepsilon^{-1}t),z^\varepsilon_{k^-}(\varepsilon^{-1}t)\big)\mathrm{d}s\mathrm{d}\sigma\mathrm{d}k. \tag{5.17}$$

On the other hand, from (5.12), (5.13), and (5.14) it follows that

$$\varepsilon\cdot\left(\frac{\partial\bar{\psi}^{\varepsilon,\delta}}{\partial t}+\bar{v}^{\varepsilon,\delta}\frac{\partial\bar{\psi}^{\varepsilon,\delta}}{\partial x}\right) = \bar{\dot{\psi}}^{\varepsilon,\delta}, \tag{5.18}$$

$$\varepsilon\cdot\left(\frac{\partial\bar{\dot{\psi}}^{\varepsilon,\delta}}{\partial t}+\bar{v}^{\varepsilon,\delta}\frac{\partial\bar{\dot{\psi}}^{\varepsilon,\delta}}{\partial x}\right) = \bar{g}^{\varepsilon,\delta}, \tag{5.19}$$

where $\bar{g}^{\varepsilon,\delta} = \bar{g}_1^{\varepsilon,\delta} + \bar{g}_2^{\varepsilon,\delta} + \frac{\bar{g}_3^{\varepsilon,\delta}}{\partial x} + \frac{\partial}{\partial x}\left(\frac{1}{\bar{\rho}^{\varepsilon,\delta}}\frac{\partial \bar{g}_4^{\varepsilon,\delta}}{\partial x}\right)$,

$$\bar{g}_1^{\varepsilon,\delta} = \int\limits_{-\infty}^{\infty}\int\limits_0^1 \left[(k-k^-)J^\delta\left(\varepsilon^{-1}\bar{\imath}^{\varepsilon,\delta}(t,x)-k+1\right) + (k-k^-)J^\delta\left(\varepsilon^{-1}\bar{\imath}^{\varepsilon,\delta}(t,x)-k\right)\right]\cdot \tag{5.20}$$
$$\cdot \sin\alpha_{k^-}^\varepsilon(\varepsilon^{-1}t)\left[d\left(z_{k^+}^\varepsilon(\varepsilon^{-1}t), z_{k^-}^\varepsilon(\varepsilon^{-1}t)\right) + d\left(z_{k^-}^\varepsilon(\varepsilon^{-1}t), z_{k^--1}^\varepsilon(\varepsilon^{-1}t)\right)\right]\mathrm{d}s\mathrm{d}\sigma\mathrm{d}k,$$

$$\bar{g}_2^{\varepsilon,\delta} = \int\limits_{-\infty}^{\infty}\int\limits_0^1 \left[(k-k^-)J^\delta\left(\varepsilon^{-1}\bar{\imath}^{\varepsilon,\delta}(t,x)-k+1\right) + (k-k^-)J^\delta\left(\varepsilon^{-1}\bar{\imath}^{\varepsilon,\delta}(t,x)-k\right)\right]\cdot \tag{5.21}$$
$$\cdot \sin\alpha_{k^-}^\varepsilon(\varepsilon^{-1}t)\left[c\left(z_{k^+}^\varepsilon(\varepsilon^{-1}t), z_{k^-}^\varepsilon(\varepsilon^{-1}t)\right) + c\left(z_{k^-}^\varepsilon(\varepsilon^{-1}t), z_{k^--1}^\varepsilon(\varepsilon^{-1}t)\right)\right]\mathrm{d}s\mathrm{d}\sigma\mathrm{d}k,$$

$$\bar{g}_3^{\varepsilon,\delta} = \varepsilon\cdot\int\limits_{-\infty}^{\infty}\int\limits_0^1 J^\delta\left(\varepsilon^{-1}\bar{\imath}^{\varepsilon,\delta}(t,x)-k-s\right) b\left(z_{k^+}^\varepsilon(\varepsilon^{-1}t), z_{k^-}^\varepsilon(\varepsilon^{-1}t)\right)\mathrm{d}s\mathrm{d}k, \tag{5.22}$$

$$\bar{g}_4^{\varepsilon,\delta} = \varepsilon^2\cdot\int\limits_{-\infty}^{\infty}\int\limits_0^1 (k-k^\pm)J^\delta\left(\varepsilon^{-1}\bar{\imath}^{\varepsilon,\delta}(t,x)-k-s\right) \alpha\left(z_{k^+}^\varepsilon(\varepsilon^{-1}t), z_{k^-}^\varepsilon(\varepsilon^{-1}t)\right)\mathrm{d}s\mathrm{d}\sigma\mathrm{d}k. \tag{5.23}$$

Based on the numerical observations of the preceding section we expect a macroscopic model having measure valued solutions, which will be described in section 6.

By taking the limit $\varepsilon \to 0$, and denoting the smooth limiting fields by ρ, v, ψ and $\dot{\psi}$, respectively, we arrive at the following system of equations, which we call in analogue of what is called cold closure in [3] of the atomic chain:

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}(\rho v) = 0 \tag{5.24}$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}\left\{\rho v^2 + A(\rho,\psi)\right\} = 0\,, \tag{5.25}$$

$$\frac{\partial}{\partial t}(\rho\psi) + \frac{\partial}{\partial x}(\rho v\psi) = \rho\dot{\psi} \tag{5.26}$$

$$\frac{\partial}{\partial t}(\rho\dot{\psi}) + \frac{\partial}{\partial x}(\rho v\dot{\psi}) = B(\rho,\psi) \tag{5.27}$$

$$A(\rho,\psi) = \tag{5.28}$$

$$-\frac{1}{2}\varphi'\left(\frac{1}{\rho}\right) - \frac{1}{4}\frac{\varphi'\left(\frac{1}{\rho}\sqrt{1-2d\rho\cos\psi+d^2\rho^2}\right)}{\sqrt{1-2d\rho\cos\psi+d^2\rho^2}}(1-d\rho\cos\psi) - \tag{5.29}$$

$$-\frac{1}{4}\frac{\varphi'\left(\frac{1}{\rho}\sqrt{1+2d\rho\cos\psi+d^2\rho^2}\right)}{\sqrt{1+2d\rho\cos\psi+d^2\rho^2}}(1+d\rho\cos\psi) \tag{5.30}$$

$$= -\varphi'\left(\frac{1}{\rho}\right) - \frac{1}{4}d^2\left[\left(\rho\varphi'\left(\frac{1}{\rho}\right)\right)'\sin^2\psi + \varphi'''\left(\frac{1}{\rho}\right)\cos^2\psi\right] + O(d^4) \tag{5.31}$$

$$B(\rho,\psi) = \tag{5.32}$$

$$\frac{1}{d}\left\{\frac{\varphi'\left(\frac{1}{\rho}\sqrt{1+2d\rho\cos\psi+d^2\rho^2}\right)}{\sqrt{1+2d\rho\cos\psi+d^2\rho^2}} - \frac{\varphi'\left(\frac{1}{\rho}\sqrt{1-2d\rho\cos\psi+d^2\rho^2}\right)}{\sqrt{1-2d\rho\cos\psi+d^2\rho^2}}\right\}\rho\sin\psi \tag{5.33}$$

$$= \left(\rho\varphi'\left(\frac{1}{\rho}\right)\right)'\sin(2\psi) + O(d^2)\ . \tag{5.34}$$

We propose to interpret the sequence of solutions observed in the preceding section (in the limit $\varepsilon \to 0$, $\delta \to 0$) as a Young-measure solution of this system. It should be mentioned, however, that we are not aware of any rigorous proof of convergence. The properties of the system will be studied in a forthcoming paper.

6 Towards Young measure solutions for the atomic chain

In order to illustrate the usefullness of Young measure solutions we consider a simpler example as it is given by the spin system.

Let $I \subseteq \mathbb{R}$ be an open interval, $I \neq \emptyset$, and let be $\Phi\colon I \longrightarrow \mathbb{R}$ a smooth function. In the following we consider a Hamilton function $H\colon I \times \mathbb{R} \longrightarrow \mathbb{R}$, which is defined by

$$H(q,p) := \frac{1}{2}p^2 + \Phi(q), \tag{6.1}$$

and corresponding initial value problems

$$\dot{q} = p\ , \tag{6.2}$$

$$\dot{p} = -\Phi'(q)\ , \tag{6.3}$$

$$q(0) = q_0\ , \tag{6.4}$$

$$p(0) = p_0 \tag{6.5}$$

with given $q_0 \in I$ and $p_0 \in \mathbb{R}$. We interprete $q(t)$, $p(t)$ as position and momentum, respectively, of a particle at time $t \geq 0$, which is subjected to the potential Φ.

Note that, for any smooth solution $q = q(t)$, $p = p(t)$ of (6.2), (6.3) there holds $\frac{d}{dt}H(q(t), p(t)) \equiv 0$. Thus there holds

$$H(q(t), p(t)) = H_0 := H(q_0, p_0) \tag{6.6}$$

for all t from the maximal domain of existence of the solution from (6.2)–(6.5). We now make additional assumptions regarding the function Φ, in order to guarantee the existence of a global periodic solution. We require

$$\lim_{q \to \partial I} \Phi(q) = +\infty. \tag{6.7}$$

The function Φ is assumed to have a unique global minimum Φ_* at q_*, thus

$$\Phi_* = \min_I \Phi = \Phi(q_*). \tag{6.8}$$

Furthermore we assume

$$(q - q_*)\Phi'(q) > 0 \text{ for all } q \in I,\ q \neq q_* . \tag{6.9}$$

In particular $\Phi(q)$ is thus strict monotone increasing and decreasing for $q > q_*$ and $q < q_*$, respectively. In fact, unter these assumptions the initial value problem (6.2)–(6.5) has a unique smooth solution $q = q(t)$, $p = p(t)$, $t \geq 0$.

Periodicity: due to the assumptions regarding Φ there are two uniquely determined real numbers $q_-, q_+ \in I$ with $q_- \leq q_* \leq q_+$, so that

$$H_0 = \Phi(q_-) = \Phi(q_+). \tag{6.10}$$

If either $p_0 \neq 0$ or $q_0 \neq q_*$, then there holds $q_- < q_* < q_+$. Furthermore we define $p_-, p_+ \in \mathbb{R}$ by

$$p_\pm := \pm\sqrt{2H_0 - 2\Phi_*}. \tag{6.11}$$

Finally we define T_0 by

$$T_0 := \int_{q_-}^{q_+} \frac{\mathrm{d}q}{\sqrt{2H_0 - 2\Phi_*(q)}}. \tag{6.12}$$

The solution of (6.2)–(6.5) represents a periodic motion with the half period T_0 of the considered particle. The minimal and maximal positions are q_- and q_+, respectively, and the minimal and maximal momenta are p_- and p_+, respectively.

More precisely: There exist smooth functions $\tilde{q} : [0, t_0] \longrightarrow I$ and $\tilde{p} : [0, T_0] \longrightarrow \mathbb{R}$, so that with $t_0; + \inf\{t \geq 0; p(t) = 0\}$ and $t_{k+1} := t_k + T_0$ for $k \in \mathbb{N}_0 = \{0, 1, \dots\}$ there holds

$$\begin{aligned} q(t) &= \tilde{q}(t - t_{2k}), & (6.13) \\ p(t) &= \tilde{p}(t - t_{2k}), & (6.14) \end{aligned}$$

if $t \in [t_{2k}, t_{2k+1}]$ and

$$
\begin{aligned}
q(t) &= \tilde{q}(t_{2k+2} - t), && (6.15)\\
p(t) &= -\tilde{p}(t_{2k+2} - t), && (6.16)
\end{aligned}
$$

if $t \in [t_{2k+1}, t_{2k+2}]$. The two last relations remain valid for $k = -1$ if we set $t_1 := 0$. There holds $\tilde{q}' = \tilde{p}$, $\tilde{p}' = -\Phi'(\tilde{q})$.

The function $\tilde{q}$ maps the interval $[0, T_0]$ bijectively onto the interval $[q_-, q_+]$. Furthermore we have $T_0 = T_{0,-} + T_{0,+}$ with

$$T_{0,-} := \int_{q_-}^{q_*} \frac{\mathrm{d}q}{\sqrt{2H_0 - 2\Phi_*(q)}}, \quad T_{0,+} := \int_{q_*}^{q_+} \frac{\mathrm{d}q}{\sqrt{2H_0 - 2\Phi_*(q)}}. \tag{6.17}$$

If $p_0 > 0$ and $p_0 < 0$, respectively, then the function $\tilde{p}$ maps the intervals $[0, T_{0,-}]$ and $[T_{0,-}, T_0]$ bijectively onto the interval $[p_-, 0]$ and $[0, p_+]$, respectively. If $p_0 = 0$ and if additionally there holds $q_0 > q_*$ and $q_0 < q_*$, respectively, than the function $\tilde{p}$ maps the intervals $[0, T_{0,-}]$ and $[T_{0,-}, T_0]$, again bijectively onto the interval $[p_-, 0]$ and $[0, p_+]$, respectively.

In the following $\varepsilon > 0$ denotes a small real parameter. We start from the solution $q = q(t)$, $p = p(t)$ of the initial value problem (6.2)–(6.5) and define rescaled maps $q^\varepsilon = q^\varepsilon(t)$ and $p^\varepsilon = p^\varepsilon(t)$ by the definitions

$$
\begin{aligned}
q^\varepsilon(t) &:= q(\varepsilon^{-1} t), && (6.18)\\
p^\varepsilon(t) &:= p(\varepsilon^{-1} t). && (6.19)
\end{aligned}
$$

We now pose the question, whether at all and in which sense the limit $\varepsilon \to 0$ can be established.

We set $\mathbb{R}_+ := (0, +\infty)$, and in a first step we introduce continuous functions $\varphi : \mathbb{R}_+ \times [q_-, q_+] \longrightarrow \mathbb{R}$ with compact support and study the integrals

$$\int_0^\infty \varphi(t, q^\varepsilon(t)) \mathrm{d}t. \tag{6.20}$$

For simplicity we consider at first functions φ with the representation

$$\varphi(t, x) = \varphi_1(t) \varphi_2(x), \tag{6.21}$$

and we try to evaluate the limit of (6.20) for $\varepsilon \to 0$. To this end we rely on the introduced notations without mentioning this in each case. There holds

$$\int_0^\infty \varphi(t, q^\varepsilon(t))\mathrm{d}t \tag{6.22}$$

$$= \sum_{k=0}^\infty \left\{ \int_{\varepsilon t_{2k}}^{\varepsilon t_{2k+1}} \varphi_1(t)\varphi_2(q^\varepsilon(t))\mathrm{d}t + \int_{\varepsilon t_{2k+1}}^{\varepsilon t_{2k+2}} \varphi_1(t)\varphi_2(q^\varepsilon(t))\mathrm{d}t \right\} \tag{6.23}$$

$$= \sum_{k=0}^\infty \left\{ \int_{\varepsilon t_{2k}}^{\varepsilon t_{2k+1}} \varphi_1(t)\varphi_2(\tilde{q}(\varepsilon^{-1}t - t_{2k}))\mathrm{d}t + \int_{\varepsilon t_{2k+1}}^{\varepsilon t_{2k+2}} \varphi_1(t)\varphi_2(\tilde{q}(t_{2k+2} - \varepsilon^{-1}t))\mathrm{d}t \right\} \tag{6.24}$$

$$= \sum_{k=0}^\infty \left\{ \int_0^{T_0} \varphi_1(\varepsilon t_{2k} + \varepsilon t)\varphi_2(\tilde{q}(t))\varepsilon\mathrm{d}t + \int_0^{T_0} \varphi_1(\varepsilon t_{2k+2} + \varepsilon t)\varphi_2(\tilde{q}(t))\varepsilon\mathrm{d}t \right\} \tag{6.25}$$

$$= \sum_{k=0}^\infty \int_{q_-}^{q_+} \varphi_1(\varepsilon t_{2k} + \varepsilon\tilde{q}^{-1}(s))\varphi_2(s)\frac{\varepsilon}{\sqrt{2H_0 - 2\Phi(s)}}\mathrm{d}s + \tag{6.26}$$

$$+ \sum_{k=0}^\infty \int_{q_-}^{q_+} \varphi_1(\varepsilon t_{2k+2} - \varepsilon\tilde{q}^{-1}(s))\varphi_2(s)\frac{\varepsilon}{\sqrt{2H_0 - 2\Phi(s)}}\mathrm{d}s. \tag{6.27}$$

In the limiting case $\varepsilon \to 0$, each of the both sums converges to the expression

$$\int_0^\infty \int_{q_-}^{q_+} \varphi_1(t)\varphi_2(s)\frac{1}{2T_0}\frac{1}{\sqrt{2H_0 - 2\Phi(s)}}\mathrm{d}s\mathrm{d}t. \tag{6.28}$$

Thus we have proved

$$\lim_{\varepsilon\to 0}\int_0^\infty \varphi(t, q^\varepsilon(t))\mathrm{d}t = \int_0^\infty \int_{q_-}^{q_+} \varphi_1(t)\varphi_2(s)\frac{1}{2T_0}\frac{1}{\sqrt{2H_0 - 2\Phi(s)}}\mathrm{d}s\mathrm{d}t, \tag{6.29}$$

however, only for those continuous functions φ with compact support of the kind (6.21). For a better reading we define

$$F(s) := \frac{1}{T_0}\frac{1}{\sqrt{2H_0 - 2\Phi(s)}}. \tag{6.30}$$

Relying on the notation of measure theory we alternatively reformulate the limit (6.29): We denote by μ_{q^ε} the Young measure that is induced by the function $q^\varepsilon : \mathbb{R}_+ \to [q_-, q_+]$, i.e.

$$\langle \mu_{q^\varepsilon}, \varphi\rangle = \int_0^\infty \varphi(t, q^\varepsilon(t))\mathrm{d}t, \qquad \varphi \in C_0^0(\mathbb{R}_+ \times [q_-, q_+]). \tag{6.31}$$

Furthermore we introduce $\nu_F \in \mathcal{M}^1_+([q_-, q_+])$ which represents the probability measure that is induced by the probability density F:

$$\langle \nu_F, \varphi \rangle = \int_{q_-}^{q_+} \varphi(s) F(s) \mathrm{d}s, \qquad \varphi \in C^0_0([q_-, q_+]). \tag{6.32}$$

Finally we introduce the Lebesgue measure λ, restricted to the positive half line $\mathbb{R}_+$. Then the statement (6.29) can be written as

$$\lim_{\varepsilon \to 0} \mu_{q^\varepsilon} = \lambda \otimes \nu_F \tag{6.33}$$

in the sense of convergence of measures. Note that (6.29) remains valid if the function φ has the representation (6.21) with an integrable function φ_1 and a continuous function φ_2. Thus for any continuous function $\varphi_2 : [q_-, q_+] \to \mathbb{R}$ the limit

$$\lim_{\varepsilon \to 0} \varphi_2(q^\varepsilon(.)) = \int_{q_-}^{q_+} \varphi(s) F(s) \mathrm{d}s, \tag{6.34}$$

exist in the sense of weak-* convergence in $L^\infty(\mathbb{R}_+)$.

Next we derive the corresponding limit for the rescaled momenta $p^\varepsilon(t)$. For simplicity we consider only the case $p_0 = 0$, $q_0 = q_*$. Other cases can be treated analogously. Obviously we have as before

$$\int_0^\infty \varphi(t, p^\varepsilon(t)) \mathrm{d}t \tag{6.35}$$

$$= \sum_{k=0}^\infty \left\{ \int_{\varepsilon t_{2k}}^{\varepsilon t_{2k+1}} \varphi_1(t) \varphi_2(p^\varepsilon(t)) \mathrm{d}t + \int_{\varepsilon t_{2k+1}}^{\varepsilon t_{2k+2}} \varphi_1(t) \varphi_2(p^\varepsilon(t)) \mathrm{d}t \right\} \tag{6.36}$$

$$= \sum_{k=0}^\infty \left\{ \int_{\varepsilon t_{2k}}^{\varepsilon t_{2k+1}} \varphi_1(t) \varphi_2(\tilde{p}(\varepsilon^{-1} t - t_{2k})) \mathrm{d}t + \int_{\varepsilon t_{2k+1}}^{\varepsilon t_{2k+2}} \varphi_1(t) \varphi_2(-\tilde{p}(t_{2k+2} - \varepsilon^{-1} t)) \mathrm{d}t \right\} \tag{6.37}$$

$$= \sum_{k=0}^\infty \left\{ \int_0^{T_0} \varphi_1(\varepsilon t_{2k} + \varepsilon t) \varphi_2(\tilde{p}(t)) \varepsilon \mathrm{d}t + \int_0^{T_0} \varphi_1(\varepsilon t_{2k+2} + \varepsilon t) \varphi_2(-\tilde{p}(t)) \varepsilon \mathrm{d}t \right\} . \tag{6.38}$$

We denote by Ψ_+ and Ψ_-, respectively, the inverse mappings of the functions

$\Phi\big|_{I\cap[q_*,+\infty)}$ and $\Phi\big|_{I\cap(+\infty,q_*]}$, respectively. It follows:

$$\int_0^{T_0} \varphi_1(\varepsilon t_{2k}+\varepsilon t)\varphi_2(\tilde p(t))\varepsilon \mathrm{d}t \tag{6.39}$$

$$= \int_0^{T_{0,-}} \varphi_1(\varepsilon t_{2k}+\varepsilon t)\varphi_2(\tilde p(t))\varepsilon \mathrm{d}t + \int_{T_{0,-}}^{T_{0,+}} \varphi_1(\varepsilon t_{2k}+\varepsilon t)\varphi_2(\tilde p(t))\varepsilon \mathrm{d}t \tag{6.40}$$

$$= \int_0^{p_-} \varphi_1(\varepsilon t_{2k}+\varepsilon \tilde p^{-1}(s))\varphi_2(s)\frac{\varepsilon}{-\Phi'(\tilde q(\tilde p^{-1}(s)))}\mathrm{d}s + \tag{6.41}$$

$$+\int_{p_-}^{0} \varphi_1(\varepsilon t_{2k}+\varepsilon \tilde p^{-1}(s))\varphi_2(s)\frac{\varepsilon}{-\Phi'(\tilde q(\tilde p^{-1}(s)))}\mathrm{d}s \tag{6.42}$$

$$= \int_{p_-}^{0} \varphi_1(\varepsilon t_{2k}+\varepsilon \tilde p^{-1}(s))\varphi_2(s)\frac{\varepsilon}{\Phi'(\Psi_+(H_0-\frac{1}{2}s^2))}\mathrm{d}s - \tag{6.43}$$

$$-\int_{p_-}^{0} \varphi_1(\varepsilon t_{2k}+\varepsilon \tilde p^{-1}(s))\varphi_2(s)\frac{\varepsilon}{\Phi'(\Psi_-(H_0-\frac{1}{2}s^2))}\mathrm{d}s. \tag{6.44}$$

In an analogous manner we proceed with

$$\int_0^{T_0} \varphi_1(\varepsilon t_{2k+2}+\varepsilon t)\varphi_2(-\tilde p(t))\varepsilon \mathrm{d}t \tag{6.45}$$

$$= \int_0^{T_{0,-}} \varphi_1(\varepsilon t_{2k+2}-\varepsilon t)\varphi_2(-\tilde p(t))\varepsilon \mathrm{d}t + \int_{T_{0,-}}^{T_{0,+}} \varphi_1(\varepsilon t_{2k+2}-\varepsilon t)\varphi_2(-\tilde p(t))\varepsilon \mathrm{d}t \tag{6.46}$$

$$= \int_0^{p_+} \varphi_1(\varepsilon t_{2k+2}-\varepsilon \tilde p^{-1}(-s))\varphi_2(s)\frac{\varepsilon}{\Phi'(\tilde q(\tilde p^{-1}(-s)))}\mathrm{d}s + \tag{6.47}$$

$$+\int_{p_+}^{0} \varphi_1(\varepsilon t_{2k+2}-\varepsilon \tilde p^{-1}(-s))\varphi_2(s)\frac{\varepsilon}{\Phi'(\tilde q(\tilde p^{-1}(-s)))}\mathrm{d}s \tag{6.48}$$

$$= \int_0^{p_+} \varphi_1(\varepsilon t_{2k+2}-\varepsilon \tilde p^{-1}(-s))\varphi_2(s)\frac{\varepsilon}{\Phi'(\Psi_+(H_0-\frac{1}{2}s^2))}\mathrm{d}s - \tag{6.49}$$

$$+\int_0^{p_+} \varphi_1(\varepsilon t_{2k+2}-\varepsilon \tilde p^{-1}(-s))\varphi_2(s)\frac{\varepsilon}{\Phi'(\Psi_-(H_0-\frac{1}{2}s^2))}\mathrm{d}s. \tag{6.50}$$

We end up with

$$\lim_{\varepsilon\to 0}\int_0^\infty \varphi(t,p^\varepsilon(t))\mathrm{d}t = \int_0^\infty\int_{p_-}^{p_+}\varphi(t,s)G(s)\mathrm{d}s\,\mathrm{d}t, \tag{6.51}$$

where the probability density is defined by

$$\begin{aligned} G(s) &= \frac{1}{2T_0}\left\{\frac{1}{\Phi'(\Psi_+(H_0-\frac{1}{2}s^2))}-\frac{1}{\Phi'(\Psi_-(H_0-\frac{1}{2}s^2))}\right\} & (6.52)\\ &= \frac{1}{2T_0}\left\{\Phi'\left(\Psi_+(H_0-\frac{1}{2}s^2)\right)-\Phi'\left(\Psi_-(H_0-\frac{1}{2}s^2)\right)\right\}. & (6.53)\end{aligned}$$

Let μ_{p^ε} be the Young measure that is induced by the function $p^\varepsilon : \mathbb{R}_+ \to [p_-, p_+]$ and let furthermore be ν_G the probability measure that is induced by the probability density G, so that in analogy to the former case:

$$\lim_{\varepsilon\to 0}\mu_{p^\varepsilon} = \lambda\otimes\nu_G \tag{6.54}$$

in the sense of convergence of measures. Furthermore there holds

$$\lim_{\varepsilon\to 0}\varphi_2(p^\varepsilon(.)) = \int_{p_-}^{p_+}\varphi_2(s)G(s)\mathrm{d}s \tag{6.55}$$

for any continuous function $\varphi_2 : [p_-, p_+] \to \mathbb{R}$ in the sense of weak-*-convergence of $L^\infty(\mathbb{R}_+)$.

We now consider a continuous function with compact support $\varphi : \mathbb{R}_+[q_-, q_+] \times [p_-, p_+] \to \mathbb{R}$. Then we can write

$$\begin{aligned}\lim_{\varepsilon\to 0}\int_0^\infty (t,q^\varepsilon(t),p^\varepsilon(t))\mathrm{d}t = \int_0^\infty\int_{q_-}^{q_+}&\left\{\varphi\left(t,s,\sqrt{2H_0-2\Phi(s)}\right)+\right. & (6.56)\\ &\left.+\varphi\left(t,s,-\sqrt{2H_0-2\Phi(s)}\right)\right\}\frac{1}{2T_0}\frac{1}{\sqrt{2H_0-2\Phi(s)}}\mathrm{d}s\,\mathrm{d}t.\end{aligned}$$

We set

$$\mathcal{C} := \left\{(q,p)\in\mathbb{R}^2 : H(q,p)=H_0\right\}. \tag{6.57}$$

There holds $\mathcal{C} = \mathcal{C}_-\cup\mathcal{C}_+$ where $\mathcal{C}_-$ and $\mathcal{C}_+$ are given in parameter representation as follows:

$$\mathcal{C}_+ : \quad \left\{\begin{array}{lcl} q(s) &=& s\\ p(s) &=& \sqrt{2H_0-2\Phi(s)}\end{array}\right., s\in[q_-,q_+], \tag{6.58}$$

$$\mathcal{C}_- : \quad \left\{\begin{array}{lcl} q(s) &=& q_-+q_+-s\\ p(s) &=& -\sqrt{2H_0-2\Phi(q_-+q_+-s)}\end{array}\right., s\in[q_-,q_+]. \tag{6.59}$$

For any continuous functions $f : \mathcal{C} \to \mathbb{R}$ we may thus write

$$\int_{\mathcal{C}} f(q,p)\mathrm{d}\mathcal{C} = \int_{q_-}^{q_+} \left(f\left(s, \sqrt{2H_0 - 2\Phi(s)}\right) + \right. \tag{6.60}$$

$$\left. + f\left(s, -\sqrt{2H_0 - 2\Phi(s)}\right)\right) \sqrt{1 + \frac{\Phi'(s)^2}{2H_0 - 2\Phi(s)}}\mathrm{d}s$$

to obtain

$$\int_{\mathcal{C}} f(q,p)\frac{1}{\sqrt{p^2 + \Phi'(q)^2}} = \tag{6.61}$$

$$= \int_{q_-}^{q_+} \left(f\left(s, \sqrt{2H_0 - 2\Phi(s)}\right) + f\left(s, -\sqrt{2H_0 - 2\Phi(s)}\right)\right) \frac{1}{\sqrt{2H_0 - 2\Phi(s)}}\mathrm{d}s.$$

In the sense of convergence of measures the result (6.61) can be written as

$$\lim_{\varepsilon \to 0} \mu_{(q^\varepsilon, p^\varepsilon)} = \lambda \otimes \nu_A. \tag{6.62}$$

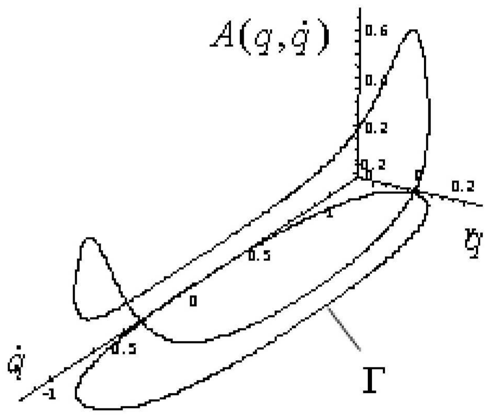
Here $\mu_{(q^\varepsilon, p^\varepsilon)}$ denotes the Young measure corresponding to the mapping $(q^\varepsilon, p^\varepsilon) : \mathbb{R}_+ \to [q_-, q_+] \times [p_-, p_+]$ again we denote the Lebesgue measure restricted to the positive half line $\mathbb{R}_+$ by λ, and ν_A denotes the measure on $\mathcal{C}$ that is induced by the probability density

$$A(q,p) = \frac{1}{2T_0}\frac{1}{\sqrt{p^2 + \Phi'(q)^2}}, \quad (q,p) \in \mathcal{C}, \tag{6.63}$$

so that we may write

$$\langle \nu_A, \varphi \rangle = \int_{\mathcal{C}} \varphi(q,p)A(q,p)\mathrm{d}\mathcal{C}, \quad \varphi \in C^0(\mathcal{C}). \tag{6.64}$$

It is important to note that the functions F and G have weak (integrable) singularities, whereas the function A, which is depicted in the figure, is regular in all points of its domain of definition $\mathcal{C}$.



Phase space of the single oscillator

References

[1] W. Dreyer, M. Herrmann, *A simple but rigourous micro-macro transitions*, WIAS-Preprint No. **723** (1998).

[2] W. Dreyer, M. Herrmann, *Towards rigorous micro-macro transitions: The microscopic oscillator motion.*, WIAS-Preprint No. 724 (2002).

[3] Dreyer, W.; Kunik, M.: Cold, thermal and oscillator closure of the atomic chain; *J. Phys. A: Math. Gen.* **33** (2000), 2097–2129, 2458

[4] Friesecke, G.; Pego, R. L.: Solitary waves on FPU lattices: I. Qualitative properties, renormalization and continuum limit; *Nonlinearity* **12** (1999), 1601–1627

[5] A. Mielke, *Flow properties for Young-measure solutions of semilinear hyperbolic problems.* Proc. Roy. Soc. Edinburgh Sect. A **129** no. 1, 85–123, 1999.

[6] Skeel, R. D.; Zhang, G.; Schlick, T.: A Family of Symplectic Integrators: Stability, Accuracy, and Molecular Dynamics Applications; *SIAM J. Sci. Comput.* **18** (1997), 203–222

[7] Taylor, M. E.: *Partial Differential Equations. 2: Nonlinear Equations;* Springer