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# Micro-macro transitions in the atomic chain via Whitham's modulation equation


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**Abstract**

The subject matter of this paper is the thermodynamic description of the nonlinear atomic chain with temperature. For this reason we consider special approximate solutions of Newton's equations, in which the atoms perform microscopic oscillations in form of modulated traveling waves. We start with an existence result for periodic traveling wave with arbitrary large amplitudes, and study several examples including the harmonic chain, the hard sphere model, and the small-amplitude approximation. Then we discuss the thermodynamic properties of traveling waves, and derive the corresponding Gibbs equation. Afterwards we focus on the macroscopic evolution of modulated traveling waves. For this purpose we apply Whitham's modulation theory to the atomic chain, and derive the modulation equation, which turns out to be a system of four macroscopic conservation laws. The last part is devoted to the justification problem: We state a conjecture for the general case, and prove this conjecture for the harmonic chain and the hard sphere model.

# 1 Introduction

We consider an atomic chain with $N$ identical particles, whose dynamics is given by an ODE system, which consists of Newton's equation of motion. The focus of this study is the establishment of the macroscopic limit $N \to \infty$ in case that the microscopic motion generates temperature on the macroscopic scale. This phenomenon leads on the macroscopic scale to a coupling of fast oscillations and slowly varying processes.

The particles of the chain, see Figure 1 have the mass $m = 1$, and they are indexed by $\alpha$. At time $t$ the particles have the positions $x_\alpha(t)$. The basic variables are the distances $r_\alpha(t) = x_{\alpha+1}(t) - x_\alpha(t)$ and the velocities $v_\alpha(t) = \dot{x}_\alpha(t)$. The particles move according to nearest neighbour interactions with interaction potential $\Phi(r)$. Their motion is determined by Newton's equation of motion

$$\ddot{x}_\alpha = \Phi'(x_{\alpha+1} - x_\alpha) - \Phi'(x_\alpha - x_{\alpha-1}), \tag{1.1}$$

which can be written in conservative form as

$$\dot{r}_\alpha = v_{\alpha+1} - v_\alpha \qquad \dot{v}_\alpha = \Phi'(r_\alpha) - \Phi'(r_{\alpha-1}). \tag{1.2}$$

In the following we will mainly consider convex interaction potentials, so that the force $\Phi'$ is a monotone increasing function. For instance, the harmonic chain is governed by a quadratic interaction potential, and the famous Toda chain ([Tod70, Tod81]) results, if we set

$$\Phi(r) = \exp(1 - r) - (1 - r). \tag{1.3}$$

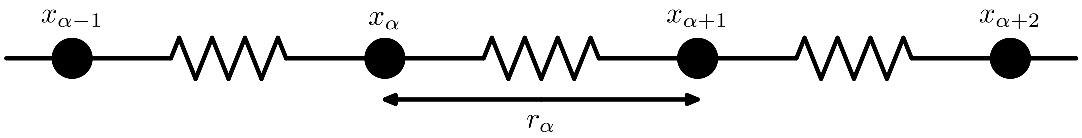


Figure 1: The atomic chain with nearest neighbour interaction.

The system (1.2) describes the evolution of the atomic chain on the *microscopic scale*, where $t$ and $x$ denote the microscopic time and space, respectively. The discrete particle index $\alpha$ may be interpreted as the microscopic Lagrange coordinate.

Thermodynamics describes a physical system, which consists of a very large number of particle, on the *macroscopic scale*. There are several possibilities to establish a transition from the microscopic to the macroscopic scale, which correspond to different scalings. In this study we focus on the hyperbolic scaling, where time, position and Lagrange coordinate are scaled in the same manner, see [DK00]. We introduce the scaling parameter $\varepsilon = 1/N$, and we define the macroscopic time, the macroscopic position and the macroscopic Lagrange coordinate by

$$\tau = \varepsilon t, \quad \xi = \varepsilon x, \quad y = \varepsilon\alpha, \tag{1.4}$$

respectively.

We mention two other scalings. The scaling $\tau = \varepsilon^2 t$, $y = \varepsilon(\alpha - ct)$ was studied by Giannoulis & Mielke in connection to the micro-macro transition for the atomic chain that leads on the macroscopic scale to the nonlinear Schrödinger equation, see [GM05, GM04]. Friesecke and Pego considered the Korteweg/de Vries scaling $\tau = \varepsilon^3 t$, $y = \varepsilon(\alpha - ct)$, in order to establish the Korteweg/deVries equation in the macroscopic limit, see [FP99]. Note that the various macroscopic limits only exist, if the chosen scaling fits to the microscopic initial data. For example, the Korteweg/deVries scaling requires initial data of the type $r_\alpha(0) = 1 + \varepsilon^2\bar{g}(\varepsilon\alpha)$, where $\bar{g}$ is a macroscopic function.

The derivation of the thermodynamic limit is currently too difficult, if we allow arbitrary microscopic oscillations. For this reason we only consider a restricted class of oscillations, namely those which are generated by *traveling waves*. A traveling wave is an exact solution of the atomic chain satisfying

$$x_\alpha(t) \;\;=\;\; r\alpha + vt + \mathbb{X}(k\alpha + \omega t). \tag{1.5}$$

Here $r$, $v$, $k$ and $\omega$ are constant parameters, which we call the *mean distance*, *mean velocity*, the *wave number* and the *frequency*, respectively, and the *wave profile* $\mathbb{X}$ is assumed to be periodic w.r.t. the phase $\varphi = k\alpha + \omega t$. Since the periodicity length $\varphi_{\text{per}}$ can be chosen arbitrarily, we usually suppose $\varphi_{\text{per}} = 1$. Only in Section 5.4 we set $\varphi_{\text{per}} = 2\pi$.

Next we discuss the notion of the modulation theory, which is best suited to pass from a microscopic ODE system to a macroscopic PDE system, if the macroscopic oscillations are generated by traveling waves. Modulation theory is a generalization of the passage from the Maxwell equations to geometric optics due to Kelvin, see Whitham's textbook on waves [Whi74], and is already applied to many microscopic systems including lattice models as well as nonlinear PDEs, but containing linear differential operators. For formal derivations we refer to [HLM94, FV98] for lattice models and to [Whi74] for PDEs. For rigorous mathematical justifications of Hamiltonian modulation equations see [GM05, GM04] and [KSM92, Sch98].

Within the modulation theory for the atomic chain we consider *modulated traveling waves*, which are *approximate* solutions of (1.1). They result from (1.5), if the traveling wave parameter vary on the macroscopic scale. This gives rise to the following ansatz

$$x_\alpha^{\mathrm{app}}(t) \;=\; \frac{1}{\varepsilon}X(\varepsilon t,\, \varepsilon\alpha) + \mathbb{X}\bigg(\varepsilon t,\, \varepsilon\alpha;\, \frac{1}{\varepsilon}\Theta(\varepsilon t,\, \varepsilon\alpha)\bigg), \tag{1.6}$$

where $X(\tau,\, y)$ and $\Theta(\tau,\, y)$ are the modulated position and phase, respectively, and $\tilde{\mathbb{X}}$ is a family of periodic traveling waves. The modulated traveling wave parameter now are fields depending on $(\tau,\, y)$, and are determined by $X$ and $\Theta$ via

$$v = \frac{\partial X}{\partial \tau}, \quad r = \frac{\partial X}{\partial y}, \quad \omega = \frac{\partial \Theta}{\partial \tau}, \quad k = \frac{\partial \Theta}{\partial y}.$$

The modulation equations are macroscopic PDEs, which describe the macroscopic evolution of the modulated traveling wave parameters $(r,\, v,\, k,\, \omega)$. As discussed in Section 4, they result as four macroscopic conservation laws:

$$\frac{\partial}{\partial \tau}(r,\, v,\, k,\, S)^T + \frac{\partial}{\partial y}(-v,\, +p,\, -\omega,\, +g)^T \;=\; 0. \tag{1.7}$$

Moreover, the constitutive relations closing (1.7) are given by the Gibbs equation

$$\mathrm{d}F = S\,\mathrm{d}\omega \,+\, p\,\mathrm{d}r \,+\, g\,\mathrm{d}k, \tag{1.8}$$

where $F = F(r,\, k,\, \omega)$ is the internal action of a traveling wave.

However, up to now there is no rigorous derivation of the modulation equations for the nonlinear case. For this reason we address the justification problem in Section 6. At first we present a conjecture for the general case, which claims, roughly spoken, that one can estimate the difference between the approximate solution (1.6) and a corresponding exact solution of atomic chain. Finally, we prove this conjecture for the harmonic chain and for the hard sphere model.

The paper is organized as follows:

In Section 2 we describe traveling waves as exact solutions of a difference-differential equation, and present an existence proof for traveling waves. Our proof relies on a result of Filip and Venakides, see [FV98], but simplifies some of their arguments.

The thermodynamics of traveling waves is established in Section3, where we introduce the thermodynamic quantities like temperature, internal energy, entropy and so on. Furthermore, we consider different sets of basic variables and derive the corresponding variants of the Gibbs equations (1.8).

Section 4 is devoted to modulated traveling waves and to the formal derivation of the modulation equations (1.7) via the principle of least action. The strategy is again similar to [FV98]; the new results regard the thermodynamic interpretation of the modulation system. Moreover, we find the additional conservation law for the energy, so that we can transform the system into the symmetric form. However, we can not guarantee that we have at hand a symmetric hyperbolic system, because in general the energy is not a convex function.

In Section 5 we consider three different interaction potentials that give rise to three examples with traveling waves of quite simple structure. These examples include the harmonic chain and the hard sphere model. For all three examples we exploit the modulation equations explicitly. Finally, in Section 5.4 we study the small-amplitude approximation of traveling waves, and obtain an explicit criterion for the hyperbolicity of the modulation equations.

Section 6 regards the justification problem mentioned above. In particular, we formulate the conjecture, and prove it in two cases.

# 2 Traveling waves

Recall that any traveling wave is an exact solution of (1.1), which satisfies the ansatz (1.5). If we plug in (1.5) into Newton's equation, we obtain a difference-differential equation for the *wave profile* $\mathbb{X}$, namely

$$\omega^2 \frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}\mathbb{X}(\varphi) = \Phi'\Big(r + \mathbb{X}(\varphi + k) - \mathbb{X}(\varphi)\Big) - \Phi'\Big(r + \mathbb{X}(\varphi) - \mathbb{X}(\varphi - k)\Big), \qquad (2.1)$$

where $\varphi = k\alpha + \omega t$ is the phase variable, and $(r,\, v,\, k,\, \omega)$ are four parameters. Note that the velocity $v$ does not enter in (2.1), because Newton's equations are invariant under Galilei transformations. However, in modulation theory it is necessary to consider the parameter $v$ explicitly.

We define the *traveling velocity wave* $\mathbb{V}$ and the *traveling distance wave* $\mathbb{R}$ by

$$\mathbb{V}(\varphi) = \frac{\mathrm{d}}{\mathrm{d}\varphi}\mathbb{X}(\varphi), \quad \mathbb{R}(\varphi) = \mathbb{X}\Big(\varphi + \frac{k}{2}\Big) - \mathbb{X}\Big(\varphi - \frac{k}{2}\Big), \qquad (2.2)$$

so that the atomic distances and velocities in a traveling wave read

$$r_\alpha(t) = r + \mathbb{R}(k\alpha + \omega t + k/2) \quad \text{and} \quad v_\alpha(t) = v + \omega\mathbb{V}(k\alpha + \omega t). \qquad (2.3)$$

Note that any traveling wave is completely determined by its traveling velocity wave.

**Existence of traveling waves**

The existence of traveling waves is a non-trivial and subtle problem. Many authors have studied this problem for different potentials, see for instance [FW94, FP99, FV98, IK00, Ioo00], and the references therein. Here we present a variational approach to this problem that is quite elementary but restricted to convex interaction potentials. Our existence proof is similar to that given in [FV98], but simplifies some arguments.

In order to avoid technical difficulties, we assume that the convex interaction potential $\Phi$ is in $\mathcal{C}^2$, and that it is defined on the whole real axis. Furthermore, we suppose that the second derivative $\Phi''$ is bounded. These regularity assumptions imply, that the following nonlinear operator $\partial\Phi$ is well defined and Lipschitz continuous

$$\partial\Phi \ : \ L^2([0,\,1]) \to L^2([0,\,1]), \quad \partial\Phi(\mathbb{V})(\varphi) \ := \ \Phi'(\mathbb{V}(\varphi)). \tag{2.4}$$

In what follows all functions from $L^p([0,\,1])$, $1 \leq p \leq \infty$, are supposed to be 1-periodic. For any $0 < k < 1$ we introduce two integral operators $A_k$ and $\hat{A}_k$ by

$$(A_k\mathbb{V})(\varphi) := \int\limits_{\varphi-k/2}^{\varphi+k/2} \mathbb{V}(\varphi')\,\mathrm{d}\varphi', \quad \hat{A}_k\mathbb{V} := A_k\mathbb{V} - k\int\limits_0^1 \mathbb{V}(\varphi')\,\mathrm{d}\varphi'. \tag{2.5}$$

Both integral operators are compact, symmetric, and map $L^2([0,\,1])$ into $L^\infty([0,\,1])$. Furthermore we define

$$B_k = \partial_k A_k, \quad \text{i.e.} \quad B_k\mathbb{V}(\varphi) \ := \ \frac{1}{2}(\mathbb{V}(\varphi+k/2) + \mathbb{V}(\varphi-k/2)) \tag{2.6}$$

$$\tag{2.7}$$

which is a bounded automorphism of $L^2([0,\,1])$. The traveling wave equation (2.1) can now be written as

$$\frac{\mathrm{d}\,\mathbb{R}}{\mathrm{d}\varphi}(\varphi) \ = \ \mathbb{V}(\varphi+k/2) - \mathbb{V}(\varphi-k/2), \tag{2.8}$$

$$\omega^2\frac{\mathrm{d}\,\mathbb{V}}{\mathrm{d}\varphi}(\varphi) \ = \ \Phi'\big(r+\mathbb{R}(\varphi+k/2)\big) - \Phi'\big(r+\mathbb{R}(\varphi-k/2)\big), \tag{2.9}$$

or, equivalently,

$$\mathbb{R} = \hat{A}_k\mathbb{V}, \quad \omega^2\mathbb{V} = \hat{A}_k\partial\Phi\Big(r+\mathbb{R}\Big). \tag{2.10}$$

In order to prove the existence of traveling waves, we consider the following optimization problem.

**Problem 2.1** *For fixed $r$, $0 < k < 1$ and $\gamma > 0$, we maximize the functional*

$$\mathbb{V} \in L^2([0,\,1]) \ \mapsto \ \mathcal{W}(r,\,k,\,\mathbb{V}) \ := \ \int\limits_0^1 \Phi\Big(r + \hat{A}_k\mathbb{V}(\varphi)\Big)\,\mathrm{d}\varphi \tag{2.11}$$

*under the constraint* $\mathbb{V} \in H_\gamma$ *with*

$$H_\gamma \;:=\; \Big\{ \mathbb{V} \in L^2([0,\,1]) \;:\; \frac{1}{2}\int\limits_0^1 \mathbb{V}(\varphi)^2\,\mathrm{d}\varphi \le \gamma \Big\}. \tag{2.12}$$

**Theorem 2.2** *For all* $r$, $0 < k < 1$ *and* $\gamma > 0$ *there exists a maximizer* $\tilde{\mathbb{V}}$ *of Problem 2.1 such that*

$$\frac{1}{2}\int\limits_0^1 \tilde{\mathbb{V}}(\varphi)^2\,\mathrm{d}\varphi \;=\; \gamma \tag{2.13}$$

*Furthermore, there exists a positive Lagrangian multiplier* $\tilde{\omega}^2$ *so that* $\tilde{\mathbb{V}}$ *is a traveling velocity wave with frequency* $\tilde{\omega}$, *i.e.*

$$\tilde{\omega}^2\tilde{\mathbb{V}} = \hat{A}_k \partial\Phi\Big(r + \hat{A}_k\tilde{\mathbb{V}}\Big). \tag{2.14}$$

*Proof.* Since the operator $\hat{A}_k$ maps $L^2([0,\,1])$ compactly into itself, the functional (2.11) is weakly continuous on the weakly compact set $H_\gamma$. Therefore there exists a maximizer $\tilde{\mathbb{V}} \in H_\gamma$. Since (2.11) is convex, the maximizer is an element of the boundary of $H_\gamma$, which implies (2.13). Moreover, there exists a Lagrangian multiplier $\tilde{\omega}^2$ such that (2.14) is satisfied. $\square$

We conclude with two remarks: (*i*). The maximizer $\tilde{\mathbb{V}}$ from Theorem 2.2 is not unique, because any shift of a maximizer is also a maximizer. It remains an open problem to characterize all maximizers of problem 2.1. (*ii*). We have constructed traveling waves as maximizers of the functional (2.11). We mention that any stationary point of (2.11) is a traveling wave, as long as it is an element of the boundary of $H_\gamma$. The existence of non-maximizing traveling waves is another open question.

### Binary oscillations

For an arbitrary potential $\Phi$, it is hard to solve the difference-differential equations (2.1) or the optimization problem 2.1. However, if we restrict the wave number to $k = \frac{1}{2}$, we can do this explicitly.

**Lemma 2.3** *If* $k = 1/2$ *the difference-differential equations* (2.8) *and* (2.9) *become ordinary differential equations, namely*

$$\omega\mathbb{R}'(\varphi) \;=\; -2\mathbb{V}(\varphi - k/2) \tag{2.15}$$
$$\omega\mathbb{V}'(\varphi - k/2) \;=\; \Phi'(r + \mathbb{R}(\varphi)) - \Phi'(r - \mathbb{R}(\varphi)) \tag{2.16}$$

*Proof.* Since $\mathbb{R}$ and $\mathbb{V}$ are 1-periodic, the equations (2.8) and (2.9) yield

$$\omega\mathbb{R}'(\varphi+1/2)+\omega\mathbb{R}'(\varphi)=0, \quad \omega\mathbb{V}'(\varphi+1/2)+\omega\mathbb{V}'(\varphi)=0. \tag{2.17}$$

We conclude that $\mathbb{R}(\varphi+1/2)+\mathbb{R}(\varphi)$ and $\mathbb{V}(\varphi+1/2)+\mathbb{V}(\varphi)$ are constant. Integrating over one period shows that both constants are zero. Thus we can eliminate the delay terms, in (2.8)-(2.9) and we obtain (2.15), (2.16). □

Any traveling wave with $k = 1/2$, i.e. any solution of (2.15)-(2.16), is called a *binary oscillation.*

# 3 Thermodynamics of traveling waves

In this section we study the physical properties of traveling waves. In particular,

1. we will identify the usual thermodynamic fields as energy, temperature, pressure and so on,
2. we study the constitutive relations, i.e. the dependence of thermodynamic fields on the parameters of the traveling waves.

Since on the macroscopic scale the atomic data in a traveling wave are highly oscillating, we consider suitable microscopic mean values of the physical fields. All thermodynamic fields in a traveling wave are constant in the macroscopic Lagrangian space-time. However, in Section 4 these fields depend on the macroscopic variables, and we use the modulation theory to derive their macroscopic evolution equations.

Let $\mathbb{X} = (\mathbb{V}, \mathbb{R})$ be a traveling wave with parameters $r$, $v$, $k$ and $\omega$. We introduce the following thermodynamic quantities:

$$\begin{array}{lcll} W & := & \displaystyle\int_0^1 \Phi(r+\mathbb{R}(\varphi))\,\mathrm{d}\varphi & \text{specific internal potential energy,} \\ \gamma & := & \displaystyle\frac{1}{2}\int_0^1 \mathbb{V}(\varphi)^2\,\mathrm{d}\varphi & \text{parameter } \gamma, \\ p & := & \displaystyle-\int_0^1 \partial\Phi(r+\mathbb{R}(\varphi))\,\mathrm{d}\varphi, & \text{pressure,} \end{array}$$

and

$$\begin{array}{lcll} K & := & \omega^2\gamma & \text{specific internal kinetic energy,} \\ T & := & 2K & \text{temperature,} \\ F & := & K-W & \text{specific internal action,} \\ U & := & K+W & \text{specific internal energy.} \end{array}$$

Furthermore, we define

$$\begin{array}{rcll} S & := & 2\omega\gamma & \text{specific entropy,} \\ g & := & -\displaystyle\int_0^1 \Phi'(r+\mathbb{R}(\varphi))(B_k\mathbb{V})(\varphi)\,\mathrm{d}\varphi & \text{entropy flux.} \end{array} \tag{3.1}$$

At a first glance, these definitions may look very artificial. However, in the following we show, that $(S,\, g)$ has all macroscopic properties of an entropy density-flux pair.

Next we consider (smooth) families $\mathbb{X}$ of traveling waves, which depend on a parameter set $\vec{u}$. All physical fields then become functions in $\vec{u}$. In order to have a clear distinction between the parameter dependence and the $\varphi$-dependence, we write $\mathbb{X}(\vec{u};\, \varphi)$ as well as $\mathbb{V}(\vec{u};\, \varphi)$ and $\mathbb{R}(\vec{u};\, \varphi)$ for the corresponding families of velocity and distance waves, respectively. In Theorem 2.2 we have proved, that there exists a family of traveling waves depending on $\vec{u} = (r,\, k,\, \gamma)$. However, sometimes it is convenient to consider other set of parameters.

The parameter dependence of the physical quantities lead to constitutive relations, that become important in Section 4. In the following we derive these constitutive laws for different sets of parameters. However, in all cases we will identify a thermodynamic potential, given by the *equation of state*, and a corresponding Gibbs equation, that establishes the constitutive relations. We summarize the results as follows:

| independent variables | thermodynamic potential | Gibbs equation |
|---|---|---|
| $(r,\, k,\, \gamma)$ | $W = W(r,\, k,\, \gamma)$ | $\mathrm{d}W = \omega^2\,\mathrm{d}\gamma \,-\, p\,\mathrm{d}r \,-\, g\,\mathrm{d}k$ |
| $(r,\, k,\, \omega)$ | $F = F(r,\, k,\, \omega)$ | $\mathrm{d}F = S\,\mathrm{d}\omega \,+\, p\,\mathrm{d}r \,+\, g\,\mathrm{d}k$ |
| $(r,\, k,\, S)$ | $U = U(r,\, k,\, S)$ | $\mathrm{d}U = \omega\,\mathrm{d}S \,-\, p\,\mathrm{d}r \,-\, g\,\mathrm{d}k$ |

(3.2)

In particular, if the equation of state is known, all other constitutive relations can be determined by means of the corresponding Gibbs equation.

### The parameter set $\vec{u} = (r,\, k,\, \gamma)$

Let $\mathbb{V}(r,\, k,\, \gamma;\, \cdot)$ be a family of traveling velocity waves that is parameterized by $(r,\, k,\, \gamma)$. Recall that the existence of such families is provided by Theorem 2.2. We define a function $W$ by

$$W(r,\, k,\, \gamma) \;=\; \mathcal{W}(r,\, k,\, \mathbb{V}(r,\, k,\, \gamma;\, \cdot)), \tag{3.3}$$

where $\mathcal{W}$ is given by (2.11).

**Theorem 3.1** *The function $W = W(r,\, k,\, \gamma)$ is nondecreasing w.r.t $\gamma$, and there holds*

$$\mathrm{d}W = \omega^2\,\mathrm{d}\gamma \,-\, p\,\mathrm{d}r \,-\, g\,\mathrm{d}k, \tag{3.4}$$

*i.e.* $\omega^2 = \partial_\gamma W$, $p = -\partial_r W$, *and* $g = -\partial_k W$.

*Proof.* The functional $\mathcal{W}$ is smooth in $(r,\, k)$ and Gateaux-differentiable with respect to its variable $\mathbb{V}$. Since the family $\mathbb{V}(r,\, k,\, \gamma;\, \cdot)$ is assumed to be smooth, we find that $W$ is differentiable with respect to $(r,\, k,\, \gamma)$. We differentiate $W$ with respect to $\gamma$, and obtain

$$\partial_\gamma W = \int_0^1 \Phi'\Big(r + \hat{A}_k \mathbb{V}(\varphi)\Big) \cdot \hat{A}_k \, \partial_\gamma \mathbb{V}(\varphi) \, \mathrm{d}\varphi = \omega^2 \int_0^1 \mathbb{V}(\varphi) \, \partial_\gamma \mathbb{V}(\varphi) \, \mathrm{d}\varphi = \omega^2 \partial_\gamma \gamma > 0.$$

Here we did not write explicitly the dependence of $\mathbb{V}$ on $r$, $k$ and $\gamma$. Differentiating $W$ with respect to $r$ yields

$$\begin{aligned} \partial_r W &= \int_0^1 \Phi'\Big(r + \hat{A}_k \mathbb{V}(\varphi)\Big)\Big(1 + \hat{A}_k \, \partial_\gamma \mathbb{V}(\varphi)\Big) \, \mathrm{d}\varphi \\ &= -p + \omega^2 \int_0^1 \mathbb{V}(\varphi) \, \partial_r \mathbb{V}(\varphi) \, \mathrm{d}\varphi = \omega^2 \partial_r \gamma = -p. \end{aligned}$$

Similarly, $\partial_k W = -g$. □

According to this theorem, the internal potential energy $W$ is the thermodynamic potential, and (3.3) and (3.4) are the equation of state and the corresponding Gibbs equation, respectively.

**The parameter set** $\vec{u} = (r,\, k,\, \omega)$

We now consider smooth families $\mathbb{V}(r,\, k,\, \omega;\, \cdot)$ of traveling velocity waves that are generated by the parameters $(r,\, k,\, \omega)$. In section 4 we will describe the modulation theory of traveling waves and there we will start with such a family of traveling waves. First we derive a variational result.

**Lemma 3.2** *Any traveling velocity wave* $\mathbb{V}(r,\, k,\, \omega;\, \cdot)$ *is a stationary point of the functional*

$$\mathbb{V} \in L^2([0,\, 1]) \;\mapsto\; \mathcal{F}(r,\, k,\, \omega,\, \mathbb{V}) = \frac{1}{2}\omega^2 \int_0^1 \mathbb{V}(\varphi)^2 \, \mathrm{d}\varphi - \int_0^1 \Phi\Big(r + \hat{A}_k \mathbb{V}(\varphi)\Big) \, \mathrm{d}\varphi. \quad (3.5)$$

*Proof.* The functional $\mathcal{F}$ is Gateaux-differentiable w.r.t. its variable $\mathbb{V}$, and the derivative reads

$$\partial_{\mathbb{V}} \mathcal{F}(r,\, k,\, \omega,\, \mathbb{V}) \;=\; \omega^2 \mathbb{V} - \tilde{A}_k \partial \Phi\Big(r + \hat{A}_k \mathbb{V}\Big). \quad (3.6)$$

We conclude, that (2.2) is just the Euler-Lagrange equation corresponding to (3.5). □

If $(r,\,k,\,\omega)$ are the independent variables, the thermodynamic potential is the internal action $F$ with equation of state

$$F(r,\,k,\,\omega) \;=\; \mathcal{F}(r,\,k,\,\omega,\,\mathbb{V}(r,\,k,\,\omega)), \tag{3.7}$$

and the corresponding Gibbs equation reads

$$\mathrm{d}F \;=\; \gamma\,\mathrm{d}\omega^2 + g\,\mathrm{d}k + p\,\mathrm{d}r. \tag{3.8}$$

Both assertions can be proved similarly to Theorem 3.1.

**The parameter set** $\vec{u} = (r,\,k,\,S)$

Sometimes it is convenient to consider a third family of traveling waves, that is parameterized by $(r,\,k,\,S)$. In section 4 it will turn out, that the modulation equations for these parameters exhibit a very symmetric structure.

**Lemma 3.3** *Any traveling velocity wave $\mathbb{V}(r,\,k,\,S,\,\cdot)$ is a stationary point of the functional*

$$\mathbb{V} \in L^2([0,\,1])\backslash\{0\} \;\mapsto\; \mathcal{U}(r,\,k,\,S,\,\mathbb{V}) = \frac{S^2}{2\int\limits_0^1 \mathbb{V}(\varphi)^2\,\mathrm{d}\varphi} + \int\limits_0^1 \Phi\Big(r + \tilde{A}_k\mathbb{V}(\varphi)\Big)\,\mathrm{d}\varphi. \tag{3.9}$$

*Proof.* Equation (2.2) is the Euler-Lagrange equation of the functional (3.9). □

In this case, the thermodynamic potential is the internal energy $U$, given by the equation of state

$$U(r,\,k,\,S) \;=\; \mathcal{U}(r,\,k,\,S,\,\mathbb{V}(r,\,k,\,S)), \tag{3.10}$$

and the Gibbs Equation reads

$$\mathrm{d}U \;=\; \omega\,\mathrm{d}S - g\,\mathrm{d}k - p\,\mathrm{d}r. \tag{3.11}$$

**Macroscopic changes of parameters**

In classical thermodynamics, the transformation from a given set of independent variables to another one is done by means of Legendre transforms (LT) of the thermodynamic potentials. Within the thermodynamics of traveling waves we find following analogue.

**Lemma 3.4** *Let $r$ and $k$ be fixed.*

1. *If $\omega^2 = \omega^2(\gamma)$ is invertible there holds: $F$ is LT of $W$ with respect to $\gamma$ and $W$ is LT of $F$ with respect to $\omega^2$.*
2. *If $S = S(\omega)$ is invertible there holds: $U$ is LT of $F$ with respect to $\omega$ and $F$ is LT of $U$ with respect to $S$.*

*Proof.* All propositions follow immediately from some basic calculations. $\square$

We mention that it remains an open problem to validate the invertibility assumptions for arbitrary atomic interaction potentials.

### Thermodynamics of binary oscillations

Let $r$ and $\omega$ be fixed and let $\mathbb{V}(\varphi)$, $\mathbb{R}(\varphi)$ be a binary oscillation, i.e. a solution of (2.15)-(2.16). The system (2.15)-(2.16) is equivalent to an Hamiltonian system. To show this, we define new functions $V(\sigma) = \omega\mathbb{V}(\omega\sigma/2 - 1/2)$ and $R(\sigma) = \mathbb{R}(\omega\sigma/2)$, and introduce the *oscillator energy* $H_{\mathrm{osc}}$ by

$$H_{\mathrm{osc}}(V,\, R) = \frac{1}{2}\omega^2 V^2 + \Phi_{\mathrm{osc}}(R), \quad \Phi_{\mathrm{osc}}(R) = \frac{1}{2}\Phi(r+R) + \frac{1}{2}\Phi(r-R). \tag{3.12}$$

The ODE system (2.8)-(2.9) then reads

$$\frac{\mathrm{d}}{\mathrm{d}\,\sigma}R(\sigma) = -\frac{\partial\, H_{\mathrm{osc}}}{\partial\, V}(V(\sigma),\, R(\sigma)), \quad \frac{\mathrm{d}}{\mathrm{d}\,\sigma}V(\sigma) = +\frac{\partial\, H_{\mathrm{osc}}}{\partial\, R}(V(\sigma),\, R(\sigma)). \tag{3.13}$$

This Hamiltonian system describes the motion of a particle in the symmetric and convex potential $\Phi_{\mathrm{osc}}$. Note that $R(\sigma)$ and $V(\sigma)$ are $2/\omega$-periodic functions.

The Hamiltonian structure allows to parameterize the binary oscillation of an atomic chain by the variables $r$ and $H_{\mathrm{osc}}$, where the oscillator energy is equal to the internal energy $U$ in the sense of Section 3.

**Theorem 3.5** *For binary oscillations there holds:*

1. *The entropy flux vanishes, i.e. $g = 0$.*
2. *The Gibbs equation reduces to $\mathrm{d}U = \omega\,\mathrm{d}S - p\,\mathrm{d}r$.*
3. *The frequency $\omega$ and the entropy $S$ are given by*

$$\frac{1}{\omega} = \int_{-R^\star}^{+R^\star} \frac{\mathrm{d}R}{\sqrt{2(U - \Phi_{\mathrm{osc}}(R))}}, \qquad S = \int_{-R^\star}^{+R^\star} \sqrt{2(U - \Phi_{\mathrm{osc}}(R))}\,\mathrm{d}R, \tag{3.14}$$

*where $R^\star > 0$ is determined by $U = \Phi_{\mathrm{osc}}(R^\star)$.*

*Proof.* From (2.17) we conclude $B_k\mathbb{V} \equiv 0$ and hence $g = 0$. Since $g = 0$, the Gibbs equation (3.14) follows immediately from (3.11). Since $H_{\rm osc}$ is an integral of motion for (3.13), we find

$$U \;=\; \int_0^1 \frac{1}{2}\mathbb{V}(\varphi)^2 + \Phi(r+\mathbb{R}(\varphi))\,\mathrm{d}\varphi \;=\; \frac{\omega}{2}\int_0^{2/\omega} H_{\rm osc}(V(\sigma),\,R(\sigma))\,\mathrm{d}\sigma \;=\; H_{\rm osc}. \tag{3.15}$$

We may assume that $V(\sigma) > 0$ within the first half period. This implies $R(\sigma = 0) = -R^\star$ and $R(\sigma = 1/\omega) = +R^\star$. Hence

$$\frac{2}{\omega} = 2\int_0^{1/\omega} \mathrm{d}\sigma = 2\int_{-R^\star}^{+R^\star} \frac{\mathrm{d}R}{V} = 2\int_{-R^\star}^{+R^\star} \frac{\mathrm{d}R}{\sqrt{2(U-\Phi_{\rm osc}(R))}}. \tag{3.16}$$

Furthermore, the definitions of $S$ and $\gamma$ imply

$$S = \frac{1}{\omega}\int_0^1 \omega^2\mathbb{V}^2(\varphi)\,\mathrm{d}\varphi = \int_0^{1/\omega} \omega^2 V^2(\sigma)\,\mathrm{d}\sigma = \int_{-R^\star}^{+R^\star} 2(U-\Phi_{\rm osc}(R))\frac{\mathrm{d}R}{\sqrt{2(U-\Phi_{\rm osc}(R))}},$$

which was claimed in (3.14). $\square$

# 4 Modulation equations

As described in the introduction, a *modulated traveling wave* is an approximate solution of (1.1), that satisfies

$$x_\alpha(t) \;=\; \frac{1}{\varepsilon}X(\varepsilon t,\,\varepsilon\alpha) + \tilde{\mathbb{X}}\Big(\varepsilon t,\,\varepsilon\alpha;\,\frac{1}{\varepsilon}\Theta(\varepsilon t,\,\varepsilon\alpha)\Big), \tag{4.1}$$

where $X(\tau,\,y)$ and $\Theta(\tau,\,y)$ are macroscopic functions. The wave profile $\tilde{\mathbb{X}}(\tau,\,y;\,\varphi)$ is assumed to be 1-periodic w.r.t to $\varphi$, and depends explicitly $\tau$ and $y$. The generic traveling wave parameters $(r,\,v,\,k,\,\omega)$ now are macroscopic fields and read

$$\omega(\tau,\,y) = \frac{\partial\,\Theta}{\partial\,\tau}(\tau,\,y), \qquad k(\tau,\,y) = \frac{\partial\,\Theta}{\partial\,y}(\tau,\,y) \tag{4.2}$$

and

$$v(\tau,\,y) = \frac{\partial\,X}{\partial\,\tau}(\tau,\,y), \qquad r(\tau,\,y) = \frac{\partial\,X}{\partial\,y}(\tau,\,y) \tag{4.3}$$

Furthermore, we assume that the wave profile describes periodic traveling waves, i.e. we set

$$\tilde{\mathbb{X}}(\tau,\,y;\,\varphi) \;=\; \mathbb{X}(r(\tau,\,y),\,v(\tau,\,y),\,k(\tau,\,y),\,\omega(\tau,\,y),\,a(\tau,\,y);\,\varphi), \tag{4.4}$$

where $\mathbb{X}(r,\, v,\, k,\, \omega,\, a;\, \varphi)$ is a smooth family of traveling waves as in Section 3. Here, $a$ denotes an additional parameter as for instance the energy $E$, the entropy $S$ or the parameter $\gamma$. To ensure that no further degree of freedom is allowed, we have to impose a further algebraic equation. The most prominent example is the *dispersion relation*, which provides the frequency

$$\omega \;=\; \Omega(r,\, k,\, a). \tag{4.5}$$

Recall that the family (4.4) does rather not depend on $v$, but some notations simplify, if we introduce the formal dependence on $v$.

The modulation equations are macroscopic PDEs that describe the macroscopic evolution of the traveling wave parameter $(r,\, v,\, k,\, \omega,\, a)$. They are determined so that the ansatz (4.1) provides in fact approximate solutions of the atomic chain. Since the dispersion relation eliminates one degree of freedom, we have to identify four further macroscopic equations. In what follows we apply a variational approach to derive these equations.

**Formal derivation of the modulation equations**

Let $\mathbb{X} = \mathbb{X}(r,\, v,\, k,\, \omega,\, a;\, \cdot) \in L^2([0,\, 1])$ be a smooth family of periodic traveling waves. In what follows, we abbreviate the parameters by $\vec{u} = (r,\, v,\, k,\, \omega,\, a)$. Moreover, let $\mathbb{V}(\vec{u};\, \cdot)$ and $\mathbb{R}(\vec{u};\, \cdot)$ be the corresponding families of traveling velocity and traveling distance waves, respectively.

We now insert the ansatz (4.1) into the expression for the total action in the atomic chain. The discrete sum w.r.t. $\alpha$ yields integrals over the microscopic phase $\varphi$ as well as integrals over the macroscopic Lagrangian coordinate $y$. There results

$$\text{total action} = \mathbb{L}(X,\, \Theta) := \int_0^{\tau_{\text{fin}}} \int_0^1 L(\vec{u}(\tau,\, y))\,\mathrm{d}y\,\mathrm{d}\tau \tag{4.6}$$

where $L(\vec{u}) = \mathcal{L}(\vec{u},\, \mathbb{X}(\vec{u};\, \cdot))$. The functional $\mathcal{L}$ is defined by

$$\mathcal{L}(\vec{u},\, \mathbb{X}) \;=\; \int_0^1 \left(\frac{1}{2}(v + \omega\mathbb{X}'(\varphi))^2 - \Phi(r + \nabla_k\mathbb{X}(\varphi))\right) \mathrm{d}\varphi, \tag{4.7}$$

where $\mathbb{X}$ is arbitrary in $L^2([0,\, 1])$. Recall that '$'$' denotes the derivative with respect to $\varphi$ and $\nabla_k$ is given by $(\nabla_k\mathbb{X})(\varphi) = \mathbb{X}(\varphi + k) - \mathbb{X}(\varphi)$. The modulation equations result if we apply the principle of least action to (4.6). The variations with respect to $X$ and $\Theta$ yield

$$0 \;=\; \frac{\partial}{\partial\,\tau}\partial_v L(\vec{u}(\tau,\, y)) + \frac{\partial}{\partial\, y}\partial_r L(\vec{u}(\tau,\, y)) \tag{4.8}$$

$$0 \;=\; \frac{\partial}{\partial\,\tau}\partial_\omega L(\vec{u}(\tau,\, y)) + \frac{\partial}{\partial\, y}\partial_k L(\vec{u}(\tau,\, y)) \tag{4.9}$$

respectively. Furthermore, there exist two compatibility conditions, which result from (4.2) and (4.3), namely

$$\frac{\partial\, r(\vec{u})}{\partial\, \tau}(\tau,\, y) = \frac{\partial\, v}{\partial\, y}(\tau,\, y), \qquad\qquad \frac{\partial\, k(\vec{u})}{\partial\, \tau}(\tau,\, y) = \frac{\partial\, \omega(\vec{u})}{\partial\, y}(\tau,\, y). \tag{4.10}$$

In the next step we evaluate the constitutive relation in more detail. The Gateaux differential of $\mathcal{L}$ w.r.t. an arbitrary function $\mathbb{X} \in L^2([0,\, 1])$ reads

$$\partial_{\mathbb{X}}\mathcal{L}(\vec{u},\, \mathbb{X}) \;=\; -\omega^2\mathbb{X}'' + \nabla_k^\star\partial\Phi(r + \nabla_k\mathbb{X}), \tag{4.11}$$

which is just the traveling wave equation with free parameter $\omega$. The family $\mathbb{X}(\vec{u};\, \cdot)$ satisfies the traveling wave equation, if the parameter $\omega$ is replaced by the dispersion relation. Thus there holds

$$\partial_{\mathbb{X}}\mathcal{L}(\vec{u},\, \mathbb{X}(\vec{u};\, \cdot)) \;=\; \big(\Omega^2(r,\, k,\, a) - \omega^2\big)\mathbb{X}(\vec{u};\, \cdot)''. \tag{4.12}$$

Since $\mathcal{L}$ does not explicitly depend on $a$ we find

$$\begin{aligned} \partial_a L(\vec{u}) \;&=\; \langle\partial_{\mathbb{X}}\mathcal{L}(\vec{u},\, \mathbb{X}(\vec{u};\, \cdot)),\, \partial_a\mathbb{X}(\vec{u};\, \cdot)\rangle_{\,L^2([0,1])} \\ &=\; \big(\Omega^2(r,\, k,\, a) - \omega^2\big)\int_0^1 \mathbb{X}'(\vec{u};\, \varphi)\partial_a\mathbb{X}'(\vec{u};\, \varphi)\,\mathrm{d}\varphi. \end{aligned} \tag{4.13}$$

We conclude that the dispersion relation is equivalent to $\partial_a L(\vec{u}) = 0$. Moreover, it implies

$$\partial_{\mathbb{X}}\mathcal{L}(\vec{u},\, \mathbb{X}(\vec{u};\, \cdot)) = 0 \quad \text{as well as} \quad \partial_x L(\vec{u}) = \partial_x\mathcal{L}(\vec{u},\, \mathbb{X}(\vec{u};\, \cdot)) \tag{4.14}$$

for all $x \in \{r,\, v\; k,\, \omega\}$. This yields

$$\partial_r L(\vec{u}) \;=\; -\int_0^1 \partial\Phi(r + \nabla_k\mathbb{X}(\vec{u};\, \varphi))\,\mathrm{d}\varphi \;=\; -\int_0^1 \partial\Phi(r + \mathbb{R}(\vec{u};\, \varphi))\,\mathrm{d}\varphi, \tag{4.15}$$

$$\partial_v L(\vec{u}) \;=\; +\int_0^1 (v + \omega\mathbb{X}'(\vec{u};\, \varphi))\,\mathrm{d}\varphi \;=\; v \tag{4.16}$$

and

$$\begin{aligned} \partial_k L(\vec{u}) \;&=\; -\int_0^1 \partial\Phi(r + \nabla_k\mathbb{X}(\vec{u};\, \varphi))\mathbb{X}'(\vec{u};\, \varphi + k)\,\mathrm{d}\varphi \\ &=\; -\int_0^1 \partial\Phi(r + \mathbb{R}(\vec{u};\, \varphi))B_k\mathbb{V}(\vec{u};\, \varphi)\,\mathrm{d}\varphi, \end{aligned} \tag{4.17}$$

$$\partial_\omega L(\vec{u}) \;=\; +\int_0^1 (v + \omega\mathbb{X}'(\vec{u};\, \varphi))\mathbb{X}'(\vec{u};\, \varphi)\,\mathrm{d}\varphi \;=\; \omega\int_0^1 \mathbb{V}(\vec{u};\, \varphi)^2\,\mathrm{d}\varphi. \tag{4.18}$$

According to the definitions in Section 3, we finally obtain

$$\partial_r L(\vec{u}) = p(\vec{u}), \quad \partial_v L(\vec{u}) = v, \quad \partial_k L(\vec{u}) = g(\vec{u}), \quad \partial_\omega L(\vec{u}) = S(\vec{u}). \tag{4.19}$$

The modulation equations (4.8), (4.9) and (4.10) now read

$$\frac{\partial}{\partial\,\tau}\begin{pmatrix} r \\ v \\ k \\ S(\vec{u}) \end{pmatrix}(\tau,\, y) + \frac{\partial}{\partial\, y}\begin{pmatrix} -v \\ +p(\vec{u}) \\ -\omega \\ +g(\vec{u}) \end{pmatrix}(\tau,\, y) \;\; = \;\; 0. \tag{4.20}$$

Note that we did not eliminate the frequency $\omega$ by the algebraic dispersion relation (4.5). According to Section 3, we may interpret the four PDEs as the macroscopic conservation laws for mass, momentum, wave vector and entropy.

Let us now consider the fields $r$, $v$, $k$ and $\omega$ as the independent variables. We set $a := \omega$ and the dispersion relation (4.5) reads $\omega = a$. The resulting modulation equations are the same as (4.20), but now all constitutive relations are given by the Gibbs Equation (3.8). In this form, the modulation system for the atomic chain was derived by Filip and Venakides in [FV98]. Moreover, we find the same formal structure as in the context of modulated traveling waves for PDEs, cf. [Whi74].

**The modulation equations for** $(r,\, v,\, k,\, S)$

Here we consider the independent parameters $r$, $k$, $v$ and $S$, i.e. we choose $a = S$. In densities of (4.20) are the independent variables, and the fluxes are given by the Gibbs Equation

$$\mathrm{d}E \;\; = \;\; \omega\,\mathrm{d}S - g\,\mathrm{d}k - p\,\mathrm{d}r + v\,\mathrm{d}v, \tag{4.21}$$

where $E := \frac{1}{2}v^2 + U(r,\, k,\, S)$ is the specific total energy. The system (4.20) now can be written as

$$\frac{\partial}{\partial\,\tau}\vec{v} + B\frac{\partial}{\partial\, y}\partial_{\vec{v}}E(\vec{v}) \;\; = \;\; 0, \tag{4.22}$$

where

$$\vec{v} = \begin{pmatrix} r \\ v \\ k \\ S \end{pmatrix}, \qquad B = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{4.23}$$

In fact, this is a very nice structure of the modulation equation. Moreover, the set of variables $(r,\, v,\, k,\, S)$ provide further information about the modulation equations.

**Theorem 4.1** *Let a smooth solution of (4.22) be given. Then, the energy $E$ is conserved according to*

$$\frac{\partial E}{\partial \tau} + \frac{\partial}{\partial y}\big(pv + g\omega\big) \;=\; 0. \tag{4.24}$$

*Furthermore, there holds a further conservation law*

$$\frac{\partial}{\partial \tau}\big(rv + kS\big) - \frac{\partial E^\star}{\partial y} \;=\; 0, \tag{4.25}$$

*where $E^\star$ is the Legendre transform of $E$ with respect to all variables, i.e.*

$$E^\star \;=\; -rp + v^2 - kg + \omega S - E. \tag{4.26}$$

*Proof.* Equation (4.21) yields

$$\begin{aligned}\frac{\partial E}{\partial \tau} &= \omega\frac{\partial S}{\partial \tau} - p\frac{\partial r}{\partial \tau} - g\frac{\partial k}{\partial \tau} + v\frac{\partial v}{\partial \tau} \\ &= -\omega\frac{\partial g}{\partial y} - p\frac{\partial v}{\partial y} - g\frac{\partial \omega}{\partial y} - v\frac{\partial p}{\partial y} \;=\; -\frac{\partial}{\partial y}(pv + \omega g).\end{aligned}$$

Let $E^\star$ be given as in (4.26). Then there holds $dE^\star = S\,d\omega - r\,dp - k\,dg + v\,dv$. Finally, we find

$$\begin{aligned}\frac{\partial E^\star}{\partial y} &= S\frac{\partial \omega}{\partial y} - r\frac{\partial p}{\partial y} - k\frac{\partial g}{\partial y} + v\frac{\partial v}{\partial y} \\ &= S\frac{\partial k}{\partial \tau} + r\frac{\partial v}{\partial \tau} + k\frac{\partial S}{\partial \tau} + v\frac{\partial r}{\partial \tau} \;=\; \frac{\partial}{\partial \tau}\big(rv + kS\big).\end{aligned}$$

□

# 5 Examples of traveling waves

## 5.1 Harmonic chain

The most prominent example for an atomic chain with $\Phi(x) = a^2x^2/2$, where $a > 0$ is a constant. It is easy to prove, that there exists the following family of traveling waves, parameterized by $(r,\, k,\, \gamma)$,

$$\mathbb{V}(\gamma;\, \varphi) \;=\; 2\sqrt{\gamma}\sin(2\pi\varphi), \qquad \mathbb{R}(k,\, \gamma;\, \varphi) \;:=\; \frac{\sin(\pi k)}{\pi}\mathbb{V}(\varphi). \tag{5.1}$$

The dispersion relation $\omega(k) = a\sin(\pi k)/\pi$ provides the frequency $\omega$ as function of $k$, and does not depend on $r$ or $\gamma$. Furthermore, the equation of state reads

$$W(r,\, k,\, \gamma) \;=\; \frac{1}{2}a^2r^2 + \omega(k)^2\gamma, \tag{5.2}$$

and implies

$$g(r,\, k,\, \gamma) = -a^2\sin(2\pi k)\gamma,\; F(r,\, k,\, \gamma) = -\frac{1}{2}a^2r^2,\; S(r,\, k,\, \gamma) = 2\omega(k)\gamma. \tag{5.3}$$

## 5.2 Hard sphere model

Here we consider the hard sphere model of the atomic chain, which describes all interaction by hard sphere collisions. As long as the distance between two adjacent atoms is larger than a fixed interaction distance $r_{\min} > 0$, there is no interaction between the atoms. If the distance meets the interaction distance, both atoms will interact by an elastic collision, i.e. they will exchange their velocities. Although there is no corresponding smooth interaction potential, we may apply the notion of traveling waves and modulated traveling waves. There are three motivations for studying this simple model: (*i*). We can derive explicit expressions for families of traveling waves and thus also for the modulation equations. (*ii*). According to [FM02], the model describes the high energy limit for certain potentials. (*iii*). In Section 6 we can justify the modulation equations.

Using basic physical arguments, one can derive the following family of traveling velocity waves, parameterized by $(r, k, \omega)$,

$$\mathbb{V}(r, k; \varphi) = \begin{cases} -\dfrac{(r - r_{\min})}{k} & \text{if} \quad 0 \le \varphi < k \\ +\dfrac{(r - r_{\min})}{1-k} & \text{if} \quad k \le \varphi < 1 \end{cases}. \tag{5.4}$$

Recall that the frequency $\omega > 0$ is a free parameter and may be chosen independently of $r$ and $k$.The equation of state reads

$$F(r, k, \omega) = \frac{(r - r_{\min})^2 \omega^2}{2k(1-k)}, \tag{5.5}$$

and implies

$$S(r, k, \omega) = \frac{(r - r_{\min})^2 \omega}{k(1-k)}, \quad U = U(r, k, S) = \frac{S^2 k(1-k)}{2(r - r_{\min})^2}. \tag{5.6}$$

Since there is no internal potential energy, there holds $U = F$.

**Theorem 5.1** *The modulation equations in the variables $\vec{u} = (r, v, k, \omega)^T$ read*

$$\frac{\partial}{\partial \tau}\vec{u} + C(\vec{u})\frac{\partial}{\partial y}\vec{u} = 0, \tag{5.7}$$

*where*

$$C(\vec{u}) = \begin{pmatrix} 0 & -1 & 0 & 0 \\ \frac{\omega^2}{k(1-k)} & 0 & -\frac{(1-2k)r\omega^2}{k^2(1-k)^2} & \frac{2(r-r_{\min})\omega}{k(1-k)} \\ 0 & 0 & 0 & -1 \\ -\frac{(1-2k)\omega^2}{(r-r_{\min})k(1-k)} & \frac{2\omega}{(r-r_{\min})} & \frac{(1-4k(1-k))\omega^2}{k^2(1-k)^2} & -\frac{(1-2k)\omega}{k(1-k)} \end{pmatrix}. \tag{5.8}$$

*The system is hyperbolic with two linearly degenerate eigenvalues*

$$\lambda_1 = -\frac{\omega}{k}, \quad \lambda_2 = \frac{\omega}{1-k}. \tag{5.9}$$

*Proof.* See Theorem 5.2. □

### 5.3 Harmonic interactions, interrupted by periods of free flight

We consider an atomic chain in which the atomic interactions are given by the potential

$$\Phi(r) \;=\; \begin{cases} \dfrac{\delta^2 (r - r_{\min})^2}{4} & \text{iff} \quad r \le r_{\min}, \\ 0 & \text{iff} \quad r > r_{\min}, \end{cases} \tag{5.10}$$

where $\delta$ and $r_{\min}$ are two fixed constants. This model combines properties of the harmonic chain and of the hard sphere model. Next we give a family of traveling velocity waves that is parameterized by $(r,\, v,\, k,\, \omega)$. To this end we set $\sigma = \pi\omega/\delta$, and define a 1-periodic auxiliary function $\tilde{V}$ by

$$\tilde{V}(\varphi) \;=\; \begin{cases} +\cos\big(\sigma^{-1}\pi\varphi\big) & \text{iff} \quad 0 \le \varphi \le \sigma, \\ -1 & \text{iff} \quad \sigma \le \varphi \le k, \\ -\cos\big(\sigma^{-1}\pi(\varphi - k)\big) & \text{iff} \quad k \le \varphi \le k + \sigma, \\ +1 & \text{iff} \quad k + \sigma \le \varphi \le 1. \end{cases} \tag{5.11}$$

The family of traveling velocity waves results as

$$\mathbb{V}(\varphi) \;=\; \frac{r - r_{\min}}{2k(1-k) - \pi\delta^{-1}\omega}\Big(\tilde{V}(\varphi) - (1 - 2k)\Big). \tag{5.12}$$

Note that the corresponding family of distance waves is given by $\mathbb{R} = \hat{A}_k \mathbb{V}$. In order to ensure that (5.12) is well defined, the frequency must be sufficiently small, i.e.

$$\sigma = \pi\delta^{-1}\omega \le \min\{k,\, 1-k\}. \tag{5.13}$$

This condition corresponds to the physical restriction, that all interactions in the chain due to the harmonic part of $\Phi$ incorporate only two atoms. In other words, as long as the atomic distance $r_\alpha$ is smaller that $r_{\min}$, the adjacent distances $r_{\alpha-1}$ and $r_{\alpha+1}$ are larger than $r_{\min}$. We mention that there exist traveling waves violating this condition, but for these the explicit expressions become more complicate.

The family (5.12) yields the following equation of state

$$F = F(r,\, v,\, k,\, \omega) \;=\; \frac{(r - r_{\min})^2 \omega^2}{2k(1-k) - \pi\delta^{-1}\omega}, \tag{5.14}$$

which implies

$$S \;=\; \frac{(r - r_{\min})^2 \omega}{\big(2k(1-k) - \pi\delta^{-1}\omega\big)^2}\big(4k(1-k) - \pi\delta^{-1}\omega\big). \tag{5.15}$$

Moreover, if $\sigma = \pi\delta^{-1}\omega$ tends to zero, we obtain both for the traveling waves and for the equation of state the same expressions as in the hard sphere model.

**Theorem 5.2** *The modulation equations in the variables $\vec{u} = (r,\, v,\, k,\, \omega)^T$ read*

$$\frac{\partial}{\partial \tau}\vec{u} + A^{-1}(\vec{u})B(\vec{u})\frac{\partial}{\partial y}\vec{u} \;=\; 0, \tag{5.16}$$

*where*

$$A \;=\; \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \frac{2r\omega\left(4k(1-k)-\pi\delta^{-1}\omega\right)}{\left(2k(1-k)-\pi\delta^{-1}\omega\right)^2} & 0 & \frac{8r^2\omega k(1-k)(1-2k)}{\left(2k(1-k)-\pi\delta^{-1}\omega\right)^3} & \frac{8r^2k^2(1-k)^2}{\left(2k(1-k)-\pi\delta^{-1}\omega\right)^3} \end{pmatrix}, \tag{5.17}$$

$$B \;=\; \begin{pmatrix} 0 & -1 & 0 & 0 \\ \frac{2\omega^2}{(2k(1-k)-\pi\delta^{-1}\omega)} & 1 & -\frac{4r\omega^2(1-2k)}{\left(2k(1-k)-\pi\delta^{-1}\omega\right)^2} & \frac{2r\omega\left(4k(1-k)-\pi\delta^{-1}\omega\right)}{\left(2k(1-k)-\pi\delta^{-1}\omega\right)^2} \\ 0 & 0 & 0 & -1 \\ -\frac{4r\omega^2(1-2k)}{\left(2k(1-k)-\pi\delta^{-1}\omega\right)^2} & 0 & \frac{4r^2\omega^2\left(2-6(1-k)-\pi\delta^{-1}\omega\right)}{\left(2k(1-k)-\pi\delta^{-1}\omega\right)^3} & -\frac{8r^2\omega k(1-k)(1-2k)}{\left(2k(1-k)-\pi\delta^{-1}\omega\right)^3} \end{pmatrix}.$$

*The system is hyperbolic with two eigenvalues*

$$\lambda_1 = -\frac{\omega}{k}, \quad \lambda_2 = \frac{\omega}{1-k}, \tag{5.18}$$

*which both are linearly degenerate.*

*Proof.* The matrices $A$ and $B$ may be calculated directly from (4.22) and (5.14). The characteristic polynomial of the matrix $A^{-1}B$ is

$$P(\lambda) \;=\; \frac{(\omega + k\lambda)^2(\omega - (1-k)\lambda)^2}{k^2(1-k)^2}. \tag{5.19}$$

Hence, the system (5.16) has four real eigenvalues which are given by (5.18). The right eigenvectors $\vec{u_1}$ and $\vec{u_2}$ of $A^{-1}B$ corresponding to $\lambda_1$ and $\lambda_2$, respectively, are twofold degenerate and read

$$\vec{u_1} \;=\; \left(c_1,\, c_1\frac{\omega}{k},\, 1,\, \frac{\omega}{k}\right)^T, \quad c_1 = -\frac{2(r - r_{\min})k}{2k(1-k) - \pi\delta^{-1}\omega}, \tag{5.20}$$

$$\vec{u_2} \;=\; \left(c_2,\, -c_2\frac{\omega}{1-k},\, 1,\, -\frac{\omega}{1-k}\right)^T, \quad c_2 = \frac{2(r - r_{\min})(1-k)}{2k(1-k) - \pi\delta^{-1}\omega}. \tag{5.21}$$

It is easy to check that both eigenvectors are perpendicular to the gradients of the corresponding eigenvalues, which implies that both $\lambda_1$ and $\lambda_2$ are linearly degenerate.
□

## 5.4 Small-amplitude traveling waves

We now consider the small-amplitude approximation of traveling waves. This gives an example where we can explicitly determine a criterion for the hyperbolicity of the modulation equations. In order to simplify the notations we set the periodicity length of traveling waves to $2\pi$. At first we calculate the specific internal action, $F$, in the small-amplitude approximation. We have shown in Section 3 that $F$ does not depend on the velocity $\upsilon$, so that we can set $\upsilon = 0$ in the following calculation. The traveling wave representations (4.1) and (4.4) will now be written

$$x_\alpha(t) = r\alpha + \mathbb{X}(r,k,\delta;k\alpha + \Omega(r,k,\delta)t). \tag{5.22}$$

Note that within this section all traveling waves have period $\varphi_{\text{per}} = 2\pi$. The dispersion relation $\Omega(r,k,\delta)$ is given here with a different parameter set as in Section 3. The newly introduced parameter $\delta$ defines the amplitude of the wave. Furthermore we assume

$$\begin{aligned} \mathbb{X}(r,k,\delta;\varphi+2\pi) &= \mathbb{X}(r,k,\delta;\varphi) && (5.23)\\ \int_0^{2\pi} \mathbb{X}(r,k,\delta;\varphi)\,\mathrm{d}\varphi &= 0 && (5.24)\\ \int_0^{2\pi} \mathbb{X}(r,k,\delta;\varphi)\mathrm{e}^{-\mathrm{i}\varphi}\,\mathrm{d}\varphi &= 4\pi\delta. && (5.25) \end{aligned}$$

In fact, assuming that $\Phi$ is sufficiently smooth, we construct $\mathbb{X}$ as a power series expansion with respect to $\delta$. The dispersion relation $\omega = \Omega(r,k,\delta)$ is then also expanded in $\delta$. The small-amplitude approximation relies on the ansatz

$$\mathbb{X}(\varphi) = 2\delta\cos(\varphi) + \sum_{n=2}^{N} \delta^n \sum_{m=-n}^{n} A_{n,m}\mathrm{e}^{\mathrm{i}m\varphi} + \mathcal{O}(\delta^{N+1})_{\delta\to 0}, \tag{5.26}$$

$$\omega = \Omega(r,k,\delta) = \Omega_0 + \sum_{n=1}^{N} \delta^n\Omega_n + \mathcal{O}(\delta^{N+1})_{\delta\to 0}. \tag{5.27}$$

Here, we assume $A_{n,0} = A_{n,1} = 0$ as well as $A_{n,-m} = \overline{A}_{n,m}$. Of course, all $A_{n,m}$ and $\Omega_n$ will depend on $r$ and $k$. Inserting this into (5.22) and (2.1) and equating to 0 the terms associated with $\delta^n\mathrm{e}^{\mathrm{i}m\varphi}$ yields equations for the desired coefficients:

$$\delta^1\mathrm{e}^{\mathrm{i}\varphi} : \Omega_0^2 = \Phi''(r)2(1-\cos(k)) \tag{5.28}$$

$$\delta^2\mathrm{e}^{\mathrm{i}\varphi} : \Omega_1 = 0 \tag{5.29}$$

$$\delta^2\mathrm{e}^{\mathrm{i}2\varphi} : A_{2,2} = \frac{\mathrm{i}\sin k}{1-\cos k}\frac{\Phi'''(r)}{\Phi''(r)} \tag{5.30}$$

$$\delta^3\mathrm{e}^{\mathrm{i}\varphi} : \Omega_2 = \frac{1}{2\Omega_0}\left(12(1-\cos k)^2\Phi^{(4)}(r) + 8(\sin k)^2\frac{\Phi'''(r)^2}{\Phi''(r)}\right) \tag{5.31}$$

$$\delta^3\mathrm{e}^{\mathrm{i}2\varphi} : A_{3,2} = 0 \tag{5.32}$$

$$\delta^3\mathrm{e}^{\mathrm{i}3\varphi} : A_{3,3} = \frac{2\Phi''(r)\Phi^{(4)}(r)(\cos(2k)-\cos k) - 4\Phi'''(r)^2(\cos(2k)+3\cos k+2)}{\Phi''(r)^2(6-4\cos k-2\cos 2k)} \tag{5.33}$$

This expansion can now be inserted into the internal action $\tilde{F}$ as a function of $(r,k,\delta)$:

$$\tilde{F}(r,k,\omega,\delta) = \frac{1}{2\pi}\int_0^{2\pi} \frac{\omega^2}{2}\left[\mathbb{X}'(r,k,\delta;\varphi)\right]^2 - \Phi\left(r + \mathbb{X}(r,k,\delta;\varphi+k) - \mathbb{X}(r,k,\delta;\varphi)\right)\mathrm{d}\varphi. \tag{5.34}$$

This resuls in the following expansion

$$\tilde{F}(r,k,\omega,\delta) = -\Phi(r) + \sum_{n=1}^{N/2} \delta^{2n}\big(\omega^2 K_n(r,k) - V_n(r,k)\big) + \mathcal{O}\big(\delta^{N+2}\big), \tag{5.35}$$

with

$$K_1(r,k) = 1, \tag{5.36}$$

$$V_1(r,k) = \Phi''(r)2(1-\cos k), \tag{5.37}$$

$$K_2(r,k) = \left(\frac{\Phi'''(r)}{\Phi''(r)}\right)^2 \frac{1+\cos k}{1-\cos k}, \tag{5.38}$$

$$V_2(r,k) = \Phi^{(4)}(r)(1-\cos k)^2 + \frac{(\Phi'''(r))^2}{\Phi''(r)}\left[3 + 2\cos k - (\cos k)^2\right]. \tag{5.39}$$

Note that the function $\Omega(r,k,\delta)$ appears here from solving $\frac{\partial}{\partial\delta}\tilde{F}(r,k,\omega,\delta) = 0$ for $\omega$ as a function of $(r,k,\delta)$, namely

$$\Omega(r,k,\delta) = \big(V_1(r,k) + 2\delta^2(V_2(r,k) - V_1(r,k)K_2(r,k)) + \mathcal{O}(\delta^4)\big)^{1/2}. \tag{5.40}$$

However, we rather consider $\omega$ as independent variable and eliminate $\delta$ instead. We let $\Omega_0(r,k) = \sqrt{V_1(r,k)}$ and assume that

$$\begin{aligned} M(r,k) &\stackrel{\text{def}}{=} V_1(r,k)K_2(r,k) - V_2(r,k) \\ &= \Omega_0(r,k)^2 K_2(r,k) - V_2(r,k) \\ &= -\frac{(\Phi'''(r))^2}{\Phi''(r)}\left[1 - (\cos k)^2\right] - \Phi^{(4)}(r)[1-\cos k]^2 \end{aligned} \tag{5.41}$$

is different from 0. Then, $\frac{\partial}{\partial\delta}\tilde{F}(r,k,\omega,\delta) = 0$ can be solved for $\delta$ as a function $\delta = D(r,k,\omega)$ near $\omega = \Omega_0(r,k)$, namely

$$\delta^2 = D(r,k,\omega)^2 = -\frac{\omega^2 - \Omega_0(r,k)^2}{2[\Omega_0(r,k)^2 K_2(r,k) - V_2(r,k)]} + \mathcal{O}\left((\omega - \Omega(r,k))^4\right). \tag{5.42}$$

Thus, the reduced functional $F(r,k,\omega) = \tilde{F}(r,k,\omega,E(r,k,\omega))$ takes the form

$$F(r,k,\omega) = -\Phi'(r) + G(r,k)(\omega - \Omega_0(r,k))^2 + \mathcal{O}\left((\omega - \Omega(r,k))^4\right), \tag{5.43}$$

where

$$\begin{aligned} G(r,k) &= \frac{\Omega_0(r,k)^2}{V_2(r,k) - \Omega_0(r,k)^2 K_2(r,k)} = -\frac{\Omega_0(r,k)^2}{M(r,k)} \\ &= \frac{2(\Phi''(r))^2}{\Phi''(r)\Phi^{(4)}(r)(1-\cos k) + (\Phi'''(r))^2(1+\cos k)}. \end{aligned} \tag{5.44}$$

Of course, $F$ is only correctly related to the atomic chain when $\delta^2 \geq 0$ is satisfied, i.e.

$$\omega < \Omega_0(r,k) \quad \text{if } G(r,k) < 0 \tag{5.45}$$

and

$$\omega > \Omega_0(r,k) \quad \text{if } G(r,k) > 0. \tag{5.46}$$

Finally, we consider Whitham's modulation equation for the set of parameters from Section 3.2

$$\frac{\partial}{\partial t}\begin{pmatrix} r \\ v \\ k \\ \partial_\omega F(r,k,\omega) \end{pmatrix} = \frac{\partial}{\partial y}\begin{pmatrix} v \\ -\partial_r F(r,k,\omega) \\ \omega \\ -\partial_k F(r,k,\omega) \end{pmatrix}. \tag{5.47}$$

Hyperbolicity is checked by calculating the characteristic speeds $\lambda$ from

$$0 = p(\lambda) \overset{\text{def}}{=} \det\left[\lambda \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \partial_r\partial_\omega F & 0 & \partial_k\partial_\omega F & \partial_\omega^2 F \end{pmatrix} + \begin{pmatrix} 0 & -1 & 0 & 0 \\ \partial_r^2 F & 0 & \partial_r\partial_k F & \partial_r\partial_\omega F \\ 0 & 0 & 0 & -1 \\ \partial_r\partial_k F & 0 & \partial_k^2 F & \partial_k\partial_\omega F \end{pmatrix}\right] \tag{5.48}$$

An expansion in terms of $\omega - \Omega_0(r,k)$ yields

$$p(\lambda) = 2G(r,k)\left(\lambda - \partial_k\Omega_0(r,k)\right)^2\left(\lambda^2 - \Phi''(r)\right) + \mathcal{O}(\omega - \Omega_0). \tag{5.49}$$

For the case $\delta = 0$ we obtain the two macroscopic wave speeds $\lambda_{1,2} = \pm\sqrt{\Phi''(r)}$ and $\lambda_{3,4} = \partial_k\Omega_0(r,k)$, i.e., the group velocity is a double eigenvalue. The important question is how this pair behaves for small $\delta$. To this end we fix $\lambda = \partial_k\Omega_0(r,k)$ and expand in terms of $\omega - \Omega_0(r,k)$:

$$p(\partial_k\Omega_0(r,k)) = -2G(r,k)\partial_k^2\Omega_0(r,k)N(r,k)(\omega - \Omega_0(r,t)) + \mathcal{O}\left((\omega - \Omega_0)^2\right) \tag{5.50}$$

with

$$N(r,k) = \partial_k\Omega_0(r,k)^2 - \Phi''(r) + G(r,k)\partial_r\Omega_0(r,k)^2. \tag{5.51}$$

An explicit calculation gives

$$\begin{aligned} N(r,k) &= \hat{N}(r,k)G(r,k)/\Phi''(r) \quad \text{with} && (5.52)\\ \hat{N}(r,k) &= \Phi'''(r)^2[7 - 8\cos k + \cos(2k)] + \Phi''(r)\Phi^{(4)}(r)[4\cos k - 3 - \cos(2k)] && (5.53) \end{aligned}$$

Since $\partial_k^2\Omega_0(r,k) = -\frac{1}{4}\Omega_0(r,k) < 0$ and $(\partial_k\Omega_0(r,k))^2 - \Phi''(r) < 0$, we conclude that the double zero $\lambda = \partial_k\Omega_0(r,k)$ splits into two real eigenvalues if $\hat{N}(r,k) > 0$; and it splits into a pair of complex conjugate eigenvalues if $\hat{N}(r,k) < 0$. In the latter case the Whitham equation is no longer hyperbolic and hence ill-posed. This indicates, at least on a formal level, that the traveling waves are unstable due to the Benjamin-Feir instability, see e.g. [BM95].

For binary oscillations we have $k = \pi$ and obtain

$$\hat{N}(r,\pi) = 8\left(2\Phi'''(r)^2 - \Phi''(r)\Phi^{(4)}(r)\right). \tag{5.54}$$

Similarly, for $k = \frac{\pi}{3}$ we have $\hat{N}\left(r, \frac{\pi}{3}\right) = \frac{1}{2}\left(5\Phi'''(r)^2 - \Phi''(r)\Phi^{(4)}(r)\right)$. Using (5.54) it is easy to construct examples where all binary oscillations with small amplitude are unstable. In general one expects that the range of wave numbers $k$, which leads to stable small-amplitude oscillations, depends on the specific length $r$.

For the Toda lattice (1.3) we have $\left(\Phi'''(r)\right)^2 = \Phi''(r)\Phi^{(4)}(r) = \mathrm{e}^{2-2r}$ and hence

$$\hat{N}_{\mathrm{Toda}}(r,k) = \mathrm{e}^{2-2r}[4 - 4\cos k] \geq 0. \tag{5.55}$$

This coincides with the fact of complete integrability which leads to stability of the traveling waves.

# 6 On the justification of Whitham's modulation equation

The mathematical justification of Whitham's equation addresses the question whether solutions which start at time $t = 0$ as a modulated traveling wave will stay in the form of a modulated traveling wave on macroscopically long time scales, i.e., for $t \in [0, \tau_0/\varepsilon]$ for a $\tau_0 > 0$. If this is the case, then the above formal arguments show that the macroscopic quantities $(r, v, k, \omega)$ have to satisfy Whitham's equation. Of course, the relevant $\tau_0$ cannot be larger than the existence time of smooth solutions for Whitham's equation. Since this is a system of hyperbolic conservation laws, it is to be expected that shocks develop and it is clear that the modulation ansatz will not be suitable to describe such cases.

## 6.1 The generally expected justification result

We believe that the following conjecture is in the heart of the matter. However, at the moment we are far from being able to prove it in this general form. To formulate the conjecture we assume that the potential $\Phi$ is sufficiently smooth (e.g., $\Phi \in \mathrm{C}^5(\mathbb{R},\mathbb{R})$) and that a smooth family of traveling waves defined via $\mathbb{X}(r,k,\omega;\cdot) : \mathbb{S}^1 \to \mathbb{R}$ exists for $(r,k,\omega) \in \mathcal{D} \subset \mathbb{R}^3$ such that the action functional $F$, see (3.7), can be constructed. Thus, Whitham's equation can be formulated and we may define

$$\begin{aligned}\mathcal{M} := \{(r,k,\omega) \in \mathcal{D} \mid\ & \text{Whitham's equation is strictly hyperbolic} \\ & \text{in } (r,0,k,\omega) \text{ and the traveling wave} \\ & \mathbb{X}(r,k,\omega;\cdot) \text{ is linearly stable}\},\end{aligned}$$

and assume that $\mathcal{M}$ is an open set.

Our conjecture follows similar justification results for partial differential equations [KSM92, Sch98, Mie02] or for discrete systems [FP99, SW00, GM04, GM05].

For a given solution $\left(\widetilde{r},\, \widetilde{v},\, \widetilde{k},\, \widetilde{\omega}\right)$ of the Whitham equation we define the modulation ansatz $M^\varepsilon$ via the global deformation $X$ and the global phase $\Theta$ which are defined as follows:

$$X(0,0) = 0,\ \frac{\partial X}{\partial \tau} = \widetilde{v},\ \frac{\partial X}{\partial y} = \widetilde{r}, \quad \Theta(0,0) = 0,\ \frac{\partial \Theta}{\partial \tau} = \widetilde{\omega},\ \frac{\partial \Theta}{\partial y} = \widetilde{k}.$$

For a given scale parameter $\varepsilon \in (0, \varepsilon_0)$ we define

$$M^\varepsilon\left(\widetilde{r},\, \widetilde{v},\, \widetilde{k},\, \widetilde{\omega}\right)_\alpha(t) = \left(\begin{array}{c} \widetilde{r}(\varepsilon t, \varepsilon\alpha) + \mathbb{R}\Big((\widetilde{r}, \widetilde{k}, \widetilde{\omega})|_{(\varepsilon t, \varepsilon\alpha)};\, \tfrac{1}{\varepsilon}\Theta(\varepsilon t, \varepsilon\alpha) + \tfrac{1}{2}\widetilde{k}(\varepsilon t, \varepsilon\alpha)\Big) \\ \widetilde{v}(\varepsilon t, \varepsilon\alpha) + \widetilde{\omega}(\varepsilon t, \varepsilon\alpha)\mathbb{V}\Big((\widetilde{r}, \widetilde{k}, \widetilde{\omega})|_{(\varepsilon t, \varepsilon\alpha)};\, \tfrac{1}{\varepsilon}\Theta(\varepsilon t, \varepsilon\alpha)\Big) \end{array}\right) \tag{6.1}$$

where

$$\begin{aligned} \mathbb{R}\Big(\widetilde{r},\, \widetilde{k},\, \widetilde{\omega};\, \varphi\Big) &= \mathbb{X}\Big(\widetilde{r},\, \widetilde{k},\, \widetilde{\omega};\, \varphi + \frac{1}{2}\widetilde{k}\Big) - \mathbb{X}\Big(\widetilde{r},\, \widetilde{k},\, \widetilde{\omega};\, \varphi - \frac{1}{2}\widetilde{k}\Big), \\ \mathbb{V}\Big(\widetilde{r},\, \widetilde{k},\, \widetilde{\omega};\, \varphi\Big) &= \mathbb{X}'\Big(\widetilde{r},\, \widetilde{k},\, \widetilde{\omega};\, \varphi\Big), \end{aligned}$$

which is the modulation ansatz associated with the macroscopic solution of Whitham's equation.

**Conjecture 6.1** *Let $(\widetilde{r}, \widetilde{v}, \widetilde{k}, \widetilde{\omega}) : [0, \tau_{\text{fin}}] \times \mathbb{R} \to \mathbb{R}^4$ be a smooth solution of Whitham's equation such that $(\widetilde{r}(\tau, y), \widetilde{k}(\tau, y), \widetilde{\omega}(\tau, y)) \in \mathcal{M}$ for all $(\tau, y) \in [0, \tau_{\text{fin}}] \times \mathbb{R}$. Moreover, let $(r^\varepsilon,\, v^\varepsilon) : \mathbb{R} \to Y_\varepsilon$ be the solution of Newton's equations* (1.2) *with the initial condition*

$$(r^\varepsilon(0), v^\varepsilon(0))^\mathsf{T} = M^\varepsilon\Big(\widetilde{r},\, \widetilde{v},\, \widetilde{k},\, \widetilde{\omega}\Big)(0),$$

*where $\Upsilon_\varepsilon$ is a Banach space, such that*

$$\|\, (r^\varepsilon(0),\, v^\varepsilon(0))^\mathsf{T} \,\|_{\Upsilon_\varepsilon} \;=\; \mathcal{O}(1).$$

*Then, there exist constants $C, \varepsilon_0, \alpha > 0$ such that for all $\varepsilon \in (0, \varepsilon_0)$ and all $t \in [0, \tau_{\text{fin}}/\varepsilon]$ there holds the estimate*

$$\Big\|(r^\varepsilon(t), v^\varepsilon(t))^\mathsf{T} - M^\varepsilon\Big(\widetilde{r},\, \widetilde{v},\, \widetilde{k},\, \widetilde{\omega}\Big)(t)\Big\|_{\Upsilon_\varepsilon} \leq C\varepsilon^\alpha.$$

A possible choice for $\Upsilon_\varepsilon$ is $\Upsilon_\varepsilon = \ell^2_\varepsilon \times \ell^2_\varepsilon$, where $\ell^2_\varepsilon$ is equipped with the norm

$$\|\, r \,\|_{\ell^2_\varepsilon} \;=\; \left(\varepsilon \sum_\alpha (r_\alpha)^2\right)^{1/2}.$$

We prove this conjecture in two cases. However, in none of these cases the assumption concerning $\mathcal{M}$ is satisfied. Instead, the Whitham equation is degenerate and explicitly solvable.

## 6.2 Justification in the linear case

In Section 5.1 we studied the case of the harmonic potential $\Phi : x \to \frac{\alpha^2}{2}x^2$ leading to the linear oscillator chain

$$\ddot{x}_\alpha = a^2(x_{\alpha+1} - 2x_\alpha + x_{\alpha-1}). \tag{6.2}$$

It is now convenient to write (6.2) in discrete conservation form. We define $R_\alpha = x_{\alpha+1} - x_\alpha, V_\alpha = \dot{x}_\alpha$, and obtain the system

$$\dot{R}_\alpha = V_{\alpha+1} - V_\alpha, \quad \dot{V}_\alpha = a^2(R_\alpha - R_{\alpha-1}). \tag{6.3}$$

The linear system is degenerate since the frequency $\omega$ depends on $k$ via the dispersion relation

$$\omega = \Omega(k) = 2a \sin \frac{k}{2}.$$

Moreover, the amplitude $\rho = \sqrt{\gamma}$ plays the role of the fifth independent variable. The Whitham equation takes the form

$$\frac{\partial}{\partial \tau}\begin{pmatrix} r \\ \partial_v L \\ k \\ \partial_\omega L \end{pmatrix} = \frac{\partial}{\partial y}\begin{pmatrix} v \\ -\partial_r L \\ \omega \\ -\partial_k L \end{pmatrix} \quad \text{and} \quad \partial_\rho L = 0$$

where $L(r, v, k, \omega, \rho) = \frac{1}{2}v^2 + \frac{\omega^2\rho^2}{4} - \frac{a^2}{2}r^2 - \frac{2a^2(1-\cos k)}{4}\rho^2$. More explicitly, after inserting $\omega = \Omega(k)$ this reads

$$\frac{\partial}{\partial \tau}\begin{pmatrix} r \\ v \\ k \\ \Omega(k)\rho^2 \end{pmatrix} = \frac{\partial}{\partial y}\begin{pmatrix} v \\ a^2 r \\ \Omega(k) \\ \Omega'(k)\Omega(k)\rho^2 \end{pmatrix}. \tag{6.4}$$

Note that the characteristic speeds of this system are $\lambda_{1,2} = \pm a$ (the macroscopic wave speeds) and $\lambda_{3,4} = \Omega'(k)$ since both, the wave number and local energy, are transported with the group velocity $\Omega'(k)$.

Associated with the scale parameter $\varepsilon > 0$ and a solution $(r, v, k, \rho)$ of (6.4) is the modulation ansatz:

$$\begin{pmatrix} R_\alpha \\ V_\alpha \end{pmatrix}(t) = M^\varepsilon(r, v, k, \rho)_\alpha(t) := \begin{pmatrix} r + \rho^{+1}\mathrm{e}^{\mathrm{i}\Theta^{+1}} - \rho \mathrm{e}^{\mathrm{i}\Theta/\varepsilon} \\ v + (\mathrm{i}\rho\Omega(k) + \varepsilon\frac{\partial \rho}{\partial \tau})\,\mathrm{e}^{\mathrm{i}\Theta/\varepsilon} \end{pmatrix},$$

where the functions $r, v, k$ and $\rho$ are evaluated at $(\tau, y) = (\varepsilon t, \varepsilon\alpha)$, where $\rho^{+1}$ and $\Theta^{+1}$ are evaluated at $(\varepsilon t, \varepsilon(\alpha{+}1))$. As above, the phase function $\Theta : [0, \tau_{\text{fin}}] \times \mathbb{R} \to \mathbb{R}$ is defined via $\Theta(0, 0)$ and $\partial_\tau\Theta = \Omega \circ k$ and $\partial_y\Theta = k$, where we use that the third component of (6.4) gives $\partial_\tau\partial_y\Theta = \partial_\tau k = \partial_y(\Omega \circ k) = \partial_y\partial_\tau\Theta$.

Our justification result now reads as follows

**Theorem 6.2** *Let $(r,v,k,\rho):[0,\tau_{\rm fin}]\to \mathrm{C}^3_{\rm b}(\mathbb{R})$ be a solution of (6.4) with $(r,v,\rho)\in \mathrm{C}^0([0,\tau_{\rm fin}],\mathrm{H}^4(\mathbb{R}))$. Then, there exists a constant $C>0$ such that for all $\varepsilon>0$ the solution $(R^\varepsilon,V^\varepsilon)\in \mathrm{C}^0([0,\tau_{\rm fin}/\varepsilon],\ell^2_\varepsilon\times\ell^2_\varepsilon)$ of (6.3) with initial condition $(R^\varepsilon(0),V^\varepsilon(0))=M^\varepsilon(r,v,k,\rho)(0)$ satisfies, for all $t\in[0,\tau_{\rm fin}/\varepsilon]$, the estimate*

$$\left\|(R^\varepsilon(t),V^\varepsilon(t))^{\mathsf{T}}-M^\varepsilon\left((r(\varepsilon t),v(\varepsilon t),k(\varepsilon t),v(\varepsilon t))\right)\right\|_{\ell^2_\varepsilon\times\ell^2_\varepsilon}\le Ct\varepsilon^2\le C\tau_{\rm fin}\varepsilon.$$

*Note that the solutions $(R^\varepsilon,V^\varepsilon)$ and $M^\varepsilon$ are of order 1 in $\ell^2_\varepsilon\times\ell^2_\varepsilon$.*

*Proof.* We establish the result in the standard way of justifications of modulation equations, cf. [KSM92, Sch98, Mie02, GM04, GM05]. Another proof using Wigner measures is provided in [Mie05]. We first insert the ansatz $M^\varepsilon$ into (6.3) and calculate the residuum "res". Then we estimate the error $(R^{\rm err},V^{\rm err})$ by the smallness of the residuum and by stability.

Since the problem at hand is linear we split the calculation of the residuum into two parts.

*(i) The macroscopic part:* Let $(r,v)$ be the solution of $\partial_\tau r=\partial_y v$ and $\partial_\tau v=a^2\partial_y r$ and $\begin{pmatrix}\hat R\\ \hat V\end{pmatrix}=M^\varepsilon_1(r,v)_\alpha(t):=\begin{pmatrix}r(\varepsilon t,\varepsilon\alpha)\\ v(\varepsilon t,\varepsilon\alpha)\end{pmatrix}$. Insertion into (6.3) yields

$$\begin{aligned}\mathrm{res}(M^\varepsilon_1(r,v))_\alpha&=\begin{pmatrix}\frac{\mathrm d}{\mathrm dt}\hat R_\alpha-\hat V_{\alpha+1}+\hat V_\alpha\\ \frac{\mathrm d}{\mathrm dt}\hat V_\alpha-a^2(\hat R_\alpha-R_{\alpha-1})\end{pmatrix}\\&=\begin{pmatrix}\varepsilon\partial_\tau r(\varepsilon t,\varepsilon\alpha)-\varepsilon\frac{1}{\varepsilon}[v(\varepsilon t,\varepsilon(\alpha+1))-v(\varepsilon t,\varepsilon\alpha)]\\ \varepsilon\partial_\tau v(\varepsilon t,\varepsilon\alpha)-\varepsilon\frac{a^2}{\varepsilon}[r(\varepsilon t,\varepsilon\alpha)-r(\varepsilon t,\varepsilon(\alpha-1))]\end{pmatrix}\\&=\varepsilon\begin{pmatrix}\partial_y v(\varepsilon t,\varepsilon\alpha)-\frac{1}{\varepsilon}[v(\varepsilon t,\varepsilon(\alpha+1))-v(\varepsilon t,\varepsilon\alpha)]\\ a^2(\partial_y r(\varepsilon t,\varepsilon\alpha)-\frac{1}{\varepsilon}[r(\varepsilon t,\varepsilon\alpha)-r(\varepsilon t,\varepsilon(\alpha-1))]\end{pmatrix},\end{aligned}$$

where we have used that $(r,v)$ satisfies (6.4). Using $(r,v)\in\mathrm{C}^2(\mathbb{R})$ we obtain

$$\mathrm{res}(M^\varepsilon_1(r,v))_\alpha=\mathcal{O}(\varepsilon^2)$$

and employing Prop. 3.3 in [GM04] gives

$$\|\,\mathrm{res}(M^\varepsilon_1(r,v))\|_{\ell^2_\varepsilon\times\ell^2_\varepsilon}\le C\varepsilon^2\|(r,v)\|_{\mathrm{H}^3(\mathbb{R})}.$$

*(ii) The microscopic oscillations:* We insert

$$\begin{pmatrix}\tilde R_\alpha\\ \tilde V_\alpha\end{pmatrix}=M^\varepsilon_2(k,\rho)_\alpha:=\begin{pmatrix}\rho^{+1}\mathrm{e}^{\mathrm{i}\Theta^{+1}/\varepsilon}-\rho\,\mathrm{e}^{\mathrm{i}\Theta/\varepsilon}\\ [\mathrm{i}\Omega\rho+\varepsilon\partial_\tau\rho]\mathrm{e}^{\mathrm{i}\Theta/\varepsilon}\end{pmatrix}$$

into (6.3) and obtain $\mathrm{res}(M^\varepsilon_2(k,\rho))_\alpha=(0,\frac{\mathrm d}{\mathrm dt}\tilde V_\alpha-a^2(\tilde R_\alpha-\tilde R_{\alpha-1}))^{\mathsf{T}}$ with $\frac{\mathrm d}{\mathrm dt}\tilde V_\alpha=[-\Omega^2\rho+\mathrm{i}\varepsilon(\partial_\tau(\Omega\rho)+\Omega\partial_\tau\rho)+\varepsilon^2\partial_\tau^2\rho]\mathrm{e}^{\mathrm{i}\Theta/\varepsilon}$ and

$$\begin{aligned}\tilde R_\alpha-\tilde R_{\alpha-1}&=\rho\left[\mathrm{e}^{\mathrm{i}\Theta^{+1}/\varepsilon}-2\mathrm{e}^{\mathrm{i}\Theta/\varepsilon}+\mathrm{e}^{\mathrm{i}\Theta^{-1}/\varepsilon}\right]+\left(\rho^{+1}-\rho\right)\mathrm{e}^{\mathrm{i}\Theta^{+}/\varepsilon}+\left(\rho^{-1}-\rho\right)\mathrm{e}^{\mathrm{i}\Theta^{-1}/\varepsilon}\\&=\rho(2\cos k-2)\mathrm{e}^{\mathrm{i}\Theta/\varepsilon}+\mathrm{i}\varepsilon[\rho\partial_y k\cos k+\partial_y\rho 2\sin k]\mathrm{e}^{\mathrm{i}\Theta/\varepsilon}+\mathcal{O}(\varepsilon^2).\end{aligned}$$

The fourth component of (6.4) reads $\partial_\tau(\Omega\rho^2) = \partial_y(\Omega\Omega'\rho^2)$ and thus provides

$$\partial_\tau(\Omega\rho) + \Omega\partial_\tau\rho = \partial_y(\Omega\Omega')\rho + 2\Omega\Omega'\partial_y\rho = a^2(\rho\partial_y k\cos k + 2\partial_y\rho\sin k).$$

From this we obtain $\mathrm{res}(M_2^\varepsilon((k,\rho)))_\alpha = \mathcal{O}(\varepsilon^2)$ and conclude as above

$$\|\mathrm{res}\,(M_2^\varepsilon((k,\rho)))\|_{\ell^2_\varepsilon\times\ell^2_\varepsilon} \leq C\varepsilon^2\left(1 + \|k\|_{\mathrm{C}^3(\mathbb{R})}\right)\|\rho\|_{\mathrm{H}^3(\mathbb{R})}.$$

To control the error

$$\begin{pmatrix} R^{\mathrm{err}}(t) \\ V^{\mathrm{err}}(t)\end{pmatrix} = \begin{pmatrix} R^\varepsilon(t) \\ V^\varepsilon(t)\end{pmatrix} - M^\varepsilon((r,v,k,\rho))(t)$$

we use that it satisfies the linear problem (6.3) with initial data equal to 0, but with the residuum as an inhomogeneity:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} R^{\mathrm{err}}_\alpha \\ V^{\mathrm{err}}_\alpha\end{pmatrix} = \begin{pmatrix} V^{\mathrm{err}}_{\alpha+1} - V^{\mathrm{err}}_\alpha \\ a^2(R^{\mathrm{err}}_\alpha - R^{\mathrm{err}}_{\alpha-1})\end{pmatrix} + \mathrm{res}\,(M_1^\varepsilon + M_2^\varepsilon) \text{ and } \begin{pmatrix} R^{\mathrm{err}}(0) \\ V^{\mathrm{err}}(0)\end{pmatrix} = \begin{pmatrix} 0 \\ 0\end{pmatrix}.$$

The energy norm provides a simple error control. Defining

$$e(t) := \varepsilon\sum_{\alpha\in\mathbb{Z}}\left(\frac{1}{2}\left(V^{\mathrm{err}}_\alpha(t)\right)^2 + \frac{a^2}{2}\left(R^{\mathrm{err}}_\alpha(t)\right)^2\right)$$

we find $e(0) = 0$ and

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}e(t) &= \varepsilon\sum_{\alpha\in\mathbb{Z}} V^{\mathrm{err}}_\alpha\left(a^2\left(R^{\mathrm{err}}_\alpha - R^{\mathrm{err}}_{\alpha-1}\right) + \mathrm{Res}^V_\alpha\right) + a^2 R^{\mathrm{err}}_\alpha\left(V^{\mathrm{err}}_{\alpha+1} - V^{\mathrm{err}}_\alpha + \mathrm{Res}^R_\alpha\right) \\ &= \varepsilon\sum_{\alpha\in\mathbb{Z}} V^{\mathrm{err}}_\alpha\mathrm{Res}^V_\alpha + a^2 R^{\mathrm{err}}_\alpha\mathrm{Res}^R_\alpha \;\leq\; C_a\sqrt{2e(t)}\,\|\mathrm{res}\,(M_1^\varepsilon + M_2^\varepsilon)\|_{\ell^2_\varepsilon\times\ell^2_\varepsilon}\end{aligned}$$

with $C_a = \max\{1, a\}$. Together with $\|\,\mathrm{res}(M_1^\varepsilon + M_2^\varepsilon)\|_{\ell^2\_\varepsilon\times\ell^2_\varepsilon} \leq C_{\mathrm{res}}\varepsilon^2$ this yields

$$\left\|(R^{\mathrm{err}}(t), V^{\mathrm{err}}(t))^{\mathsf{T}}\right\|_{\ell^2_\varepsilon\times\ell^2_\varepsilon} \leq C_a\sqrt{2e(t)} \leq C_a^2 C_{\mathrm{res}}\varepsilon^2 t,$$

which is the desired result. □

## 6.3 Justification for the hard sphere model

The hard sphere model, which was introduced in Section 5.2, will here be used to establish a rigorous justification of the micro-macro transition. For simplicity we set $r_{\min} = 0$, so that $\Phi(d) = +\infty$ for $d < 0$ and $\Phi(d) = 0$ for $d > 0$. As in the linear case the microscopic discrete model as well as the associated Whitham equation are explicitly solvable. This fact enables us to compare solutions of the microscopic model with corresponding solutions of the modulation equations. To this end we pass from the Lagrange representation to the Euler representation of thermodynamics. Recall that in the Lagrange representation time $t$ and particle index $\alpha$ are the independent variables, where in the Euler representation the motion is studied in the plane spanned by time $t$ and physical space (position) $x$. Correspondingly, in the macroscopic Lagrange representation all fields depend on $\tau$ and $y$, where in the macroscopic Euler representation they depend on $\tau$ and $\xi$.

**Microscopic dynamics in the Euler representation**

The microscopic dynamics can be characterized very simple (cf. Figure 2), if only two particle collisions are involved.

1. Since we set $r_0 = 0$, all atomic distances are nonnegative. As long as $r_{\alpha-1}$ and $r_\alpha$ are positive, the atom $\alpha$ moves along a free flight trajectory.

2. If the distance $r_\alpha$ vanishes at a certain time $t$, the particles $\alpha$ and $\alpha + 1$ interact by an elastic collision, i.e. both particles will exchange their velocities. In particular, the particle $\alpha + 1$ moves after the collision on the free flight trajectory, which was occupied before the collision by the particle $\alpha$ and vice versa.

3. All free flight trajectories are uniquely determined by the initial positions and velocities. Any particle moves along a zig-zag curve on the pattern which is generated by all free flight trajectories.

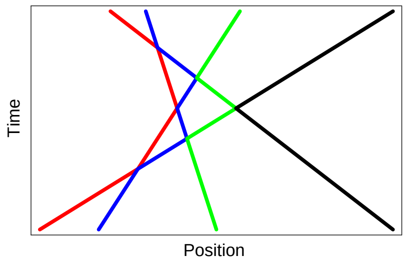


Figure 2: Schematic representation of the microscopic dynamics in the Euler representation. Any particle moves along a zig-zag curve on the free flight trajectories of phonons.

In the sequel we refer to the free flight trajectories as *phonons*, and we label them by the index $\beta$. At $\tau = 0$, any particle $\alpha$ defines uniquely a phonon $\beta$, whose motion is given by $t \mapsto x_\alpha(0) + t\, v_\alpha(0)$. Any solution of the microscopic dynamics associates to any phonon $\beta$ a function $t \mapsto \alpha_\beta(t)$, so that $\alpha_\beta(t)$ gives the index of the atom, which moves at time $t$ on the free flight trajectory of phonon $\beta$. Recall that for all $\beta$ the integer $\alpha_\beta(t)$ is well defined for almost all times $t$. Since we are free to choose the initial labeling of phonons arbitrarily, we set $\alpha_\beta(0) = \beta$.

The atomic interactions take place at the intersection points of free flight trajectories and can be described as follows. Let $\beta_1$ and $\beta_2$ be two phonons, whose free flight trajectories intersect at a certain time $t$. Moreover, let $t{-}0$ and $t{+}0$ denote two times immediately *before* and *after* the collision, respectively. Before the collision there holds either $\alpha_{\beta_1}(t-0) = \alpha_{\beta_2}(t-0) - 1$ or $\alpha_{\beta_1}(t-0) = \alpha_{\beta_2}(t-0) + 1$, depending on whether $\beta_2$ is faster or slower than $\beta_1$. After the collision there holds $\alpha_{\beta_1}(t+0) = \alpha_{\beta_2}(t-0)$ and $\alpha_{\beta_2}(t+0) = \alpha_{\beta_1}(t-0)$. The atomic collision is thus equivalent to an increment/decrement of $\alpha_{\beta_1}$ and $\alpha_{\beta_2}$. The reformulation of the microscopic dynamics in terms of phonons has the advantage, that we can compute both time and spatial positions of the atomic interactions directly from the initial data. For fixed phonons $\beta_1$ and $\beta_2$, the *collision time* $t_{\mathrm{coll}}(\beta_1,\,\beta_2)$ and the *collision position* $x_{\mathrm{coll}}(\beta_1,\,\beta_2)$ are given by

$$t_{\mathrm{coll}}(\beta_1,\,\beta_2) \;=\; -\frac{x_{\beta_2}(0)-x_{\beta_1}(0)}{v_{\beta_2}(0)-v_{\beta_1}(0)}, \tag{6.5}$$

$$x_{\mathrm{coll}}(\beta_1,\,\beta_2) \;=\; x_{\beta_i}+t_{\mathrm{coll}}(\beta_1,\,\beta_2)\,v_{\beta_i}(0), \quad i=1,\,2. \tag{6.6}$$

Note that the collision time can take negative values or even indefinite values.

### Traveling waves in the Euler representation

Recall from Section 5.2, that the family of traveling velocity waves for the hard sphere model reads

$$\mathbb{V}(r,\,k;\,\varphi) \;=\; \begin{cases} -\dfrac{r}{k} & \text{falls} \quad 0\le\varphi<k,\\ +\dfrac{r}{1-k} & \text{falls} \quad k\le\varphi<1. \end{cases} \tag{6.7}$$

Now we characterize the structure of these traveling waves in the Euler representation, see figure 3. According to (6.7) and (2.3), in any traveling wave there appear only two velocities $v_1$ and $v_2$. Assuming $v_1>v_2$ we find

$$v_1 \;=\; v+r\frac{\omega}{1-k}, \qquad v_2 \;=\; v-r\frac{\omega}{k}. \tag{6.8}$$

Consequently, the phonons split into two families, namely a *faster* one and a *slower* one, where faster and slower phonons move with $v_2$ and $v_1$, respectively. Moreover, all phonons of the same family move on parallel and equidistant straight lines. We denote the constant spatial distance between adjacent faster and slower phonons by $r_1$ and $r_2$, respectively.

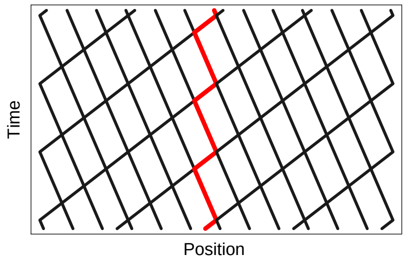


Figure 3: Schematic representation of a traveling wave in the microscopic Euler representation with periodic boundary conditions.

The distances $r_1$ and $r_2$ are related to the generic traveling wave parameters $r$, $v$, $k$, and $\omega$ via

$$r_1 \;=\; \frac{r}{1-k}, \qquad r_2 \;=\; \frac{r}{k}. \tag{6.9}$$

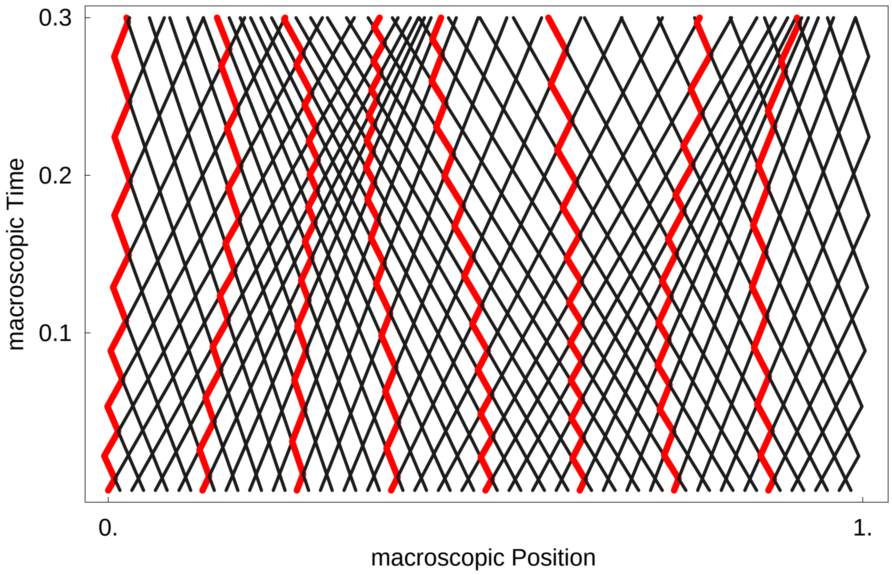


Figure 4: The microscopic dynamics in the macroscopic Euler representation for $N = 64$. The trajectories of eight selected particles are drawn with red color.

For later purposes we define

$$\varrho_i \;:=\; \frac{1}{r_i}, \quad \varrho \;:=\; \varrho_1 + \varrho_2. \tag{6.10}$$

The quantities $\varrho_1$, $\varrho_2$ can be interpreted as partial phonon densities, and their sum is the particle density $\varrho$. Any traveling wave can be characterized by $(\varrho_1, v_1, \varrho_2, v_2)$, because (6.8), (6.9), and (6.10) imply

$$r = \frac{1}{\varrho_1 + \varrho_2}, \; v = \frac{\varrho_1 v_1 + \varrho_2 v_2}{\varrho_1 + \varrho_2}, \; k = \frac{\varrho_2}{\varrho_1 + \varrho_2}, \; \omega = \frac{\varrho_1 \varrho_2 (v_1 - v_2)}{\varrho_1 + \varrho_2}. \tag{6.11}$$

### Example for the microscopic dynamics

For an illustration of the microscopic dynamics we present a numerical simulations. We consider finite particle numbers $N < \infty$ and impose periodic boundary conditions, i.e. we assume

$$r_\alpha(0) \;=\; r_{\alpha+N}(0), \quad v_\alpha(0) = v_{\alpha+N}(0) \qquad \forall \;\; \alpha. \tag{6.12}$$

For given $N$, the atomic positions and velocities are initialized by

$$x_\alpha(0) = \alpha, \quad v_\alpha(0) = \begin{cases} v_1^0(\varepsilon\alpha) & \text{if } \alpha \text{ is even,} \\ v_2^0(\varepsilon\alpha) & \text{if } \alpha \text{ is odd} \end{cases} \tag{6.13}$$

where $\alpha = 1...N$, and $v_1^0(y) = 1. + 0.2\cos(4\pi y)$, $v_2^0(y) = -1. + 0.3\sin(2\pi y)$. Figure 4 shows for $N = 64$ the exact solution in the macroscopic Euler representation. We

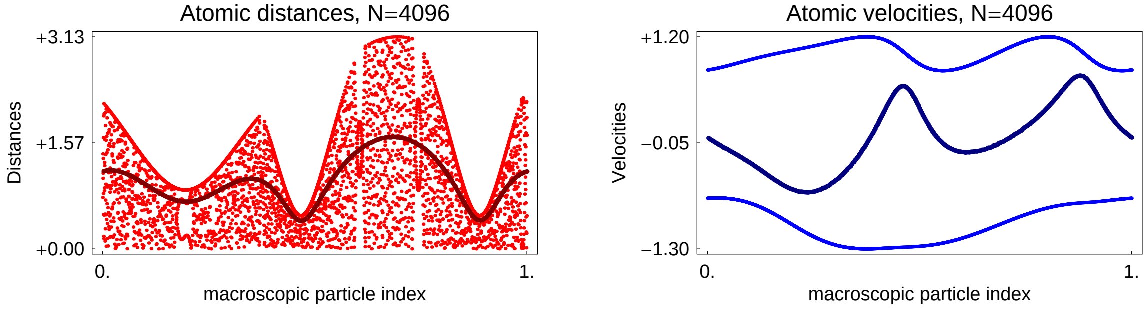


Figure 5: The microscopic dynamics in the macroscopic Lagrange representation for $N = 4096$ The atomic distances and velocities are depicted against $y$, for fixed $\tau = 0.3$. The dark colored macroscopic functions represent the macroscopic mean values, whose dynamics is governed by the modulation system.

can distinguish two families of phonons, a left going one and a right going one. All phonon trajectories of the same family are locally almost parallel. Furthermore, since the macroscopic time interval is sufficiently small, the phonon trajectories of the same family do not intersect.

For any macroscopic point $(t, x)$ there is a vicinity in space time and a traveling wave, such that the atomic motion within this vicinity can be approximated by the traveling wave data, at least for large $N$. This claim is right, because the atomic velocities are locally jumping between two (almost constant) values. It is easy to construct microscopic initial data, so that locally more than two velocities are involved. In this case we cannot expect the modulation theory to be valid. Similarly, modulation theory will fail in our example, if the macroscopic time interval is so large, that free flight trajectories of the same family intersect.

In Figure 5 we have depicted the atomic data for $\tau = 0.3$ and $N = 4096$ against the macroscopic particle index $y$. Here, the dark colored lines represent the local mean values of the highly oscillating data. Again we observe that there are locally only two velocities. For this reason we expect that the macroscopic evolution of the local mean values is governed by the modulation system (5.7).

### The modulations equations in the Euler representation

Within this subsection we study the modulation equations in the macroscopic Euler representation, which we introduce in the usual way by passing from time and particle index to time and space. The change of variables will allow us to prove the justification result.

In order to distinguish strictly between the different settings we use "$\tilde{}$" and "$\hat{}$" to denote fields in the Lagrange- and the Euler representation, respectively. With this notation the modulation system (4.20) reads

$$\frac{\partial}{\partial\tau}\begin{pmatrix}\widetilde{r}\\ \widetilde{v}\\ \widetilde{k}\\ \widetilde{S}\end{pmatrix}+\frac{\partial}{\partial y}\begin{pmatrix}-\widetilde{v}\\ +\widetilde{p}\\ -\widetilde{\omega}\\ +\widetilde{g}\end{pmatrix} \;=\; 0, \tag{6.14}$$

where $\widetilde{S} = S\Big(\widetilde{r},\,\widetilde{k},\,\widetilde{\omega}\Big)$, $\widetilde{p} = p\Big(\widetilde{r},\,\widetilde{k},\,\widetilde{\omega}\Big)$ and $\widetilde{q} = g\Big(\widetilde{r},\,\widetilde{k},\,\widetilde{\omega}\Big)$. According to the Equation of State (5.5), there hold

$$S(r,\,k,\,\omega)=\frac{r^2\omega}{k(1-k)},\quad p\,(r,\,k,\,\omega)=\frac{r\,\omega^2}{k(1-k)},\quad g(r,\,k,\,\omega)=\frac{r^2\omega^2\,(2k-1)}{2k^2(1-k)^2}.$$

Since these identities are satisfied both in the Lagrange- and Euler representation, neither "~nor "^ïs used.

The macroscopic mass balance defines the macroscopic Euler coordinate $z$ as follows. We interpret the first equation in (6.14) as an integrability condition and introduce a field $\widetilde{z}$ by

$$\frac{\partial\,\widetilde{z}}{\partial\,\tau} \;=\; \widetilde{v},\quad \frac{\partial\,\widetilde{z}}{\partial\,y} \;=\; \widetilde{r}=\frac{1}{\widetilde{\varrho}} \tag{6.15}$$

and $\widetilde{z}(0,\,0)=0$ Under the change of coordinates $(\tau,\,y)\to(\tau,\,z)$ any field $\widetilde{u}$ transforms into a field $\widehat{u}$ with

$$\widetilde{u}(\tau,\,y) \;=\; \widehat{u}(\tau,\,\widetilde{z}(\tau,\,y)). \tag{6.16}$$

Consequently, the modulation equations (6.14) can be written as

$$\frac{\partial}{\partial\tau}\begin{pmatrix}\widehat{\varrho}\\ \widehat{\varrho}\,\widehat{v}\\ \widehat{\varrho}\,\widehat{k}\\ \widehat{\varrho}\,\widehat{S}\end{pmatrix}+\frac{\partial}{\partial z}\begin{pmatrix}\widehat{\varrho}\,\widehat{v}\\ \widehat{\varrho}\,\widehat{v}^2+\widehat{p}\\ \widehat{\varrho}\,\widehat{k}\,\widehat{v}-\widehat{\omega}\\ \widehat{\varrho}\,\widehat{S}\,\widehat{v}+\widehat{g}\end{pmatrix} \;=\; 0. \tag{6.17}$$

Note that the fields $\widehat{\varrho}\,\widehat{v}$, $\widehat{\varrho}$, $\widehat{k}$, $\widehat{\varrho}$, and $\widehat{S}$ are the volume densities of momentum, wave number and entropy. Similarly as in the previous subsections we use the formulas (6.8)-(6.10) in order to define the fields $\widehat{v}_1$, $\widehat{v}_2$, $\widehat{\varrho}_1$ and $\widehat{\varrho}_2$, which now depend on the variables $(\tau,\,z)$. From (6.17) we can easily derive the equivalent system

$$\frac{\partial}{\partial\tau}\begin{pmatrix}\widehat{\varrho}_1\\ \widehat{v}_1\\ \widehat{\varrho}_2\\ \widehat{v}_2\end{pmatrix}+\frac{\partial}{\partial z}\begin{pmatrix}\widehat{\varrho}_1\,\widehat{v}_1\\ \frac{1}{2}\widehat{v}_1^2\\ \widehat{\varrho}_2\,\widehat{v}_2\\ \frac{1}{2}\widehat{v}_2^2\end{pmatrix} \;=\; 0. \tag{6.18}$$

Furthermore, we state

1. The inverse transform to (6.15) is given by

$$\frac{\partial\,\widehat{y}}{\partial\,z} = \widehat{\varrho}, \quad \frac{\partial\,\widehat{y}}{\partial\,\tau} = -\widehat{\varrho}\,\widehat{v}, \tag{6.19}$$

   with $\widehat{y}(0,\,0) = 0$, where $\widehat{\varrho} = 1/\widehat{r}$ is the mass density.

2. The systems (6.14) and (6.17)/(6.18) are equivalent, as long as all fields are smooth.

3. The quantity $z$ is the macroscopic Euler-coordinate, which up to now was abbreviated by $\xi$. We have changed the notation in order to indicate that here the macroscopic Euler-coordinate results from the mass balance in (6.14) and not by scaling of atomic positions.

For later purposes we introduce two fields $\widehat{B}_1$ and $\widehat{B}_2$ by

$$\frac{\partial\,\widehat{B}_j}{\partial\,\tau}(\tau,\,z) \;=\; -(\widehat{\varrho}_j\,\widehat{v}_j)(\tau,\,z), \qquad \frac{\partial\,\widehat{B}_j}{\partial\,z}(\tau,\,z) \;=\; +\widehat{\varrho}_j(\tau,\,z), \tag{6.20}$$

and $\widehat{B}_j(0,\,0) = 0$. We mention that the sum $\widehat{B}_1+\widehat{B}_2$ gives the macroscopic Lagrange coordinate $\widehat{y}$, i.e. $\widehat{B}_1 + \widehat{B}_2 = \widehat{y}$.

Our next task is the characterization of solutions of (6.18) in more detail. At first we observe that any solution of (6.18) is determined by the two Burgers equations

$$\frac{\partial\,\widehat{v}_j}{\partial\,\tau} + \frac{1}{2}\frac{\partial\left(\widehat{v}_j^2\right)}{\partial\,z} \;=\; 0, \quad j = 1,\,2, \tag{6.21}$$

which can be solved explicitly. In particular, for sufficiently small times $\tau$ any solution of (6.21) is given by $\widehat{v}_j(\tau,\,z) = \widehat{v}_j(0,\,\widehat{\eta}_j(\tau,\,z))$, where $\widehat{\eta}_j(\tau,\,z)$ gives the initial position of the characteristic, which crosses at time $\tau$ the position $z$. This means $\widehat{\eta}_j(\tau,\,z) + \tau\,\widehat{v}_j(0,\,\widehat{\eta}_j(\tau,\,z)) = z$, $i = 1,\,2$. The two equations in (6.21) can be solved uniquely for $\tau \in [0,\,\tau_{\mathrm{fin}}]$, as long as $\tau_{\mathrm{fin}}$ satisfies

$$1 + \tau_{\mathrm{fin}}\,\min\Big\{\inf_z \frac{\partial\,\widehat{v}_1}{\partial\,z}(0,\,z),\ \inf_z \frac{\partial\,\widehat{v}_2}{\partial\,z}(0,\,z)\Big\} > 0, \tag{6.22}$$

because this condition guaranties that (for fixed $\tau\in[0,\,\tau_{\mathrm{fin}}]$ and $z$) the functions $\eta \to \eta+\tau\widehat{v}_i(0,\,\eta)$, $i = 1,\,2$, are strictly monotone. The next Lemma summarizes important properties of solutions of (6.18), which become important in our justification result.

**Lemma 6.3**

1. *The fields $\widehat{\eta}_1$ and $\widehat{\eta}_2$ satisfy*

$$\frac{\partial\,\widehat{\eta}_j}{\partial\,\tau}(\tau,\,z) = \frac{-\widehat{v}_j(0,\,\widehat{\eta}_j(\tau,\,z))}{1+\tau\,\dfrac{\partial\,\widehat{v}_j}{\partial\,z}(0,\,\widehat{\eta}_j(\tau,\,z))}, \qquad \frac{\partial\,\widehat{\eta}_j}{\partial\,z}(\tau,\,z) = \frac{1}{1+\tau\,\dfrac{\partial\,\widehat{v}_j}{\partial\,z}(0,\,\widehat{\eta}_j(\tau,\,z))}.$$

*2. For all times* $\tau \in [0,\, \tau_{\rm fin}]$*, with* $\tau_{\rm fin}$ *satisfying* (6.22)*, we find*

$$\widehat{v}_j(\tau,\, z) = \widehat{v}_j(0,\, \widehat{\eta}_j(\tau,\, z)), \tag{6.23}$$

$$\widehat{\varrho}_j(\tau,\, z) = \frac{\widehat{\varrho}_j(0,\, \widehat{\eta}_j(\tau,\, z))}{1 + \tau \dfrac{\partial\,\widehat{v}_j}{\partial\, z}(0,\, \widehat{\eta}_j(\tau,\, z))}, \tag{6.24}$$

$$\widehat{B}_j(\tau,\, z) = \widehat{B}_j(0,\, \widehat{\eta}_j(\tau,\, z)). \tag{6.25}$$

For shortness we omit the proof of this Lemma, because all assertions follow from straight forward calculations. For the details we refer to [Her04].

For the sake of simplicity we will restrict the following considerations to a special class of solutions of (6.18).

**Assumption 6.4** *In what follows we assume:*

1. *Let* $\widehat{\varrho}_1$*,* $\widehat{\varrho}_2$*,* $\widehat{v}_1$ *and* $\widehat{v}_1$ *be a smooth solution (at least* $C^2$*) of* (6.18) *with the following properties*
   - *(a) All fields are periodic in* $z$ *with period* $\overline{L}$*.*
   - *(b) All fields are defined for macroscopic times* $\tau$ *with* $0 \le \tau \le \tau_{\rm fin}$*, where* $\tau_{\rm fin}$ *is acceptable in the sense of* (6.22)*.*
   - *(c) The fields* $\widehat{\varrho}$*,* $\widehat{r}$*,* $\widehat{r}_j$*,* $\widehat{k}$*,* $\widehat{\omega}$*,* $\widehat{B}_1$ *and* $\widehat{B}_2$ *are defined by* (6.10)*–*(6.11) *and* (6.20)*.*
   - *(d) There is a constant* $\delta > 0$*, so that the fields* $\widehat{v}_1$*,* $\widehat{v}_2$*,* $\widehat{\varrho}$*,* $\widehat{\varrho}_1$*,* $\widehat{\varrho}_2$*,* $\widehat{r}$*,* $\widehat{r}_1$*,* $\widehat{r}_2$*,* $\widehat{\omega}$*,* $\widehat{k}$*,* $1 - \widehat{k}$ *are all pointwise larger than* $2\delta$*.*
2. *Any Euler-field* $\widehat{u}$ *transforms according to* (6.16) *into a corresponding Lagrange-field* $\widetilde{u}$*. The fields* $\widetilde{r}$*,* $\widetilde{v}$*,* $\widetilde{k}$ *and* $\widetilde{\omega}$ *are thus a smooth solution of* (6.14)*.*
3. *There exist two smooth functions* $W_1$ *and* $W_2$*, defined on the hole real axis, so that*

$$\widehat{v}_j(0,\, z) = W_j\Big(\widehat{B}_j(0,\, z)\Big), \quad j = 1,\, 2. \tag{6.26}$$

### Modulated traveling waves in the Euler representation

We now insert this smooth solutions of (6.14) into the modulation ansatz (6.1) and study the resulting modulated traveling wave. We denote by $r_\alpha^{\rm TW}(t)$ and $v_\alpha^{\rm TW}(t)$ the atomic distances and velocities, respectively.

Our aim is to prove, that $r_\alpha^{\rm TW}(t)$ and $v_\alpha^{\rm TW}(t)$ indeed approximate an exact solution of the microscopic dynamics. For this, we will estimate the difference between the modulated traveling wave and a suitable exact solution.

To be consistent with the macroscopic assumptions 6.4, we consider finite particle numbers $N < \infty$ and impose periodic boundary conditions for the microscopic system, see (6.12), and recall $\varepsilon = 1/N$.

**Lemma 6.5** *There holds*

$$v_\alpha^{\mathrm{TW}}(t) \;=\; \mathbb{W}\Big(\big(\widetilde{B}_1,\, \widetilde{B}_2,\, \widetilde{k}\big)(\varepsilon t,\, \varepsilon\alpha);\, \frac{1}{\varepsilon}\widetilde{B}_2(\varepsilon t,\, \varepsilon\tau)\Big), \tag{6.27}$$

*with*

$$\mathbb{W}(B_1,\, B_2,\, k;\, \varphi) \;=\; \begin{cases} W_2(B_2) & \textit{if} \;\; 0 \le \varphi < k \mod 1, \\ W_1(B_1) & \textit{if} \;\; 1-k \le \varphi < 1 \mod 1. \end{cases}$$

*In particular, $\widetilde{B}_2$ gives the phase, i.e.*

$$\widetilde{\omega}(\tau,\, y) \;=\; \frac{\partial\, \widetilde{B}_2}{\partial\, \tau}(\tau,\, y), \quad \widetilde{k}(\tau,\, y) \;=\; \frac{\partial\, \widetilde{B}_2}{\partial\, y}(\tau,\, y). \tag{6.28}$$

*Sketch of the proof.* We transform the ansatz (4.2) into the Euler representation. Hereafter we can verify the equations (6.28) by straight forward calculations. Next we define

$$\widehat{\mathbb{V}}(\tau,\, z;\, \varphi) \;=\; \mathbb{V}\Big(\widehat{r}(\tau,\, z),\, \widehat{k}(\tau,\, z);\, \varphi\Big),$$

where $\mathbb{V}$ is given by (6.7). From (4.1) we obtain

$$\begin{aligned} v_\alpha^{\mathrm{TW}}(t) \;&=\; \widetilde{v}(\varepsilon t,\, \varepsilon\alpha) + \mathbb{V}\Big(\widetilde{r}(\varepsilon t,\, \varepsilon\alpha),\, \widetilde{k}(\varepsilon t,\, \varepsilon\alpha);\, \frac{1}{\varepsilon}\widetilde{B}_2(\varepsilon t,\, \varepsilon\alpha)\Big) \\ &=\; \widehat{v}(\varepsilon t,\, \widetilde{z}(\varepsilon t,\, \varepsilon\alpha)) + \widehat{\mathbb{V}}\Big(\varepsilon t,\, \widetilde{z}(\varepsilon t,\, \varepsilon\alpha);\, \frac{1}{\varepsilon}\widehat{B}_2(\varepsilon t,\, \widetilde{z}(\varepsilon t,\, \varepsilon\alpha))\Big), \end{aligned}$$

which finally implies (6.27). □

Similarly, we can derive explicit expressions for the atomic distances in a modulated traveling wave. There holds

$$\begin{aligned} r_\alpha^{\mathrm{TW}}(t) \;&=\; \mathbb{Z}_1\Big(\big(\widetilde{r}_1,\, \widetilde{r}_2,\, \widetilde{k}\big)(\varepsilon t,\, \varepsilon\alpha);\, \frac{1}{\varepsilon}\widetilde{B}_2(\varepsilon t,\, \varepsilon\alpha)\Big) \\ &\quad + \mathbb{Z}_2\Big(\big(\widetilde{r}_1,\, \widetilde{r}_2,\, \widetilde{k}\big)(\varepsilon t,\, \varepsilon\alpha);\, \frac{1}{\varepsilon}\widetilde{B}_2(\varepsilon t,\, \varepsilon\alpha)\Big), \end{aligned}$$

where the 1-periodic functions $\mathbb{Z}_j(r_1,\, r_2,\, k;\, \cdot)$ are given by

$$\begin{aligned} \mathbb{Z}_1(r_1,\, r_2,\, k;\, \varphi) \;&=\; \begin{cases} +r_1\varphi & \text{for} \;\; 0 \le \varphi \le 1-k, \\ -r_2(\varphi - 1 + k) & \text{for} \;\; 1-k \le \varphi \le 1, \end{cases} \\ \mathbb{Z}_2(r_1,\, r_2,\, k;\, \varphi) \;&=\; \begin{cases} +r_2\varphi & \text{for} \;\; 0 \le \varphi \le k, \\ -r_1(\varphi - k) & \text{for} \;\; k \le \varphi \le 1. \end{cases} \end{aligned}$$

The main idea for the justification result is to use the profile functions $\mathbb{W}$ from Lemma 6.5 for the construction of exact solutions of the microscopic system. To this end we define

$$\widetilde{k}^{\,\mathrm{ex}}(\tau,\,y) \;:=\; \frac{1}{\varepsilon}\Big(\widetilde{B}_2(\tau,\,y)-\widetilde{B}_2(\tau,\,y-\varepsilon)\Big) \tag{6.29}$$

and

$$\widetilde{B}_2^{\mathrm{ex}}(\tau,\,y) \;:=\; \varepsilon\,\mathrm{floor}\left(\frac{1}{\varepsilon}\widetilde{B}_2(\tau,\,y)\right), \tag{6.30}$$

$$\widetilde{B}_1^{\mathrm{ex}}(\tau,\,y) \;:=\; \varepsilon\,\mathrm{ceil}\left(\frac{1}{\varepsilon}\widetilde{B}_1(\tau,\,y)+\widetilde{k}^{\,\mathrm{ex}}(\tau,\,y)\right). \tag{6.31}$$

Here, $\mathrm{floor}\,(b)$ and $\mathrm{ceil}\,(b)$ denote integer parts of the real number $b$, and satisfy $0\le b-\mathrm{floor}\,(b)<1$ and $0\le\mathrm{ceil}\,(b)-b<1$, respectively. Obviously we have

$$\widetilde{k}^{\,\mathrm{ex}}(\tau,\,y) \;=\; \widetilde{k}(\tau,\,y)+\mathcal{O}(\varepsilon), \tag{6.32}$$

$$\widetilde{B}_j^{\mathrm{ex}}(\tau,\,y) \;=\; \widetilde{B}_j(\tau,\,y)+\mathcal{O}(\varepsilon). \tag{6.33}$$

In the next step we define velocities $v_\alpha^{\mathrm{ex}}(t)$ by

$$v_\alpha^{\mathrm{ex}}(t) \;:=\; \mathbb{W}\bigg(\Big(\widetilde{B}_1^{\mathrm{ex}},\,\widetilde{B}_2^{\mathrm{ex}},\,\widetilde{k}^{\,\mathrm{ex}}\Big)(\varepsilon t,\,\varepsilon\alpha);\,\frac{1}{\varepsilon}\widetilde{B}_2(\varepsilon t,\,\varepsilon\alpha)\bigg), \tag{6.34}$$

Note that we did *not* replace the term $\widetilde{B}_2$ in the phase variable. The main step is now to prove, that (6.34) in fact defines an exact solution of the microscopic problem.

**Theorem 6.6** *The functions $v_\alpha^{\mathrm{ex}}(t)$ determine uniquely an exact solution of the microscopic problem. In particular, there exist functions $r_\alpha^{\mathrm{ex}}(t)$ with*

$$\frac{\mathrm{d}}{\mathrm{d}t}r_\alpha^{\mathrm{ex}}(t) \;:=\; v_{\alpha+1}^{\mathrm{ex}}(t)-v_\alpha^{\mathrm{ex}}(t). \tag{6.35}$$

*Moreover, the distances $r_\alpha^{\mathrm{TW}}$ and $r_\alpha^{\mathrm{ex}}$ are "in phase", i.e. for all $t$ and all $\alpha$ there holds $r_\alpha^{\mathrm{TW}}(t)=0$ if and only if $r_\alpha^{\mathrm{ex}}(t)=0$.*

*Sketch of the proof.* We cannot present the complete proof, because it is rather technical and long, see [Her04]. The main ideas can be summarized as follows:

1. First we introduce two different phonon numbers by $b_{j,\alpha}^{\mathrm{ex}}(t):=\varepsilon^{-1}\widetilde{B}_j^{\mathrm{ex}}(\varepsilon t,\,\varepsilon\alpha)$ for $j=1,\,2$. The quantity $b_{1,\alpha}^{\mathrm{ex}}(t)$ gives the smallest number of all phonons, which belong to the first family and which are located at time $t$ on the right of particle $\alpha$. Similarly, $b_{2,\alpha}^{\mathrm{ex}}(t)$ is the largest number of all phonons of the second family left of $\alpha$.

2. From $b_{i,\alpha}^{\rm ex}(t)$ we can reconstruct for each phonon $\beta$ and for each time $t$ the information which particle moves on the free flight trajectory of $\beta$ at time $t$. This can be done by the following definition.

   (a) Let $a_\beta(0) = \beta$.

   (b) We set $a_\beta(t) = \alpha$, if either

      i. $\beta = b_{2,\alpha}^{\rm ex}(t)$ and $v_\alpha^{\rm ex}(t) = W_2(\varepsilon\beta)$, or

      ii. $\beta = b_{1,\alpha}^{\rm ex}(t)$ and $v_\alpha^{\rm ex}(t) = W_1(\varepsilon\beta)$.

   It can be shown, that the functions $a_\beta(t)$ are well defined, as long as $t < \varepsilon^{-1}\tau_{\rm fin}$.

3. In the third step we define for all particles $\alpha$ the curve $x_\alpha^{\rm ex}(t)$ by $\dot{x}_\alpha^{\rm ex}(t) = v_\alpha^{\rm ex}(t)$. Then we check, that the functions $x_\alpha^{\rm ex}(t)$ are the atomic positions of an exact solution, where we shall use the result from the first two steps. Finally we set $r_\alpha^{\rm ex}(t) = x_{\alpha+1}^{\rm ex}(t) - x_\alpha^{\rm ex}(t)$

4. Equation (6.29) implies that $r_\alpha^{\rm TW}(t) = 0$ if and only if

$$\widetilde{B}_2(\varepsilon t,\, \varepsilon\alpha) \;=\; 0. \tag{6.36}$$

   On the other hand, we have $r_\alpha^{\rm ex}(t) = 0$ if and only if both $v_\alpha^{\rm ex}(t)$ and $v_{\alpha+1}^{\rm ex}(t)$ jump simultaneously at time $t$. According to the definition (6.34), this happens if and only if (6.36) is satisfied. We have thus proved the"in phaseproperty.

Now we can formulate and prove the justification result for the hard sphere model. Note that here the space $\ell^2_\varepsilon$ has dimension $N < \infty$.

**Theorem 6.7** *Let $\left(\widetilde{r},\, \widetilde{v},\, \widetilde{k},\, \widetilde{\omega}\right)$ be a solution of (6.14) satisfying Assumption 6.4. Then, there exists a constant $C$ such that for all $N$ the following holds. For $\varepsilon = 1/N$ let $P^\varepsilon(t)$ and $Q^\varepsilon(t)$ be the vectors with components*

$$P_\alpha^\varepsilon(t) \;:=\; \left(r_\alpha^{\rm ex}(t),\, v_\alpha^{\rm ex}(t)\right), \tag{6.37}$$

$$Q_\alpha^\varepsilon(t) \;:=\; \left(r_\alpha^{\rm TW}(t),\, v_\alpha^{\rm TW}(t)\right), \tag{6.38}$$

*where $\alpha = 1, ..., N$. Then, for all $t \in [0,\, \tau_{\rm fin}/\varepsilon]$ we have*

$$\|\, Q^\varepsilon(t) - P^\varepsilon(t)\,\|_{\ell^2_\varepsilon\times\ell^2_\varepsilon} \;\leq\; \varepsilon C. \tag{6.39}$$

*Sketch of the proof.* Using the representations (6.29) we can compute $\dot{r}_\alpha^{\rm TW}(t)$ explicitly. Then we show that there holds

$$\dot{r}_\alpha^{\rm TW}(t) - \dot{r}_\alpha^{\rm ex}(t) = \mathcal{O}(\varepsilon). \tag{6.40}$$

Finally, the "in phaseproperty guaranties that (6.40) implies $r_\alpha^{\rm TW}(t) - r_\alpha^{\rm ex}(t) = \mathcal{O}(\varepsilon)$, which provides

$$\|\, r^{\rm TW}(t) - r^{\rm ex}(t)\,\|_{\ell^2_\varepsilon} \;=\; \mathcal{O}(\varepsilon). \tag{6.41}$$

Since the profile functions

$$\mathbb{W}(B_1,\, B_2,\, k;\, \cdot) \in L^2([0,\, 1]) \tag{6.42}$$

depend Lipschitz continuously on their parameters $B_1$, $B_2$, and $k$, we find

$$\| \, \mathbb{U}(\tau,\, y,\, \cdot) \, \|_{L^2([0,\,1])} \;=\; \mathcal{O}(\varepsilon) \tag{6.43}$$

where

$$\mathbb{U}(\tau,\, y,\, \cdot) \;=\; \mathbb{W}\Big(\Big(\widetilde{B}_1,\, \widetilde{B}_2,\, \widetilde{k}\Big)(\tau,\, y);\, \cdot\Big) - \mathbb{W}\Big(\Big(\widetilde{B}_1^{\,\mathrm{ex}},\, \widetilde{B}_2^{\,\mathrm{ex}},\, \widetilde{k}^{\,\mathrm{ex}}\Big)(\tau,\, y);\, \cdot\Big).$$

There follows

$$\| \, v^{\mathrm{TW}}(t) - v^{\,\mathrm{ex}}(t) \, \|_{\ell^2_\varepsilon} \;=\; \mathcal{O}(\varepsilon), \tag{6.44}$$

which completes the proof. □

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