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Towards Rigorous Micro-Macro Transitions: The Microscopic Oscillator Motion

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Abstract

The atomic chain whose dynamics evolve according to NEWTON's equations of motion serves as a simple microscopic many-particle system for an analysis of the macroscopic or thermodynamic limit. If the interaction potential has a sufficient strong repulsive part, it is possible to create a special microscopic motion, that we call *oscillator motion*, which is simpler as the *classical thermal motion*. However, also the oscillator motion leads to temperature, a GIBBS equation and an entropy.

In the current paper we derive the thermodynamics for the oscillator motion without the subtle replacement of the many-particle sytem by a single equation of motion as it is done in [4]. Furthermore we introduce a different mathematical setting for micro-macro transitions as in [4], which is better suited for a rigorous treatment.

1 Introduction

1.1 The problem

The atomic chain whose dynamics evolve according to NEWTON's equations of motion serves as a simple microscopic many-particle system for an analysis of the macroscopic limit which sometimes is also called thermodynamic limit. If the interaction potential has a sufficient strong repulsive part, it is possible to create a special microscopic motion, that we call *oscillator motion*, which is simpler as the *classical thermal motion*. We indicate by the notion *classical thermal motion* that the velocities and distances of the particles are completely uncorrelated. *Oscillator motion* denotes the other extreme case, where velocities and distances are completely correlated by the equations of motion. However, both kinds of microscopic motions have in common that they produce on the macroscopic scale an evolution which relies on the conservation laws for mass, momentum and energy and on constitutive functions obeying the laws of thermodynamics. Despite its deterministic features, the oscillator motion even leads to temperature, a GIBBS equation and an entropy.

On the other hand, the mathematical structure of the oscillator motion is much simpler as for the classical thermal motion, and this makes the former very attractive for rigorous micro-macro transitions. The oscillator motion and its properties was first observed and described by DREYER & KUNIK in [4], where they reported on an interesting scaling behaviour of the solutions of RIEMANN initial value problems in the macroscopic limit. The authors motivate by computer experiments that the many-particle problem of the oscillator motion can be reduced to a single equation of motion for a single oscillator. Relying on this assumption they derived the thermodynamics of the atomic chain.

In the current paper we derive the same thermodynamics for the oscillator motion without the subtle replacement of the many-particle sytem by a single equation of motion. Furthermore we introduce a different mathematical setting for micro-macro transitions as in [4], which is better suited for a rigorous treatment. The different setting relies on the introduction of LAGRANGE coordinates instead of EULER coordinates. LAGRANGE coordinates are the canonical coordinates for the establishment of micro-macro transitions because their microscopic counterpart is the particle index which appears explicitely in the equations of motions. They were already used by FRIESECKE & PEGO in [1] for the first rigorous transition from the microscopic equations of motion to the KORTEWEG-DEVRIES equation.

1.2 The organization of this study

In Section 2 we introduce the macroscopic conservation laws for mass, momentum and energy in EULER and LAGRANGE coordinates. The objective of this this study is formulated explicitely in Section 3. The microscopic model and the RIEMANN initial value problems are introduced in Sections 4 and 5.

In Section 6 we report on some numerical observations from [4], where the authors have identified the oscillator motion of the atomic chain.

The main part of this study is contained in Section 7, which is decomposed into several subsections. In section 7.1 we reformulate the equations of motions so that the relation of the oscillator motion to the general motion becomes apparent. The scalings of space and time and of various quantities, which appear in the equations of motion, are introduced in Section 7.2. The introduction of the scaling behaviour is the most subtle procedure, because macroscopic convergence of microscopic quantities can only be achieved if the introduced scaling fits to the considered class of initial conditions. In Section 7.3 we derive the conservation law of mass, which is in LAGRANGE coordinates simply a kinematic condition. The other conservation laws and the constitutive functions are derived in the Sections 7.6 and 7.7. To this end a prerequisite knowledge of mean values of highly oscillating functions is necessary. Mean values are introduced in Section 7.4. In 7.5. we calculate the explicit form of the phase density of the oscillator motion.

We conclude the study in section 8 with a summary and we give some perspectives.

2 The macroscopic conservation laws

The macroscopic behaviour of the atomic chain relies on the conservation laws for particle number, momentum and energy. The densities of these quantities are

$$\rho \text{ -- number densitiy}, \quad \rho v \text{ -- momentum density} \quad \text{and} \quad \rho e \text{ -- energy density}. \tag{1}$$

Here v and e are the velocity and the specific energy, respectively.

2.1 The conservation laws in Euler coordinates

In regular space time points (t, x) the conservation laws read

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x} = 0, \quad \frac{\partial \rho v}{\partial t} + \frac{\partial P}{\partial x} = 0, \quad \frac{\partial \rho e}{\partial t} + \frac{\partial Q}{\partial x} = 0. \tag{2}$$

The quantities P and Q are the momentum flux and the energy flux, respectively. It is well known that shocks may arise during the evolution of these fields, so that the considered space time region decomposes into two regions $+$ and $-$, which are seperated by a shock curve, $x_s(t)$, whose tangent gives the shock speed V_s. On singular points where this happens, the jumps $[[\psi]] := \psi_+ - \psi_-$ of the fields follow from the jump conditions

$$-V_s[[\rho]] + [[\rho v]] = 0, \quad -V_s[[\rho v]] + [[P]] = 0, \quad -V_s[[\rho e]] + [[Q]] = 0. \tag{3}$$

The principle of GALLILEI invariance implies decompositions of the energy density, the momentum flux and the energy flux so that their dependence on the velocity becomes explicit:

$$\begin{aligned} P &= \rho v^2 + p, \\ \rho e &= \frac{1}{2}\rho v^2 + \rho u, \\ Q &= (\frac{1}{2}\rho v^2 + \rho u)v + pv + q. \end{aligned} \tag{4}$$

Here p, u and q are the pressure, the specific internal energy and the heat flux, respectively. These quantities do not depend on the velocity, rather these are considered to be constitutive quantities which must be given by constitutive relations so that the conservation laws become a closed system of field equations. The given scheme represents the conservation laws in EULER coordinates t and x which are best suited for the discussion of the evolution of the fields, because the EULER coordinates give the point of view of a fixed observer.

2.2 The conservation laws in Lagrange coordinates

There are other coordinates t and α which are called LAGRANGE coordinates. These are introduced here, because LAGRANGE coordinates are more appropriate than EULER coordinates to establish micro-macro transitions.

The LAGRANGE coordinate α is defined by

$$\alpha(t,\, x) \;=\; \int\limits_0^x \rho(t,\, \xi)\, d\xi. \tag{5}$$

We conclude that for given time t, the coordinate α is a monotone function of x. There holds

$$\frac{\partial\, \alpha}{\partial\, x}(t,\, x) = \rho(t,\, x) > 0, \tag{6}$$

and we can invert $\alpha = \alpha(t,\, x)$ to obtain $x = \hat{x}(t,\, \alpha)$.

Next we define the fields ρ, v and u in LAGRANGE coordinates according to

$$\hat{\rho}(t,\, \alpha) = \rho\big(t,\, \hat{x}(t,\, \alpha)\big), \quad \hat{v}(t,\, \alpha) = v\big(t,\, \hat{x}(t,\, \alpha)\big), \quad \hat{u}(t,\, \alpha) = u\big(t,\, \hat{x}(t,\, \alpha)\big), \tag{7}$$

and in the same manner

$$\hat{p}(t,\, \alpha) = p\big(t,\, \hat{x}(t,\, \alpha)\big), \quad \hat{q}(t,\, \alpha) = q\big(t,\, \hat{x}(t,\, \alpha)\big). \tag{8}$$

These definitions can now be used to derive the conservation laws in LAGRANGE coordinates from the conservation laws in EULER coordinates. We obtain in regular points

$$\frac{\partial\, \hat{d}}{\partial\, t} - \frac{\partial\, \hat{v}}{\partial\, \alpha} = 0, \quad \frac{\partial\, \hat{v}}{\partial\, t} + \frac{\partial\, \hat{p}}{\partial\, \alpha} = 0, \quad \frac{\partial\, (\hat{u} + \frac{1}{2}\hat{v}^2)}{\partial\, t} + \frac{\partial\, (\hat{p}\hat{v} + \hat{q})}{\partial\, \alpha} = 0. \tag{9}$$

and in singular points, which move with the speed V_S with respect to LAGRANGE coordinates, there follows

$$-V_S[[\hat{d}]] - [[\hat{v}]] = 0, \quad -V_S[[\hat{v}]] + [[p]] = 0, \quad -V_S[[\hat{u} + \frac{1}{2}\hat{v}^2]] + [[\hat{p}\hat{v} + \hat{q}]] = 0. \tag{10}$$

The field $\hat{d} = 1/\, \hat{\rho}$ denotes the specific volume, which is a specific length in the $1D$ case.

3 The objective of this study

For the description of the macroscopic state of the atomic chain, we consider the specific length, the velocity and the internal energy as the basic variables. Consequently, the conservation laws become field equations if we will be able to relate the constitutive quantities pressure and heat flux to the variables.

It is the objective of this study to derive the system of conservation laws and constitutive relations from an underlying microscopic many-particle model. In general this task has not been solved up to now. In [4] it is demonstrated that the resulting macroscopic system of field equations strongly depends on the class of intial conditions for which the many-particle system is solved. The authors describe in [4] that there exists a special class of initial conditions, which induce a simple kind of microscopic motion. They call these initial conditions *cold* RIEMANN data and the resulting microscopic motion *oscillator motion.*

RIEMANN data consists of two constant states which are separated by a single discontinuity. The notion *cold* indicates that there is initially no thermal motion. However, it was numerically observed that the microscopic system develops temperature and entropy in the vicinity of the discontinuity. Furthermore it was observed that the resulting macroscopic fields exhibit a very astonishing scaling behaviour. For RIEMANN data with the initial discontinuity at $x = L/2$, the space time dependence of the macroscopic fields is simply given by the ratio $(x - L/2)/t$.

This observation motivates a special scaling which is the starting point of the current study, where we derive the macroscopic system of field equations completely from the microscopic many-particle system.

With the introduction of the microscopic model, which will be given next, there appear two time and space scales. From now on, the macroscopic coordinates are denoted by

$$\overline{t}, \quad \overline{x} \quad \text{and} \quad \overline{\alpha}, \tag{11}$$

whereas t, x, α are their corresponding microscopic counterparts.

4 The microscopic model

We consider an atomic chain consisting of N structureless particles with mass $m = 1$. At time t the particles have the positions and velocities

$$\big\{x_1(t),\, x_1(t),\, ...,\, x_N(t)\big\} \quad \text{and} \quad \big\{\dot{x}_1(t),\, \dot{x}_1(t),\, ...,\, \dot{x}_N(t)\big\}, \tag{12}$$

repectively. The first and the Nth particle are fixed at $x_1 = 0$ and $x_N = L$. The other particles move according to nearest neighbour interactions with the potential

$$\varphi(r) = \frac{1}{8}\frac{1}{r^4} - \frac{1}{4}\frac{1}{r^2}, \qquad \text{so that} \qquad \varphi'(1) = 0 \qquad \text{and} \qquad \varphi''(1) = 1. \tag{13}$$

The dynamics of the particles is described by NEWTONs law of motion

$$\ddot{x}_\alpha = \varphi'(x_{\alpha+1} - x_\alpha) - \varphi'(x_\alpha - x_{\alpha-1}) \qquad \text{with} \qquad \alpha \in \{2, N-1\}. \tag{14}$$

The initial conditions are given by the initial positions

$$\{x_1(0) = 0,\, x_2(0) = x_2^0,\, ...,\, x_{N-1}(0) = x_{N-1}^0,\, x_N(0) = L\} \tag{15}$$

and the initial velocities

$$\{\dot{x}_1(0) = 0,\, \dot{x}_2(0) = \dot{x}_2^0,\, ...,\, \dot{x}_{N-1}(0) = \dot{x}_{N-1}^0,\, \dot{x}_N(0) = 0\}. \tag{16}$$

The potential (13) may be replaced by other potentials, for instance by the TODA potential, which reads

$$\varphi(r) = \frac{a}{b}\exp(-b(r-1)) + a(r-1), \qquad \text{with} \qquad a, b > 0. \tag{17}$$

The TODA potential has some advantages regarding the analytical treatment of the many-particle problem. In the vicinity of $r = 1$, the TODA potential has the same properties as the potential (13).

5 The RIEMANN problem with cold initial data

We consider macroscopic initial data with a constant state for $\overline{x} \leq \frac{1}{2}\overline{L}$ and a different constant state for $\overline{x} > \frac{1}{2}\overline{L}$, so that there is initially a single discontinuity at $\overline{x} = \frac{1}{2}\overline{L}$.

RIEMANN initial data are best suited to exhibit the scaling behaviour that appears along with micro-macro transitions. There are special RIEMANN initial data that lead to a very interesting microscopic motion. These data are called cold initial data.

Cold initial data can be described as follows. The macroscopic state of a chain with N particles is determined by only four constants $\overline{\rho}_-$, $\overline{\rho}_+$, $\overline{v}_-$, $\overline{v}_+$. The corresponding macroscopic initial fields number density and velocity read

$$\overline{\rho}\,(0,\,\overline{x}) = \left\{ \begin{array}{ccc} \overline{\rho}_- & & \overline{x} \leq \frac{1}{2}\overline{L} \\ & \text{for} & \\ \overline{\rho}_+ & & \overline{x} > \frac{1}{2}\overline{L} \end{array} \right. , \qquad \overline{v}\,(0,\,\overline{x}) = \left\{ \begin{array}{ccc} \overline{v}_- & & \overline{x} \leq \frac{1}{2}\overline{L} \\ & \text{for} & \\ \overline{v}_+ & & \overline{x} > \frac{1}{2}\overline{L} \end{array} \right. . \tag{18}$$

According to these *macroscopic* initial data we prepare the *microscopic* initial data of the atomic chain as follows. Let be N_- and N_+ be the numbers of atoms which are initially left and right from the discontinuity, respectively, and let $L = N\overline{L}$ be the length of the chain in microscopic space units. According to [4] we can calculate N_-, N_+ and L by

$$L = 2\frac{N-1}{\overline{\rho}_- + \overline{\rho}_+}, \quad N_- + N_+ = N - 1, \quad \frac{N_-}{\overline{\rho}_-} + \frac{N_+}{\overline{\rho}_+} = L. \tag{19}$$

Finally, the microscopic initial positions of the atoms result as

$$x_\alpha^0 \;=\; \frac{\alpha - 1}{\overline{\rho}_-} \qquad \text{if} \quad \alpha = 1,\, ..,\, N-, \qquad \text{and} \tag{20}$$

$$x_\alpha^0 \;=\; \frac{N_-}{\overline{\rho}_-} + \frac{\alpha - 1 - N_-}{\overline{\rho}_+} \qquad \text{if} \quad \alpha = N_- + 1,\, ..,\, N. \tag{21}$$

Since there is initially no temperature, we set

$$\dot{x}_\alpha^0 \;=\; \overline{v}_- \qquad \text{if} \quad \alpha = 1,\, ..,\, N_-, \qquad \text{and} \tag{22}$$

$$\dot{x}_\alpha^0 \;=\; \overline{v}_+ \qquad \text{if} \quad \alpha = N_- + 1,\, ..,\, N. \tag{23}$$

6 Numerical observations

Numerical observations of the cold initial value problem in [4] has revealed the following phenomena:

- The macroscopic fields $\overline{U}(\bar{t}, \overline{x})$ scale so that there holds

$$\overline{U}(\bar{t}, \overline{x}) = \hat{U}(\frac{\overline{x} - \overline{L}/2}{\bar{t}}). \tag{24}$$

- The evolution of the macroscopic fields $\overline{U}(\bar{t}, \overline{x})$ consists of constant states, rarefaction waves and shocks, which is the usual behaviour of a quasi-linear hyperbolic sytem of conservation laws, see [5], [6] and [8] for details.

- Temperature develops in the vicinity of the shocks.

- In the space time regions with temperature, the underlying microscopic motion is the *oscillator motion*. The atoms of the chain move according to the oscillator motion, if for any α the two atomic distances

$$x_{\alpha+1}(t) - x_\alpha(t) \quad \text{and} \quad x_{\alpha+3}(t) - x_{\alpha+2}(t) \tag{25}$$

  have about the same size. In [4] the oscillator motion is modeled by only two different atomic distances $r\,(t)$ and $s\,(t)$, so that the microscopic atomic distances $y_\alpha := x_{\alpha+1} - x_\alpha$ are given by

$$..,\, y_\alpha(t),\, y_{\alpha+1}(t),\, y_{\alpha+2}(t),\, y_{\alpha+3}(t),\, .. \quad = \quad ..,r(t),\, s(t),\, r(t),\, s(t),\, \ldots$$

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

$$r\,(t) + s\,(t) = \frac{2}{\rho}. \tag{26}$$

Furthermore it was argued in [4] that there is only one representative equation of motion, viz.

$$\ddot{r}\,(t) = 2\left(\varphi'\left(\frac{2}{\rho} - r\,(t)\right) - \varphi'\,(r\,(t))\right). \tag{27}$$

Relying on this single microscopic equation, DREYER & KUNIK calulated the macroscopic system of field equations. In the current study we will also start from the reported scaling behaviour (24). However, we will not assume that only two microscopic distances may appear.

7 The macroscopic limit

7.1 Preliminary reformulation of the N-particle system

We start from (14) in the form

$$\ddot{x}_\alpha = \varphi'(x_{\alpha+1} - x_\alpha) - \varphi'(x_\alpha - x_{\alpha-1}), \tag{28}$$

where $\alpha \in \{1, .., N\}$. For simplicity we assume that $N = 2M$ is odd. Furthermore, for the theoretical setting we consider periodic boundary conditions. In particular we set

$$x_0 := x_N \quad \text{and} \quad x_{N+1} := x_1. \tag{29}$$

Note that the energy per particle, which is defined by

$$e_\alpha = \frac{1}{2}\dot{x}_\alpha^2 + \frac{1}{2}\varphi(x_{\alpha+1} - x_\alpha) + \frac{1}{2}\varphi(x_\alpha - x_{\alpha-1}), \tag{30}$$

leads to a conservation law, viz.

$$\frac{d}{dt}\left(\sum_{\alpha=1}^{N} e_\alpha\right) = 0. \tag{31}$$

Next we rearrange the particle indices according to

$$\beta = \frac{1}{2}\alpha \quad \text{with} \quad \beta \in [1, M], \tag{32}$$

and we introduce new variables, viz.

$$\begin{aligned} r_\beta &= x_{2\beta} - x_{2\beta-1}, & m_\beta &= \frac{1}{2}(x_{2\beta} + x_{2\beta-1}), \\ s_\beta &= x_{2\beta+1} - x_{2\beta}, & n_\beta &= \frac{1}{2}(x_{2\beta} + x_{2\beta+1}). \end{aligned} \tag{33}$$

Motivation

The introduction of the new particle index β is closely related to the oscillator motion, cf. [4]. The positions of the particles in an atomic chain that performs the oscillator motion, are depicted in Figure 1. In particular, the functions r_β and s_β vary slowly with respect to β.

Assumption

Within this paper we assume, that the atoms of the chain move according to the oscillator motion. All results that we will derive below, are valid only under this

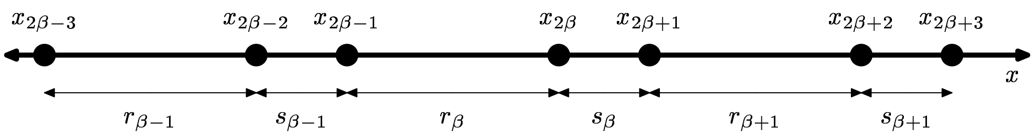

Figure 1: The atomic positions of the oscillator motion

assumption. However, this assumption can be justified numerically for a class of special initial data. For a more detailed discussion we refer to [4].

Among the new variables (33) there a several identities:

$$r_\beta + s_\beta = 2(n_\beta - m_\beta) = 2(n_\beta - n_{\beta-1/2}) = 2(m_{\beta+1/2} - m_\beta), \tag{34}$$

which will be used in the following. The variables r_β and s_β are adjacent distances, whereas m_β and n_β indicate adjacent centers of mass of two neighbouring particles.

The equations of motion for the atom with index 2β and its two neighbours read

$$\begin{aligned} \ddot{x}_{2\beta-1} &= \varphi'(r_\beta) - \varphi'(s_{\beta-1}), \\ \ddot{x}_{2\beta} &= \varphi'(s_\beta) - \varphi'(r_\beta), \\ \ddot{x}_{2\beta+1} &= \varphi'(r_{\beta+1}) - \varphi'(s_\beta). \end{aligned} \tag{35}$$

From the variables (33) we form the canonical variables for the establishment of a macroscopic limit. These are defined by

$$\begin{aligned} d_\beta &= \frac{1}{2}(r_\beta + s_\beta) = n_\beta - m_\beta, \\ q_\beta &= \frac{1}{4}(s_\beta - r_\beta) = \frac{1}{2}(d_\beta - r_\beta), \\ f_\beta &= \frac{1}{2}(m_\beta + n_\beta). \end{aligned} \tag{36}$$

The time derivative of f_β will be identified later as the macroscopic velocity. For this reason we introduce the notation

$$v_\beta = \dot{f}_\beta. \tag{37}$$

Remarks

1. Recall that it was observed in [4], that d_β is a slowly varying function of time. Variations of d_β can be observed on the macro scale only. The same holds for the variable f_β. On the other hand, the variable q_β describes rapid oscillations that can be observed exclusively on the microscale.

2. All variables vary slowly with respect to the particle index β.

3. The variables m_β, n_β and f_β depend monotonically on the particle index β.

NEWTON's equations of motion for the variables d_β, q_β and f_β read

$$
\begin{aligned}
\ddot{d}_\beta &= \frac{1}{2}(\varphi'(r_{\beta+1}) - \varphi'(r_\beta) + \varphi'(s_{\beta-1}) - \varphi'(s_\beta)), \\
\ddot{q}_\beta &= \varphi'(r_\beta) - \varphi'(s_\beta) + \ddot{f}_\beta, \\
\ddot{f}_\beta &= \frac{1}{4}(\varphi'(r_{\beta+1}) - \varphi'(r_\beta) + \varphi'(s_\beta) - \varphi'(s_{\beta-1})).
\end{aligned}
\tag{38}
$$

Interpretation

The three equations of motion (38) for the variables d_β, q_β and f_β play different roles. Equation $(38)_2$ describes the microscopic oscillators. It is used to calculate the constitutive functions. On the other hand, $(38)_1$ and $(38)_3$ form the basis for the macroscopic conservation laws of momentum and energy. In contrast to the fact that $d_\beta(t)$ is a slow function, Equation $(38)_1$ is macroscopically not directly observable, and it is only used for some preliminary calculations.

Let us use the new variables to form the energy

$$
\begin{aligned}
e_\beta &= \frac{1}{4}\dot{x}_{2\beta+1}^2 + \frac{1}{2}\dot{x}_{2\beta}^2 + \frac{1}{4}\dot{x}_{2\beta-1}^2 + \varphi(r_\beta) + \varphi(s_\beta) \\
&= \frac{1}{8}\dot{r}_\beta^2 + \frac{1}{8}\dot{s}_\beta^2 + \frac{1}{2}\dot{m}_\beta^2 + \frac{1}{2}\dot{n}_\beta^2 + \varphi(r_\beta) + \varphi(s_\beta) \\
&= \dot{q}_\beta^2 + \frac{1}{2}\dot{d}_\beta^2 + \dot{f}_\beta^2 + \varphi(r_\beta) + \varphi(s_\beta),
\end{aligned}
\tag{39}
$$

so that there holds

$$
\frac{d}{dt}\left(\sum_{\beta=1}^{M} e_\beta(t)\right) = 0. \tag{40}
$$

Note that e_β contains the energy of two particles.

7.2 Scalings, Part 1: Definitions and first conclusions

The natural scaling parameter is given by the number of particles N. In order to establish the macro limit $N \to \infty$ we introduce $\varepsilon = 1/N$ and consider the limiting case $\varepsilon \to 0$. According to the chosen class of initial conditions, namely those that lead to waves, we scale time, space and the two particle indices by

$$
\overline{t} = \varepsilon t, \qquad \overline{x} = \varepsilon x, \qquad \overline{\alpha} = \varepsilon\alpha, \qquad \overline{\beta} = \varepsilon\beta. \tag{41}
$$

There follows

$$
\overline{\alpha} \in [0,\, 1], \qquad \overline{\beta} \in [0,\, \frac{1}{2}], \qquad \overline{\beta} = \frac{1}{2}\overline{\alpha} \qquad \text{and} \qquad \frac{\partial}{\partial\,\overline{\beta}} = 2\frac{\partial}{\partial\,\overline{\alpha}}. \tag{42}
$$

We call the scaled particle index $\overline{\alpha}$ a LAGRANGE position. Obviously, for any finite N the scaled particles indices $\overline{\alpha}$ and $\overline{\beta}$ remain discrete quantities. However, $\overline{\alpha}$ as well as $\overline{\beta}$ become continuous if $N \to \infty$. The transition from discrete particle indices to continuous ones, is studied in detail in [2].

In order to obtain a more intuitive notation, we write

$$r^{\varepsilon}(t,\, \beta) \text{ instead of } r_{\beta}(t), \quad s^{\varepsilon}(t,\, \beta) \text{ instead of } s_{\beta}(t), \quad \ldots \tag{43}$$

However, recall that β is a discrete variable with $\beta \in \{1, ..., M\}$. Furthermore we write for the velocities

$$\frac{\partial r^{\varepsilon}}{\partial t}(t,\, \beta) \text{ instead of } \dot{r}_{\beta}(t), \quad \frac{\partial s^{\varepsilon}}{\partial t}(t,\, \beta) \text{ instead of } \dot{s}_{\beta}(t), \quad \ldots \tag{44}$$

There is only one exception to the latter convention. For reasons that will become obvious in Section 7.4, we define

$$\dot{q}^{\varepsilon}(t,\, \beta) \;\; := \;\; \dot{q}_{\beta}(t). \tag{45}$$

Since m_{β}, n_{β} and f_{β} are center of mass coordinates, they scale like the space coordinate. The other variables r_{β}, s_{β}, d_{β} and q_{β} represent atomic distances, thus these variables are scale invariant. We write

$$\begin{aligned}
\overline{m}^{\varepsilon}(\overline{t},\, \overline{\beta}) \;&:=\; \varepsilon m^{\varepsilon}\Big(\frac{\overline{t}}{\varepsilon},\, \frac{\overline{\beta}}{\varepsilon}\Big) \;=\; \varepsilon m^{\varepsilon}(t,\, \beta), \\
\overline{n}^{\varepsilon}(\overline{t},\, \overline{\beta}) \;&:=\; \varepsilon n^{\varepsilon}\Big(\frac{\overline{t}}{\varepsilon},\, \frac{\overline{\beta}}{\varepsilon}\Big) \;=\; \varepsilon n^{\varepsilon}(t,\, \beta), \\
\overline{f}^{\varepsilon}(\overline{t},\, \overline{\beta}) \;&:=\; \varepsilon f^{\varepsilon}\Big(\frac{\overline{t}}{\varepsilon},\, \frac{\overline{\beta}}{\varepsilon}\Big) \;=\; \varepsilon f^{\varepsilon}(t,\, \beta),
\end{aligned} \tag{46}$$

and for the other group of variables

$$\begin{aligned}
\overline{r}^{\varepsilon}(\overline{t},\, \overline{\beta}) \;&:=\; r^{\varepsilon}\Big(\frac{\overline{t}}{\varepsilon},\, \frac{\overline{\beta}}{\varepsilon}\Big) \;=\; r^{\varepsilon}(t,\, \beta), \\
\overline{s}^{\varepsilon}(\overline{t},\, \overline{\beta}) \;&:=\; s^{\varepsilon}\Big(\frac{\overline{t}}{\varepsilon},\, \frac{\overline{\beta}}{\varepsilon}\Big) \;=\; s^{\varepsilon}(t,\, \beta), \\
\overline{d}^{\varepsilon}(\overline{t},\, \overline{\beta}) \;&:=\; d^{\varepsilon}\Big(\frac{\overline{t}}{\varepsilon},\, \frac{\overline{\beta}}{\varepsilon}\Big) \;=\; d^{\varepsilon}(t,\, \beta), \\
\overline{q}^{\varepsilon}(\overline{t},\, \overline{\beta}) \;&:=\; q^{\varepsilon}\Big(\frac{\overline{t}}{\varepsilon},\, \frac{\overline{\beta}}{\varepsilon}\Big) \;=\; q^{\varepsilon}(t,\, \beta).
\end{aligned} \tag{47}$$

Furthermore we set

$$\overline{v}^{\varepsilon}(\overline{t},\, \overline{\beta}) := \frac{\partial \overline{f}^{\varepsilon}}{\partial \overline{t}}(\overline{t},\, \overline{\beta}) = \frac{\partial f^{\varepsilon}}{\partial t}\Big(\frac{\overline{t}}{\varepsilon},\, \frac{\overline{\beta}}{\varepsilon}\Big) = v^{\varepsilon}\Big(\frac{\overline{t}}{\varepsilon},\, \frac{\overline{\beta}}{\varepsilon}\Big) = v^{\varepsilon}(t,\, \beta). \tag{48}$$

The appropriate scaling of the energy will be discussed in Section 7.7.

Regarding their dependence on time, the variables must be categorized differently. There exist *slow* variables that vary on the macro time scale, and there are *fast* variables that change on the micro time scale. The group of slow variables consists of the quantities d, f, m and n. The functions

$$\overline{d}^{\varepsilon}(\overline{t},\overline{\beta}),\quad \overline{f}^{\varepsilon}(\overline{t},\overline{\beta}),\quad \overline{n}^{\varepsilon}(\overline{t},\overline{\beta})\quad\text{and}\quad \overline{m}^{\varepsilon}(\overline{t},\overline{\beta}) \tag{49}$$

have thus an immediate macroscopic meaning. Note that only $\overline{d}^{\varepsilon}$ and $\overline{f}^{\varepsilon}$ are algebraically independent, because from (36) there follow the identities

$$\begin{aligned}\overline{n}^{\varepsilon}(\overline{t},\overline{\beta}) &= \overline{f}^{\varepsilon}(\overline{t},\overline{\beta})+\frac{1}{2}\overline{d}^{\varepsilon}(\overline{t},\overline{\beta})\quad\text{and} &(50)\\ \overline{m}^{\varepsilon}(\overline{t},\overline{\beta}) &= \overline{f}^{\varepsilon}(\overline{t},\overline{\beta})-\frac{1}{2}\overline{d}^{\varepsilon}(\overline{t},\overline{\beta}). &(51)\end{aligned}$$

The quantities r, s and q are fast variables. In particular, the functions

$$\overline{r}^{\varepsilon}(\overline{t},\overline{\beta}),\quad \overline{s}^{\varepsilon}(\overline{t},\overline{\beta})\quad\text{and}\quad \overline{q}^{\varepsilon}(\overline{t},\overline{\beta}) \tag{52}$$

exhibit rapid oscillations with respect to the macro time $\overline{t}$. In the next section we shall explain, how these oscillations can be described in the limit $\varepsilon \to 0$.

Remarks

1. The classification into slow and fast variables can be justified both numerically and analytically.
2. The scaling behavior of a quantity, cf. (46) and (47), is independent from its classification as a fast or a slow variable.

7.3 Scalings, Part 2: The macroscopic conservation law of mass

The definitions of the last section immediately imply some conclusions regarding the slow variables. With (33) and (34) we find two expressions for $2d^{\varepsilon} = r^{\varepsilon} + s^{\varepsilon}$, namely

$$\begin{aligned}2d^{\varepsilon}(t,\beta) &= 2\Big(m^{\varepsilon}(t,\beta+\frac{1}{2})-m^{\varepsilon}(t,\beta)\Big)\\ &= \frac{2}{\varepsilon}\Big(\overline{m}^{\varepsilon}(\overline{t},\overline{\beta}+\frac{\varepsilon}{2})-\overline{m}^{\varepsilon}(\overline{t},\overline{\beta})\Big)\end{aligned} \tag{53}$$

and

$$\begin{aligned}2d^{\varepsilon}(t,\beta) &= 2\Big(n^{\varepsilon}(t,\beta)-n^{\varepsilon}(t,\beta-\frac{1}{2})\Big)\\ &= \frac{2}{\varepsilon}\Big(\overline{n}^{\varepsilon}(\overline{t},\overline{\beta})-\overline{n}^{\varepsilon}(\overline{t},\overline{\beta}-\frac{\varepsilon}{2})\Big).\end{aligned} \tag{54}$$

If we assume that the limits

$$\overline{d}(\overline{t},\,\overline{\beta}) \;:=\; \lim_{\varepsilon\to 0}\,\overline{d}^{\,\varepsilon}(\overline{t},\,\overline{\beta}) \quad\text{and}\quad \overline{f}(\overline{t},\,\overline{\beta}) \;:=\; \lim_{\varepsilon\to 0}\,\overline{f}^{\,\varepsilon}(\overline{t},\,\overline{\beta}) \tag{55}$$

exist, we obtain from (53) and (54)

$$\overline{d}(\overline{t},\,\overline{\beta}) = \frac{1}{2}\frac{\partial\,\overline{m}(\overline{t},\,\overline{\beta})}{\partial\,\overline{\beta}} = \frac{1}{2}\frac{\partial\,\overline{n}(\overline{t},\,\overline{\beta})}{\partial\,\overline{\beta}}, \tag{56}$$

and finally

$$\overline{d}(\overline{t},\,\overline{\beta}) = \frac{1}{2}\frac{\partial\,\overline{f}}{\partial\,\overline{\beta}}(\overline{t},\,\overline{\beta}). \tag{57}$$

Differentiating (57) with respect to $\overline{t}$ leads to

$$\frac{\partial\,\overline{d}}{\partial\,\overline{t}}(\overline{t},\,\overline{\beta}) \;=\; \frac{1}{2}\frac{\partial\,\overline{v}}{\partial\,\overline{\beta}}(\overline{t},\,\overline{\beta}). \tag{58}$$

This equation is the first of the three macroscopic conservation laws in LAGRANGE coordinates, because it can be written in the form

$$\frac{\partial\,\overline{d}}{\partial\,\overline{t}} - \frac{\partial\,\overline{v}}{\partial\,\overline{\alpha}} = 0. \tag{59}$$

The remaining two macroscopic conservation laws rely on NEWTONs equations of motion. Their derivation requires more elaborated techniques.

7.4 The microscopic oscillators

In order to study the macroscopic meaning of Equation $(38)_2$, we introduce two new auxiliary quantities $\tilde{q}^{\varepsilon}$ by $\tilde{\dot{q}}^{\varepsilon}$ by

$$\tilde{q}^{\varepsilon}(t,\,\overline{\beta}) = q^{\varepsilon}\Big(t,\,\frac{\overline{\beta}}{\varepsilon}\Big), \quad\text{and}\quad \tilde{\dot{q}}^{\varepsilon}(t,\,\overline{\beta}) = \dot{q}^{\varepsilon}\Big(t,\,\frac{\overline{\beta}}{\varepsilon}\Big). \tag{60}$$

Note that the functions $\tilde{q}^{\varepsilon}$ and $\tilde{\dot{q}}^{\varepsilon}$ depend on the *micro* time t but on the *macro* particle index $\overline{\beta}$. Equation $(38)_2$ transforms into

$$\begin{aligned}\frac{\partial^2\tilde{q}^{\varepsilon}}{\partial\,t^2}(t,\,\overline{\beta}) \;&=\; \frac{\partial\,\tilde{\dot{q}}^{\varepsilon}}{\partial\,t}(t,\,\overline{\beta})\\ &=\; \varphi'\big(\overline{d}^{\,\varepsilon}(\varepsilon t,\,\overline{\beta}) - 2\tilde{q}^{\varepsilon}(t,\,\overline{\beta})\big) - \varphi'\big(\overline{d}^{\,\varepsilon}(\varepsilon t,\,\overline{\beta}) + 2\tilde{q}^{\varepsilon}(t,\,\overline{\beta})\big) +\\ &\quad\;\varepsilon\frac{\partial^2\overline{f}^{\,\varepsilon}}{\partial\,\overline{t}^{\,2}}(\varepsilon t,\,\overline{\beta}).\end{aligned} \tag{61}$$

This equation describes a family of microscopic oscillators indexed by $\overline{\beta}$. We observe that the microscopic oscillator, which corresponds to fixed $\overline{\beta}$, is disturbed by the following two slow functions

$$t \;\rightsquigarrow\; \overline{d}^{\,\varepsilon}(\varepsilon t,\,\overline{\beta}) \quad\text{and}\quad t \;\rightsquigarrow\; \varepsilon\frac{\partial^2\overline{f}^{\,\varepsilon}}{\partial\,\overline{t}^{\,2}}(\varepsilon t,\,\overline{\beta}). \tag{62}$$

The oscillating system (61) and the influence of the slow functions have to be studied carefully. Therefore we have investigated systems like (61) in [3]. The results from [3] regard the following oscillating system

$$\frac{\partial^2 q^\varepsilon}{\partial t^2}(t) \;=\; \varphi'\big(\,g_1(\varepsilon t) - 2q^\varepsilon(t)\,\big) - \varphi'\big(\,g_1(\varepsilon t) - 2q^\varepsilon(t)\,\big) + \varepsilon g_2(\varepsilon t), \tag{63}$$

which is very similar to (61) for fixed $\overline{\beta}$. Obviously, the difference between both systems is caused by the explicit ε-dependence of the slow perturbations in (61). However, we expect that (61) and (63) behave similar if $\varepsilon \to 0$.

Before we summarize the main results from [3], we introduce further notations. With $Q = (q,\, \dot{q})$ we denote the variable in the phase space of the oscillator (61). Furthermore, we define the *oscillator energy* $e_{\mathrm{osc}} = e_{\mathrm{osc}}(Q,\, \overline{d})$ by

$$e_{\mathrm{osc}}(Q,\, \overline{d}) \;:=\; \frac{1}{2}\dot{q}^2 + \Phi_{\mathrm{osc}}(q,\, \overline{d}) \quad \text{with} \tag{64}$$

$$\Phi_{\mathrm{osc}}(q,\, \overline{d}) \;:=\; \frac{1}{2}\big(\varphi(\overline{d} - 2q) + \varphi(\overline{d} + 2q)\big), \tag{65}$$

where Φ_{osc} is the potential of the microscopic oscillator (61).

If we use the potential (13) as atomic interaction potential, we must restrict our considerations to the range

$$\overline{d} \leq \sqrt{\frac{5}{3}}. \tag{66}$$

The upper bound guarantees that the function

$$q \;\rightsquigarrow\; \Phi_{\mathrm{osc}}(q,\, \overline{d}) \tag{67}$$

has a unique global minimum.

The evolution of the oscillator energy is given by

$$\tilde{e}^{\,\varepsilon}_{\mathrm{osc}}(t,\, \overline{\beta}) \;:=\; \frac{1}{2}\Big(\dot{\tilde{q}}^{\,\varepsilon}(t,\, \overline{\beta})\Big)^2 + \Phi_{\mathrm{osc}}\Big(\overline{d}^{\,\varepsilon}(\varepsilon t,\, \overline{\beta}),\, \tilde{q}^{\,\varepsilon}(t,\, \overline{\beta})\Big). \tag{68}$$

As we will see in Section 7.7, the oscillator energy is closely related to the internal energy of the atomic chain. Finally we introduce the scaled oscillator energy by

$$\overline{e}^{\,\varepsilon}_{\mathrm{osc}}(\overline{t},\, \overline{\beta}) \;:=\; \tilde{e}^{\,\varepsilon}_{\mathrm{osc}}\Big(\frac{\overline{t}}{\varepsilon},\, \overline{\beta}\Big). \tag{69}$$

We now assume that the methods that are developed in [3] can be applied to (61). Under this assumption, the following propositions will result.

1. The macroscopic behavior of the oscillating system (61) can be described by a family of YOUNG measures indexed by $\overline{\beta}$. The corresponding family of disintegrations leads to a family of probability measures

$$(\overline{t},\,\overline{\beta}) \quad \rightsquigarrow \quad \mu(\overline{t},\,\overline{\beta},\,dQ) \;\in \mathrm{Prob}\,(\mathbb{R}^2). \tag{70}$$

2. The macroscopic influence of the term

$$\varepsilon\frac{\partial^2 \overline{f}^{\,\varepsilon}}{\partial\,\overline{t}^{\,2}}(\varepsilon t,\,\overline{\beta}) \tag{71}$$

can be neglected. This is due to the factor ε in front of the second derivative of $\overline{f}^{\,\varepsilon}$.

3. If $\varepsilon \to 0$, the scaled oscillator energy converges to a function $\overline{e}_{\mathrm{osc}}(\overline{t},\,\overline{\beta})$ that satisfies a differential equation. We will derive this equation in Section 7.7.

4. The probability measure $\mu(\overline{t},\,\overline{\beta},\,dQ)$ is completely determined by $\overline{e}_{\mathrm{osc}}(\overline{t},\,\overline{\beta})$ and $\overline{d}(\overline{t},\,\overline{\beta})$.

5. For any $(\overline{t},\,\overline{\beta})$ the measure $\mu(\overline{t},\,\overline{\beta},\,dQ)$ can be characterized in different ways. This will be explained in the following.

Let $(\overline{t},\,\overline{\beta})$ be fixed and let $\Psi = \Psi(Q)$ be an observable. There exist three different, but equivalent characterizations of $\mu(dQ) = \mu(\overline{t},\,\overline{\beta},\,dQ)$.

1. The measure $\mu(dQ)$ is the solution of the stationary LIOUVILLE equation that corresponds to the following dynamical system

$$\frac{\partial^2 q}{\partial\,\theta^2}(\theta) \;=\; \varphi'\big(\overline{d} - 2q(\theta)\big) - \varphi'\big(\overline{d} + 2q(\theta)\big), \quad \overline{d} = \overline{d}(\overline{t},\,\overline{\beta}). \tag{72}$$

Note that there is no coupling between θ and $\overline{t}$. We call (72) the *associated system* to (61). The corresponding stationary LIOUVILLE equation reads

$$\dot{q}\frac{\partial\,\mu}{\partial\,q}(dQ) + \Big(\varphi'(\overline{d} - 2q) - \varphi'(\overline{d} + 2q)\Big)\frac{\partial\,\mu}{\partial\,\dot{q}}(dQ) \;=\; 0. \tag{73}$$

2. The integral of an observable Ψ with respect to $\mu(dQ)$ can be expressed by means of temporal averaging. Let $(\varepsilon_i)_i$ and $(\gamma_j)_j$ be two sequences with $\gamma_j \to 0$ and $\varepsilon_i \to 0$. Then there holds

$$\int\limits_{\mathbb{R}^2} \Psi(Q)\,\mu(\overline{t},\,\overline{\beta},\,dQ) \;=\; \lim_{j\to\infty}\lim_{i\to\infty}\frac{1}{\gamma_j}\int\limits_{\overline{t}}^{\overline{t}+\gamma_j} \Psi\big(\overline{Q}^{\,\varepsilon_i}(\overline{s},\,\overline{\beta})\big)\,d\overline{s}. \tag{74}$$

Here $\overline{Q}^{\,\varepsilon}$ is the scaled solution of (61), i.e.

$$\overline{Q}^{\,\varepsilon}(\overline{t},\,\overline{\beta}) = \Big(\tilde{q}^{\,\varepsilon}(\frac{\overline{t}}{\varepsilon},\,\overline{\beta}),\,\tilde{\dot{q}}^{\,\varepsilon}(\frac{\overline{t}}{\varepsilon},\,\overline{\beta})\Big). \tag{75}$$

The integral on the right hand side of (74) describes time means with respect to time intervals that are microscopically extremely large but macroscopically very small. In [4], DREYER and KUNIK describe a more general setting for time averaging. To this end they introduce a windows function and scale its support with ε. However, this approach leads to the same results.

3. The measure $\mu(dQ)$ can be calculated directly from the associated system (72). For any observable Ψ we find

$$\int\limits_{\mathbb{R}^2} \Psi(Q)\, \mu(\bar{t}, \bar{\beta}, dQ) \quad = \quad \lim_{\theta_{\text{end}} \to \infty} \frac{1}{\theta_{\text{end}}} \int\limits_0^{\theta_{\text{end}}} \Psi\big(Q(\theta)\big)\, d\theta, \tag{76}$$

where $Q(\theta)$ is the solution of the associated system (72). Recall that (72) depends on $(\bar{t}, \bar{\beta})$ via the specific volume $\bar{d} = \bar{d}(\bar{t}, \bar{\beta})$. In the next section we use (76) in order to derive explicit expressions for time means.

7.5 Mean values with respect to time

We have mentioned in the last section, that

1. The macroscopic behavior of the fast variable q is governd by a family of probability measures $\mu(\bar{t}, \bar{\beta}, dQ)$.
2. The measures $\mu(\bar{t}, \bar{\beta}, dQ)$ can be evaluated by averaging with respect to time.

In this section we give a more detailed description of the resulting time means. As in the last section, $Q = (q, \dot{q})$ denotes the variable in the phase space of the oscillating system (61).

Let $\Psi = \Psi(Q)$ be an observable. For time means of Ψ we use the following notation

$$\begin{aligned} \Big\langle \Psi\big(\overline{Q}(\bar{t}, \bar{\beta})\big) \Big\rangle \quad &:= \quad \int\limits_{\mathbb{R}^2} \Psi(Q)\, \mu(\bar{t}, \bar{\beta}, dQ) \\ &= \quad \lim_{\gamma \to 0} \lim_{\varepsilon \to 0} \frac{1}{\gamma} \int\limits_{\bar{t}}^{\bar{t}+\gamma} \Psi\big(\overline{Q}^{\varepsilon}(\bar{s}, \bar{\beta})\big)\, d\bar{s}. \end{aligned} \tag{77}$$

Recall that

1. $\overline{Q}^{\varepsilon}$ denotes the scaled solution of the microscopic oscillators (61), i.e.

$$\overline{Q}^{\varepsilon}(\bar{t}, \bar{\beta}) = \Big(q^{\varepsilon}(\frac{\bar{t}}{\varepsilon}, \frac{\bar{\beta}}{\varepsilon}),\, \dot{q}^{\varepsilon}(\frac{\bar{t}}{\varepsilon}, \frac{\bar{\beta}}{\varepsilon})\Big). \tag{78}$$

2. The last identity in (77) was already stated in the last section, cf. (74).

Let $(\overline{t},\, \overline{\beta})$ be fixed. In order to derive explicit expression for the time means of Ψ, we consider the associated system (72) and Equation (76). As before,

$$Q(\theta) = \big(q(\theta),\, \dot{q}(\theta)\big) \tag{79}$$

denotes the solution of (72).

As in the last section, we restrict the range of the specific length $\overline{d}$ by $\overline{d} \le \sqrt{\frac{5}{3}}$. This leads to the following properties of the oscillator potential $\Phi_{\mathrm{osc}} = \Phi_{\mathrm{osc}}(q,\, \overline{d})$, cf. (65). The function $q \rightsquigarrow \Phi_{\mathrm{osc}}(q,\, \overline{d})$

1. is odd with respect to q,
2. has a global unique minimum at $q = 0$,
3. increases for $q > 0$ and decreases for $q < 0$.

We conclude that the oscillator (72) runs along a closed path in the $(q,\, \dot{q})$ space. There exist two turning points $q = q_-$ and $q = q_+$ in which $\dot{q} = 0$. For fixed $\overline{d}$ and given value of the oscillator energy e_{osc}, the turning points q_- and q_+ are given as solutions of the equation

$$e_{\mathrm{osc}} \;=\; \Phi_{\mathrm{osc}}(q_\pm,\, \overline{d}). \tag{80}$$

In particular, $q_+ = q_\star = -q_-$ and $2e_{\mathrm{osc}} = \varphi(\overline{d} - 2q_\star) + \varphi(\overline{d} + 2q_\star)$.

The total period θ_{per} of the motion can be decomposed into two half-periods with $\dot{q}(\theta) < 0$ and $\dot{q}(\theta) > 0$. Both half periods have the same duration $\theta_\star = \theta_\star(q_\star,\, \overline{d})$. Since the oscillator energy is conserved, the velocity $\dot{q}(\theta)$ is an algebraic function of $q(\theta)$. Within the two half-periods we find

$$\dot{q}(\theta) = \dot{q}_-\big(q(\theta)\big) \quad \text{and} \quad \dot{q}(\theta) = \dot{q}_+\big(q(\theta)\big), \tag{81}$$

respectively, where

$$\dot{q}_\pm(q) = \pm\sqrt{\varphi\left(\overline{d} - 2q_*\right) + \varphi\left(\overline{d} + 2q_*\right) - \varphi\left(\overline{d} - 2q\right) - \varphi\left(\overline{d} + 2q\right)}. \tag{82}$$

In order to establish the following limit theorem exclusively in the q space, we introduce three functions $\psi_-(q)$, $\psi_+(q)$ and $\psi(q)$ by

$$\psi_\pm(q) := \Psi\Big(q,\, \dot{q}_\pm(q)\Big) \quad \text{and} \quad \psi(q) = \frac{1}{2}\Big(\psi_-(q) + \psi_+(q)\Big). \tag{83}$$

Since the motion of the oscillator (72) is periodic, the right hand side in Equation (76) simplifies to

$$\lim_{\theta_{\mathrm{end}}\to\infty} \frac{1}{\theta_{\mathrm{end}}} \int\limits_0^{\theta_{\mathrm{end}}} \Psi\big(Q(\theta)\big)\, d\theta = \frac{1}{\theta_{\mathrm{per}}} \int\limits_0^{\theta_{\mathrm{per}}} \Psi\big(Q(\theta)\big)\, d\theta =: \big\langle \Psi \big\rangle\, . \tag{84}$$

Without loss of generality we can assume that $q(0) = q_- = -q_\star$. Using (81) we obtain

$$\langle\Psi\rangle = \frac{1}{\theta_{\text{per}}} \int\limits_0^{\theta_\star} \Psi\Big(q(\theta),\, \dot q_+\big(q(\theta)\big)\Big)\, d\theta + \frac{1}{\theta_{\text{per}}} \int\limits_{\theta_\star}^{2\theta_\star} \Psi\Big(q(\theta),\, \dot q_-\big(q(\theta)\big)\Big)\, d\theta. \tag{85}$$

In the first integral we substitute θ by $q(\theta)$. Since

$$dq = \dot q(\theta) d\theta = \dot q_+\big(q(\theta)\big) d\theta \tag{86}$$

there results

$$\int\limits_0^{\theta_\star} \Psi\Big(q(\theta),\, \dot q_+\big(q(\theta)\big)\Big)\, d\theta = \int\limits_{-q_\star}^{+q_\star} \psi_+\big(q\big) \frac{1}{\dot q_+(q)}\, dq.$$

In the same way we transform the second time integral in (85). We end up with

$$\begin{aligned} \langle\Psi\rangle &= \frac{1}{2\theta_\star} \int\limits_{-q_\star}^{+q_\star} \psi_+\big(q\big) \frac{1}{\dot q_+(q)}\, dq + \frac{1}{2\theta_\star} \int\limits_{+q_\star}^{-q_\star} \psi_-\big(q\big) \frac{1}{\dot q_-(q)}\, dq \\ &= \frac{1}{\theta_\star} \int\limits_{-q_\star}^{+q_\star} \psi\big(q\big) \frac{1}{\dot q_+(q)}\, dq. \end{aligned} \tag{87}$$

The half-period $\theta_\star$ follows from

$$\theta_\star = \int\limits_{-q_\star}^{+q_\star} \frac{1}{\dot q_+(q)}\, dq. \tag{88}$$

In the last step we introduce a phase density $W(q_\star,\, \overline{d},\, q)$ which is defined by

$$W(q_\star,\, \overline{d},\, q) \;=\; \frac{1}{\theta_\star(q_\star,\, \overline{d})\sqrt{\varphi\left(\overline{d} - 2q_*\right) + \varphi\left(\overline{d} + 2q_*\right) - \varphi\left(\overline{d} - 2q\right) - \varphi\left(\overline{d} + 2q\right)}}.$$

Finally, we obtain from (76), (84) and (87) the identity

$$\Big\langle \Psi\big(\overline{Q}(\overline{t},\, \overline{\beta})\big)\Big\rangle = \int\limits_{-q_\star(\overline{t},\overline{\beta})}^{+q_\star(\overline{t},\overline{\beta})} \psi(q) W\Big(q_\star(\overline{t},\, \overline{\beta}),\, \overline{d}(\overline{t},\, \overline{\beta}),\, q\Big)\, dq. \tag{89}$$

Recall that $q_\star$ depends algebraically on $\overline{d}$ and on the oscillator energy e_{osc}.

Next we give by a brief summary regarding the time means of the other variables. If we apply the time mean approach to slow functions, we obtain

$$\begin{aligned}
\left\langle \Psi\big(\overline{d}(\overline{t},\,\overline{\beta})\big)\right\rangle &= \lim_{\gamma\to 0}\lim_{\varepsilon\to 0}\frac{1}{\gamma}\int\limits_{\overline{t}}^{\overline{t}+\gamma}\Psi\Big(\overline{d}^{\varepsilon}(\overline{s},\,\overline{\beta})\Big)\,d\overline{s} \\
&= \Psi\Big(\overline{d}(\overline{t},\,\overline{\beta})\Big) = \lim_{\varepsilon\to 0}\Psi\Big(\overline{d}^{\,\varepsilon}(\overline{t},\,\overline{\beta})\Big). \qquad (90)
\end{aligned}$$

Similar identities hold for the other slow variables f, m, n and even for their macroscopic derivatives, as for instance for the velocity v.

The limiting behavior of the fast variables r and s must also be described by time means. However, we can express the time means of r and s by time means of q. Since $r = d - 2q$ and $s = d + 2q$, there holds

$$\begin{aligned}
\left\langle \Psi\big(\overline{r}(\overline{t},\,\overline{\beta})\big)\right\rangle &:= \lim_{\gamma\to 0}\lim_{\varepsilon\to 0}\frac{1}{\gamma}\int\limits_{\overline{t}}^{\overline{t}+\gamma}\Psi\Big(\overline{r}^{\varepsilon}(\overline{s},\,\overline{\beta})\Big)\,d\overline{s} \\
&= \lim_{\gamma\to 0}\lim_{\varepsilon\to 0}\frac{1}{\gamma}\int\limits_{\overline{t}}^{\overline{t}+\gamma}\Psi\Big(\overline{d}^{\varepsilon}(\overline{s},\,\overline{\beta}) - 2\overline{q}^{\varepsilon}(\overline{s},\,\overline{\beta})\Big)\,d\overline{s}. \qquad (91)
\end{aligned}$$

The following propositions

$$\left\langle \overline{q}(\overline{t},\,\overline{\beta})\right\rangle = 0, \quad \text{and} \quad \left\langle \varphi'\Big(\overline{r}(\overline{t},\,\overline{\beta})\Big)\right\rangle = \left\langle \varphi'\Big(\overline{s}(\overline{t},\,\overline{\beta})\Big)\right\rangle, \qquad (92)$$

are immediate consequences of (89) and (91). They will be used in the next sections.

7.6 Scalings, Part 3: The macroscopic conservation law of momentum

In this section we derive from the equation of motion $(38)_3$ for the variable f_β the second macroscopic conservation law.

Equation $(38)_3$ can be written as

$$\begin{aligned}
\frac{\partial\,\overline{v}^{\varepsilon}}{\partial\,\overline{t}}(\overline{t},\,\overline{\beta}) &= \frac{\partial^2\overline{f}^{\,\varepsilon}}{\partial\,\overline{t}^{2}}(\overline{t},\,\overline{\beta}) \\
&= \frac{1}{4\varepsilon}\Big(\varphi'\big(\overline{r}^{\,\varepsilon}(\overline{t},\,\overline{\beta}+\varepsilon)\big) - \varphi'\big(\overline{r}^{\,\varepsilon}(\overline{t},\,\overline{\beta})\big)\Big) + \\
&\quad \frac{1}{4\varepsilon}\Big(\varphi'\big(\overline{s}^{\,\varepsilon}(\overline{t},\,\overline{\beta})\big) - \varphi'\big(\overline{s}^{\,\varepsilon}(\overline{t},\,\overline{\beta}-\varepsilon)\big)\Big). \qquad (93)
\end{aligned}$$

Next we discuss the macroscopic limit of this equation. We assume as before that the limit functions exist, and form the time means of both sides to obtain

$$\frac{\partial \overline{v}(\overline{t}, \overline{\beta})}{\partial \overline{t}} = \frac{1}{4}\frac{\partial}{\partial \overline{\beta}}\Big\langle \varphi'\big(\overline{r}(\overline{t}, \overline{\beta})\big)\Big\rangle + \frac{1}{4}\frac{\partial}{\partial \overline{\beta}}\Big\langle \varphi'\big(\overline{s}(\overline{t}, \overline{\beta})\big)\Big\rangle . \tag{94}$$

This law can obviously be identified with the macroscopic conservation law of momentum, see $(9)_2$. Thus the pressure is defined by

$$\overline{p}(\overline{t}, \overline{\beta}) \;=\; -\frac{1}{2}\Big\langle \varphi'\big(\overline{r}(\overline{t}, \overline{\beta})\big)\Big\rangle - \frac{1}{2}\Big\langle \varphi'\big(\overline{s}(\overline{t}, \overline{\beta})\big)\Big\rangle . \tag{95}$$

Using this definition we can transform Equation (94) into

$$\frac{\partial \overline{v}}{\partial \overline{t}} + \frac{\partial \overline{p}}{\partial \overline{\alpha}} \;=\; 0. \tag{96}$$

The evaluation of the right hand side of (95) will lead to the constitutive law, that relates the pressure to the basic variables specific volume and specific energy. This will be done in the next section.

7.7 Scalings, Part 4: The macroscopic conservation law of energy

The macroscopic conservation law of energy is a consequence of the corresponding microscopic conservation law (40) for the energy

$$\sum_{\beta=1}^{M} e_\beta . \tag{97}$$

Recall that e_β represents the energy of two particles. For this reason we define the energy function $e^\varepsilon(t, \beta)$ by

$$e^\varepsilon(t,\beta) \;:=\; \frac{1}{2} e_\beta(t) \tag{98}$$

so that $e^\varepsilon(t, \beta)$ is a specific energy, i.e. an energy per particle. $e^\varepsilon(t,\beta)$ is thus given by

$$\begin{aligned} e^\varepsilon(t, \beta) \;=\; & \frac{1}{2}\Big(\dot{q}^\varepsilon(t, \beta)\Big)^2 + \frac{1}{4}\Big(\frac{\partial d^\varepsilon}{\partial t}(t, \beta)\Big)^2 + \frac{1}{2}\Big(\frac{\partial f^\varepsilon}{\partial t}(t, \beta)\Big)^2 + \\ & \frac{1}{2}\varphi\Big(r^\varepsilon(t, \beta)\Big) + \frac{1}{2}\varphi\Big(s^\varepsilon(t, \beta)\Big). \end{aligned} \tag{99}$$

In order that the rescaled energy has a macroscopic meaning, we define

$$\overline{e}^\varepsilon(\overline{t}, \overline{\beta}) := e^\varepsilon(\frac{\overline{t}}{\varepsilon}, \frac{\overline{\beta}}{\varepsilon}) = e^\varepsilon(t, \beta). \tag{100}$$

Next we form the time derivative of the oscillator energy, which is given by

$$e^{\varepsilon}_{\rm osc}(t,\,\beta) \;=\; \frac{1}{2}\Big(\dot q^{\,\varepsilon}(t,\,\beta)\Big)^2 + \frac{1}{2}\varphi'\Big(r^{\,\varepsilon}(t,\,\beta)\Big) + \frac{1}{2}\varphi'\Big(s^{\,\varepsilon}(t,\,\beta)\Big). \tag{101}$$

From the equations of motion (38) for d_β, q_β and f_β we obtain

$$\begin{aligned}\frac{\partial\, e^{\varepsilon}_{\rm osc}}{\partial\, t}(t,\,\beta) \;&=\; \dot q^{\,\varepsilon}(t,\,\beta)\frac{\partial^2 f^{\,\varepsilon}}{\partial\, t^2}(t,\,\beta) + \\ &\frac{1}{2}\Big(\varphi'\big(r^{\,\varepsilon}(t,\,\beta)\big) + \varphi'\big(s^{\,\varepsilon}(t,\,\beta)\big)\Big)\frac{\partial\, d^{\varepsilon}}{\partial\, t}(t,\,\beta),\end{aligned} \tag{102}$$

which transforms after rescaling to

$$\begin{aligned}\frac{\partial\, \overline{e}^{\varepsilon}_{\rm osc}}{\partial\, t}(\overline{t},\,\overline{\beta}) \;&=\; \dot{\overline{q}}^{\,\varepsilon}(\overline{t},\,\overline{\beta})\frac{\partial^2 \overline{f}^{\,\varepsilon}}{\partial\, \overline{t}^{\,2}}(\overline{t},\,\overline{\beta}) + \\ &\frac{1}{4}\Big(\varphi'\big(\overline{r}^{\,\varepsilon}(\overline{t},\,\overline{\beta})\big) + \varphi'\big(\overline{s}^{\,\varepsilon}(\overline{t},\,\beta)\big)\Big)\frac{\partial\, \overline{v}^{\,\varepsilon}}{\partial\, \overline{\beta}}(\overline{t},\,\overline{\beta}).\end{aligned} \tag{103}$$

We now form the time mean of both sides according to section 7.5 and pass to the limit $\varepsilon \to 0$. As before we assume that the limit function of the oscillator energy exists and write

$$\overline{e}_{\rm osc}(\overline{t},\,\overline{\beta}) = \lim_{\varepsilon\to 0}\overline{e}^{\,\varepsilon}_{\rm osc}(\overline{t},\,\overline{\beta}). \tag{104}$$

With (92) and (95) we obtain

$$\frac{\partial\, \overline{e}_{\rm osc}}{\partial\, \overline{t}}(\overline{t},\,\overline{\beta}) = -\frac{1}{2}\overline{p}(\overline{t},\,\overline{\beta})\frac{\partial\, \overline{v}}{\partial\, \overline{\beta}}(\overline{t},\,\overline{\beta}). \tag{105}$$

The specific energy, which is given by

$$e^{\,\varepsilon}(t,\,\beta) = e^{\varepsilon}_{\rm osc}(t,\,\beta) + \frac{1}{4}\Big(\frac{\partial\, d^{\varepsilon}}{\partial\, t}(t,\,\beta)\Big)^2 + \frac{1}{2}\Big(v^{\,\varepsilon}(t,\,\beta)\Big)^2, \tag{106}$$

reads after rescaling

$$\overline{e}^{\,\varepsilon}(\overline{t},\,\overline{\beta}) = \overline{e}^{\,\varepsilon}_{\rm osc}(\overline{t},\,\overline{\beta}) + \frac{\varepsilon^2}{4}\Big(\frac{\partial\, \overline{d}^{\,\varepsilon}}{\partial\, \overline{t}}(\overline{t},\,\overline{\beta})\Big)^2 + \frac{1}{2}\Big(\overline{v}^{\,\varepsilon}(\overline{t},\,\overline{\beta})\Big)^2. \tag{107}$$

The time derivative of $\overline{e}^{\,\varepsilon}(\overline{t},\overline{\beta})$ yields

$$\begin{aligned}\frac{\partial\, \overline{e}^{\,\varepsilon}}{\partial\, \overline{t}}(\overline{t},\,\overline{\beta}) \;&=\; \frac{\partial\, \overline{e}^{\,\varepsilon}_{\rm osc}}{\partial\, \overline{t}}(\overline{t},\,\overline{\beta}) + \overline{v}^{\,\varepsilon}(\overline{t},\,\overline{\beta})\frac{\partial\, \overline{v}^{\,\varepsilon}}{\partial\, \overline{t}}(\overline{t},\,\overline{\beta}) + \\ &\frac{\varepsilon^2}{2}\frac{\partial\, \overline{d}^{\,\varepsilon}}{\partial\, \overline{t}}(\overline{t},\,\overline{\beta})\frac{\partial^2 \overline{d}^{\,\varepsilon}}{\partial\, \overline{t}^{\,2}}(\overline{t},\,\overline{\beta}).\end{aligned} \tag{108}$$

In the limit $\varepsilon \to 0$ there results

$$\frac{\partial\, \overline{e}}{\partial\, \overline{t}}(\overline{t},\,\overline{\beta}) \;=\; \frac{\partial\, \overline{e}_{\rm osc}}{\partial\, \overline{t}}(\overline{t},\,\overline{\beta}) + \overline{v}(\overline{t},\,\overline{\beta})\frac{\partial\, \overline{v}}{\partial\, \overline{t}}(\overline{t},\,\overline{\beta}). \tag{109}$$

Using (58) and (105) we find the third conservation law

$$\begin{aligned}\frac{\partial \overline{e}}{\partial \overline{t}}(\overline{t},\, \overline{\beta}) &= -\frac{1}{2}\overline{p}(\overline{t},\, \overline{\beta})\frac{\partial \overline{v}}{\partial \overline{\beta}}(\overline{t},\, \overline{\beta}) - \frac{1}{2}\overline{v}(\overline{t},\, \overline{\beta})\frac{\partial \overline{p}}{\partial \overline{\beta}}(\overline{t},\, \overline{\beta}) \\ &= -\frac{1}{2}\frac{\partial\,(\overline{p}\,\overline{v})}{\partial \overline{\beta}}(\overline{t},\, \overline{\beta}),\end{aligned} \tag{110}$$

which can be written as

$$\frac{\partial \overline{e}}{\partial \overline{t}} + \frac{\partial\,(\overline{p}\,\overline{v})}{\partial \overline{\alpha}} = 0. \tag{111}$$

Remarks

1. A comparison with the macroscopic conservation law $(9)_3$ reveals that the heat flux is zero. In other words, the macroscopic equations describe local equilibria.

2. The specific energy is the sum of the oscillator energy and the energy of the macroscopic motion

$$\overline{e}(\overline{t},\, \overline{\beta}) = \overline{e}_{\rm osc}(\overline{t},\, \overline{\beta}) + \frac{1}{2}\Big(\overline{v}(\overline{t},\, \overline{\beta})\Big)^2. \tag{112}$$

   Thus we find that internal energy is identical to oscillator energy.

3. The pressure $\overline{p}(\overline{t},\, \overline{\beta})$ is an algebraic function of the internal energy $\overline{e}_{\rm osc}(\overline{t},\, \overline{\beta})$ and the specific volume $\overline{d}(\overline{t},\, \overline{\beta})$. This is a consequence of (80), (89), (91), (92) and (95). There results

$$\begin{aligned}\overline{p}(\overline{t},\, \overline{\beta}) &= -\Big\langle \varphi'\Big(\overline{r}(\overline{t},\, \overline{\beta})\Big)\Big\rangle \\ &= -\int\limits_{-q_\star(\overline{t},\overline{\beta})}^{+q_\star(\overline{t},\overline{\beta})} \varphi'\Big(\overline{d}(\overline{t},\, \overline{\beta}) - 2q\Big) W\Big(q_\star(\overline{t},\, \overline{\beta}),\, \overline{d}(\overline{t},\, \overline{\beta}),\, q\Big)\, dq,\end{aligned} \tag{113}$$

   where $q_\star(\overline{t},\, \overline{\beta})$ is determined by means of the oscillator potential $\Phi_{\rm osc}$, i.e.

$$\Phi_{\rm osc}\Big(q_\star(\overline{t},\, \overline{\beta}),\, \overline{d}(\overline{t},\, \overline{\beta})\Big) = \overline{e}_{\rm osc}(\overline{t},\, \overline{\beta}). \tag{114}$$

4. The conservation law of mass is a kinematic consequence of the definitions of d_β and f_β.

5. The equation of motion for f_β, cf. $(38)_3$, leads to the conservation law of momentum. However, we have used all equations of motion from (38) to derive the conservation law of energy.

6. Finally we discuss the meaning of Equation $(38)_1$ for the variable d_β. After the rescaling of this equation we end up with

$$\begin{aligned}\varepsilon\frac{\partial^2\overline{d}^\varepsilon}{\partial\overline{t}^2}(\overline{t},\overline{\beta}) &= \frac{1}{2\varepsilon}\Big(\varphi'\big(\overline{r}^\varepsilon(\overline{t},\overline{\beta}+\varepsilon)\big)-\varphi'\big(\overline{r}^\varepsilon(\overline{t},\overline{\beta})\big)\Big)+\\ &\quad\frac{1}{2\varepsilon}\Big(\varphi'\big(\overline{s}^\varepsilon(\overline{t},\overline{\beta}-\varepsilon)\big)-\varphi'\big(\overline{s}^\varepsilon(\overline{t},\overline{\beta})\big)\Big).\end{aligned} \tag{115}$$

If we pass to the limit $\varepsilon\to 0$, we obtain an identity, namely

$$0=\frac{1}{2}\frac{\partial}{\partial\overline{\beta}}\Big[\Big\langle\varphi'\big(\overline{r}(\overline{t},\overline{\beta})\big)\Big\rangle-\Big\langle\varphi'\big(\overline{s}(\overline{t},\overline{\beta})\big)\Big\rangle\Big]=0. \tag{116}$$

Consequently, Equation $(38)_1$ has no macroscopic meaning. This is a surprising fact because the limit function $\overline{d}(\overline{t},\overline{\beta})$ has such a macroscopic meaning.

7.8 The introduction of temperature and entropy

Note that we have already obtained a closed system of field equations, so that there is actually no need to introduce further variables. However, there are two more quantities which play a fundamental role in thermodynamics, and these are temperature and entropy.

As in [4], we identifiy the temperature T with two times the mean kinetic energy of the rapid oscillator motion. In particular we define

$$\overline{T}(\overline{t},\overline{\beta}):=\Big\langle\dot{\overline{q}}(\overline{t},\overline{\beta})^2\Big\rangle. \tag{117}$$

Thus having defined the specific internal energy $\overline{u}(\overline{t},\overline{\beta})$, the pressure $\overline{p}(\overline{t},\overline{\beta})$, the specific length $\overline{d}(\overline{t},\overline{\beta})$ and the temperature $\overline{T}(\overline{t},\overline{\beta})$, we may now pose the question, whether these quantities are related to each other by the GIBBS equation

$$\overline{T}\,d\overline{h}=d\overline{u}+\overline{p}\,d\overline{d}, \tag{118}$$

where $\overline{h}$ denotes the specific entropy. The existence of the GIBBS equation, and thus the definition of the specific entropy results from the study whether the integrability condition

$$\frac{\partial}{\partial\overline{d}}\Big(\frac{1}{\overline{T}}\Big)=\frac{\partial}{\partial\overline{u}}\Big(\frac{\overline{p}}{\overline{T}}\Big) \tag{119}$$

is satisfied or not.

Because we have justified in the current study the intuitive derivation of mean values in [4], we only must cite the proof of the integrability condition that is found to be in that paper. The specific entropy then follows by a simple integration of (118) and reads

$$\overline{h}(\overline{t},\overline{\beta}) = \log\Big(\int\limits_{-q_\star(\overline{t},\overline{\beta})}^{+q_\star(\overline{t},\overline{\beta})}\dot{q}_+\Big(q_\star(\overline{t},\overline{\beta}),\,\overline{d}(\overline{t},\overline{\beta}),\,q\Big)\,dq\Big) \tag{120}$$

with

$$\dot{q}_+(q_\star,\,\overline{d},\,q) = \sqrt{\varphi(\overline{d}-2q_\star)+\varphi(\overline{d}+2q_\star)-\varphi(\overline{d}-2q)-\varphi(\overline{d}+2q)}\,. \qquad (121)$$

8 Summary and perspectives

Relying on an observed scaling behaviour, which is generated by cold RIEMANN inital data and on the assumption (!) that the limit $\varepsilon \to 0$ exists, we have derived from NEWTON's equations of motion for the atomic chain

$$\ddot{x}_\alpha = \varphi'(x_{\alpha+1}-x_\alpha) - \varphi'(x_\alpha - x_{\alpha-1}) \qquad (122)$$

1. the macroscopic conservation laws in LAGRANGE coordinates

$$\frac{\partial\,\overline{d}}{\partial\,\overline{t}} - \frac{\partial\,\overline{v}}{\partial\,\overline{\alpha}} = 0, \quad \frac{\partial\,\overline{v}}{\partial\,\overline{t}} + \frac{\partial\,\overline{p}}{\partial\,\overline{\alpha}} = 0, \quad \frac{\partial\,\overline{e}}{\partial\,\overline{t}} + \frac{\partial\,(\overline{p}\,\overline{v})}{\partial\,\overline{\alpha}} = 0, \quad \text{and} \qquad (123)$$

2. the constitutive law for the pressure $\overline{p}$.

Furthermore we have introduced the quantities temperature and specific entropy, and we have shown that all these quantities are related to each other in a thermodynamic consistent way.

Up to now, a rigorous mathematical treatment of a limit, that starts from a many-particle system and ends up with some partial differential equations, is only considered for microscopic motions without temperature, cf. [1]. The simple microscopic oscillator motion develops temperature and may thus serve as the test case for a mathematical treatment with temperature. The oscillator motion is much easier to handle as classical thermal motion, because in contrast to classical thermal motion, the atomic distancies and velocities are completely coupled via the microscopic equations of motion.

The current study has provided the mathematical setting for micro-macro transitions of a simple microscopic motion with temperature. The main results are as follows

1. Derivation of the conservation laws and the contitutive equation.

2. For micro-macro transitions, the use of LAGRANGE coordinates is prior to EULER coordinates.

3. Furthermore we have justified, that the constitutive laws can be derived from a single oscillator equation, cf. (72). The full many-particle system is not needed for this purpose. DREYER's & KUNIK's conjecture from [4] could thus be verified.

However, we obtained the results under some assumptions regarding

1. the convergence of the slow variables,
2. the decoupling of fast and slow variables, cf. Section 7.4,
3. the convergence of time means of fast variables.

The verification of this assumptions is the subject of a forthcoming study. The first steps in this direction are already included in [2] and [3].

Finally we mention that the oscillator motion can even be used to study phase separation processes. Recall that we have restricted the range of the specific length $\overline{d}$ by $0 < \overline{d} \leq \sqrt{5/3}$. This condition guarantees that the oscillator potential exhibits a global unique minimum. If $\overline{d} > \sqrt{5/3}$, the oscillator potential changes to a double well potential and phase transitions may appear.

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