Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

On the approximation of periodic traveling waves for the nonlinear atomic chain

Wolfgang Dreyer[1], Michael Herrmann[2]

submitted: 26th May 2005

[1] Weierstrass Institute
for Applied Analysis and Stochastics
Mohrenstrasse 39
10117 Berlin
Germany
E-Mail: dreyer@wias-berlin.de

[2] Humboldt-Universität zu Berlin
Institut für Mathematik
Unter den Linden 6
10099 Berlin
Germany
E-Mail: michaelherrmann@math.hu-berlin.de

No. 1030
Berlin 2005

2000 *Mathematics Subject Classification.* 34K07 34K28 37J45.

Key words and phrases. atomic chain, periodic traveling waves.

This work was supported by the Deutsche Forschungsgemeinschaft (DFG) within the Priority Programme SPP 1095 *Analysis, Modeling and Simulation of Multiscale Problems*, see `http://www.mathematik.uni-stuttgart.de/~mehrskalen`.

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

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

We study a scheme from [FV99], which allows to approximate periodic traveling waves in the nonlinear atomic chain with nearest neighbour interactions. We prove a compactness result for this scheme, and derive some generalizations. Moreover, we discuss the thermodynamic properties of traveling waves.

1 Introduction

The atomic chain, see Figure 1, consists of identical particles with unit mass. These are located on the real axis and are labeled by the index α. Let N be the number of particles, which may be finite (in this case we set $\alpha \in \{1, ..., N\}$) or infinite (i.e. $\alpha \in \mathbb{Z}$). For any α, let $x_\alpha(t)$ and $v_\alpha(t) = \dot{x}_\alpha(t)$ denote the position and velocity,

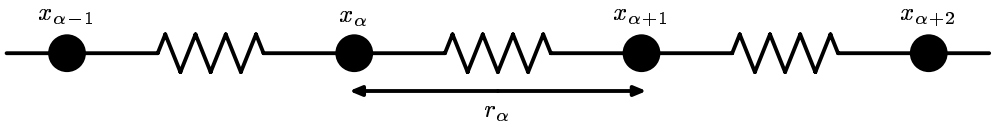

Figure 1: The atomic chain with nearest neighbor interaction.

respectively, of the atom α at time t. Moreover, let $r_\alpha(t)$ be the distance of atoms $\alpha + 1$ and α, i.e.

$$r_\alpha(t) \;:=\; x_{\alpha+1}(t) - x_\alpha(t). \tag{1.1}$$

We assume that all particles interact only with their nearest neighbors. In particular, we do not consider external forces. The dynamics in the chain is governed by Newton's equations, which read

$$\ddot{x}_\alpha(t) = \Phi'\Big(x_{\alpha+1}(t) - x_\alpha(t)\Big) - \Phi'\Big(x_\alpha(t) - x_{\alpha-1}(t)\Big), \tag{1.2}$$

where Φ is the atomic interaction potential. A prominent example for a nonlinear convex interaction potential is the Toda-potential ([Tod70, Tod81])

$$\Phi(r) \;=\; \exp(1-r) + r - 1, \tag{1.3}$$

which makes (1.2) completely integrable, cf. [Hén74, VDO91, DKKZ96, DM98].

A *traveling wave* is an exact solution of (1.2), which satisfies the ansatz

$$x_\alpha(t) \;=\; r\alpha + vt + \mathbb{X}\Big(k\alpha + \omega t\Big). \tag{1.4}$$

Here r, v, k and ω are four constant parameters and $\mathbb{X}$ is the *wave profile*. Motivated by its physical meaning we call r the *mean distance*, v the *mean velocity*, k the *wave number*, and ω the *frequency*. If we insert the Ansatz (1.4) into NEWTON's equations (1.2) we obtain a difference-differential equation for the wave profile $\mathbb{X}$, which reads

$$\begin{aligned} \omega^2 \frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}\mathbb{X}(\varphi) &= \Phi'\Big(r + \mathbb{X}(\varphi + k) - \mathbb{X}(\varphi)\Big) - \\ &\qquad \Phi'\Big(r + \mathbb{X}(\varphi) - \mathbb{X}(\varphi - k)\Big), \end{aligned} \tag{1.5}$$

where $\phi = k\alpha + \omega t$ denotes the *phase*. Note that, due to GALILEIan invariance of (1.2), v does not appear in (1.5), so that it is a free parameter. In this study we consider solely periodic functions $\mathbb{X}$. Without loss of generality we set $\varphi_{\mathrm{per}} = 1$. Furthermore, we are free to normalize $\mathbb{X}$ by

$$\int_0^1 \mathbb{X}(\varphi)\,\mathrm{d}\varphi = 0. \tag{1.6}$$

Traveling waves in discrete systems were widely studied in the last years, because they provide a lot of insight into the physics of high dimensional discrete systems. However, most of the available papers address the (nontrivial) existence problem, which was tackled by different methods (see for instance [FW94, AG96, FP99, PP00, IK00, Ioo00]). Here we concentrate on approximation schemes for travelling waves, because (*i*) explicit solutions of (1.5) are almost never available, and (*ii*) in modulation theory (which is the primary subject of our interest, see [DHM04, DH05]) one needs the information about the thermodynamicsöf travelling waves, which can be gained from numerical computations.

The paper is organized as follows. In Section 2 we summarize some basic facts about traveling waves in the atomic chain. In particular, we introduce the most important thermodynamic properties of traveling waves which become important in the modulation theory. Consequently, we will proceed with an brief overview over the modulation theory as it is developed in [FV99, DHM04, Her04], and we give the link to the Equation of State and the GIBBS-equation. Furthermore, we summarize the (for our purposes) most important existence result, which goes back to FILIP and VENAKIDES, see [FV99]. Next, in section 3 we describe a approximation scheme for periodic traveling waves and prove a compactness result for this scheme. Moreover, we will discuss some possible modifications of the scheme. Finally, in Section 4 we present some numerical simulations.

2 Properties of traveling waves - an overview

2.1 Derived quantities

We introduce two further profile functions $\mathbb{R}$ and $\mathbb{V}$ by setting

$$\mathbb{V}(\varphi) = \frac{\mathrm{d}}{\mathrm{d}\varphi}\mathbb{X}(\varphi), \qquad \mathbb{R}(\varphi) = \mathbb{X}(\varphi + k/2) - \mathbb{X}(\varphi - k/2). \tag{2.1}$$

The functions $\mathbb{R}$ and $\mathbb{V}$ are called *traveling distance wave* and *traveling velocity wave*, respectively, because (1.4) implies the following expressions for the atomic distances and velocities

$$\begin{aligned} r_\alpha(t) &= r + \mathbb{R}(k\alpha + \omega t + k/2), \\ v_\alpha(t) &= v + \omega\mathbb{V}(k\alpha + \omega t). \end{aligned} \tag{2.2}$$

Note that any traveling velocity wave provides the complete information about the the corresponding traveling wave.

Using the profile functions $\mathbb{R}$ and $\mathbb{V}$ we can define the following means values, which all have an immediate physical interpretation.

$$\begin{aligned}
W &:= \int_0^1 \Phi(r + \mathbb{R}(\varphi))\,\mathrm{d}\varphi, && \text{specific internal potential energy density,} \\
p &:= -\int_0^1 \Phi'(r + \mathbb{R}(\varphi))\,\mathrm{d}\varphi, && \text{pressure = negative specific force density,} \\
K &:= \frac{\omega^2}{2}\int_0^1 \mathbb{V}(\varphi)^2\,\mathrm{d}\varphi && \text{specific internal kinetic energy density,} \\
T &:= 2K, && \text{kinetic temperature,} \\
F &:= K - W, && \text{specific internal action density,} \\
U &:= K + W, && \text{specific internal energy density,} \\
E &:= \frac{1}{2}v^2 + U, && \text{specific energy density.}
\end{aligned}$$

All these quantities become important, if we pass from the microscopic to the macroscopic scale, where we can study the thermodynamic properties of a chain with a very large particle number. This is explained in more detail within the next section.

For later purposes we define further quantities by

$$\begin{aligned} \gamma &:= \frac{1}{2}\int_0^1 \mathbb{V}(\varphi)^2 \,\mathrm{d}\varphi, \\ S &:= 2\omega\gamma, \\ g &:= -\int_0^1 \frac{1}{2}(\mathbb{V}(\varphi + k/2) + \mathbb{V}(\varphi - k/2))\ \Phi'(r + \mathbb{R}(\varphi))\ \mathrm{d}\varphi. \end{aligned} \tag{2.3}$$

The quantity γ has no physical meaning, but it becomes important in the existence result as well as in the approximation scheme. The quantities S and g have no atomistic interpretation. However, on the macroscopic scale S and g can be shown to have all properties of an entropy density and an entropy flux, respectively (cf. [DHM04, Her04])

2.2 Summary on modulation theory

In this section we summarize the modulation theory of the nonlinear atomic chain as it is developed in [FV99, DHM04, Her04], because it is probably the most important application of periodic traveling waves and yields therefore a strong motivation for the investigation of approximation schemes. Furthermore, modulation theory clarifies the fundamental role of the thermodynamic quantities introduced above.

Modulation theory is a powerful tool which provides an effective description of the dynamics on the *macroscopic* scale, which is large in comparison to the *microscopic* (i.e. the atomic) scale. Modulation with periodic traveling waves allows to describe the macroscopic evolution of microscopic oscillations, so that finally there result some macroscopic evolution equations involving temperature. In our context, the macroscopic scale results from the *hyperbolic scaling* which reads

$$\overline{t} \;=\; \varepsilon t, \qquad \overline{\alpha} \;=\; \varepsilon\alpha \tag{2.4}$$

Here, $\overline{t}$ and $\overline{\alpha}$ are the *macroscopic* time and particle index, respectively, and $\varepsilon \ll 1$ is the *scaling parameter*. For finite chains with a particle number $N < \infty$ we set $\varepsilon = 1/N$, so that $\overline{\alpha}$ takes values in $[0,\, 1]$.

Since we scale time and particle index in the same way, we end up with hyperbolic pde's which describe the macroscopic evolution. We mention that there are other reasonable scalings for the atomic chain, as for instance the KdV-scaling in [FP99, SW00], which leads to a macroscopic KORTEWEG-DE VRIES equations, or the NSE-scaling in [GM04b, GM04a], where the macroscopic evolution is governed by the nonlinear SCHROEDINGER equation.

The main idea behind modulation theory is the construction of *approximate* solutions of the microscopic system (1.4) by allowing the traveling wave parameter

to vary on the macroscopic scale. A *modulated traveling waves* is an approximate solution of NEWTONs equations which satisfies the following ansatz for the atomic positions

$$x_\alpha(t) \;=\; \frac{1}{\varepsilon}X(\varepsilon t,\, \varepsilon\alpha) + \tilde{\mathbb{X}}\Big(\varepsilon t,\, \varepsilon\alpha;\, \frac{1}{\varepsilon}\Theta(\varepsilon t,\, \varepsilon\alpha)\Big) + \mathcal{O}(\varepsilon), \tag{2.5}$$

where X and Θ are two macroscopic functions. The modulated traveling waves parameters thus become fields depending on $\overline{t}$ and $\overline{\alpha}$. They are determined as derivatives of X and Θ, namely

$$v\big(\overline{t},\, \overline{\alpha}\big) = \frac{\partial\, X}{\partial\, \overline{t}}\big(\overline{t},\, \overline{\alpha}\big), \qquad r\big(\overline{t},\, \overline{\alpha}\big) = \frac{\partial\, X}{\partial\, \overline{\alpha}}\big(\overline{t},\, \overline{\alpha}\big), \tag{2.6}$$

$$\omega\big(\overline{t},\, \overline{\alpha}\big) = \frac{\partial\, \Theta}{\partial\, \overline{t}}\big(\overline{t},\, \overline{\alpha}\big), \qquad k\big(\overline{t},\, \overline{\alpha}\big) = \frac{\partial\, \Theta}{\partial\, \overline{\alpha}}\big(\overline{t},\, \overline{\alpha}\big). \tag{2.7}$$

The function $\tilde{\mathbb{X}}$ serves to model the microscopic oscillations and provides the link to traveling waves. In particular,

$$\tilde{\mathbb{X}}\big(\overline{t},\, \overline{\alpha};\, \varphi\big) \;=\; \mathbb{X}\big(r\big(\overline{t},\, \overline{\alpha}\big),\, v\big(\overline{t},\, \overline{\alpha}\big),\, k\big(\overline{t},\, \overline{\alpha}\big),\, \omega\big(\overline{t},\, \overline{\alpha}\big);\, \varphi\big), \tag{2.8}$$

where $\mathbb{X}$ is a family of traveling wave profiles which depends on the parameters r, v, k, ω, as well as on the phase variable φ. In order to ensure that (2.5) yields indeed approximate solutions, we can not choose X and Θ arbitrary, but we have to satisfy some restrictions. It can be shown, at least formally, that the modulated parameters have to satisfy the following version of WHITHAM's equations

$$\frac{\partial}{\partial\, \overline{t}}\begin{pmatrix} r \\ v \\ k \\ S \end{pmatrix}\big(\overline{t},\, \overline{\alpha}\big) + \frac{\partial}{\partial\, \overline{\alpha}}\begin{pmatrix} -v \\ +p \\ -\omega \\ +g \end{pmatrix}\big(\overline{t},\, \overline{\alpha}\big) \;=\; 0. \tag{2.9}$$

These equations determine the functions X and Θ, and they can be interpreted as the macroscopic conservation laws of mass, momentum, wave number and entropy. Finally, the system (2.9) implies the conservation law of energy

$$\frac{\partial}{\partial\, \overline{t}}\Big(\frac{1}{2}v^2 + U\Big)\big(\overline{t},\, \overline{\alpha}\big) + \frac{\partial}{\partial\, \overline{\alpha}}\big(vp + \omega g\big)\big(\overline{t},\, \overline{\alpha}\big) \;=\; 0. \tag{2.10}$$

The system (2.9) consists of four equations for seven variables. It is closed by the equation of state which is closely related to families of travelling waves which depend on four parameters. We summarize the main results from [DHM04]. Let $\mathbb{X} = \mathbb{X}(r,\, v,\, k,\, \omega;\, \varphi)$ a family of traveling waves which depend on the parameters r, v, k, ω and on the phase variable φ. Then the internal action F becomes a function of r, k and ω, i.e.

$$F = F(r,\, k,\, \omega) \tag{2.11}$$

This equation is the *equation of state* which intimately depends on the atomic interaction potential Φ. However, independently on Φ there holds the GIBBS equation

$$\mathrm{d}F \;=\; S\,\mathrm{d}\omega \;+\; p\,\mathrm{d}r \;+\; g\,\mathrm{d}k, \tag{2.12}$$

which establishes the closure of (2.9). Unfortunately we do not know the equation of state explicitly, except for some very special potential (see below). In all cases, where we do not know the Equations of State explicitly, we cannot characterize the properties of (2.9), as for instance strict hyperbolicity, RIEMANN-invariants and so on. Consequently, we are interested in computing the equation of state at least approximatively, in order to get a better understanding of (2.9). First steps in this direction are done in [FV99] and [Her04]. Another application of approximation schemes for traveling waves can be found in [DH05], where the authors performed detailed numerical studies on the validity of the modulation system.

Sometimes it is useful to replace the parameter ω either by S or by γ. Doing this, we shall reformulate the equation of state as well the Gibbs-equation according to the following table, which is derived in [DHM04, Her04].

variables	equation of state	GIBBS-equation
$(r,\,k,\,\gamma)$	$W \;=\; W(r,\,k,\,\gamma)$	$\mathrm{d}W \;=\; \omega^2\,\mathrm{d}\gamma \;-\; p\,\mathrm{d}r \;-\; g\,\mathrm{d}k$
$(r,\,k,\,S)$	$U \;=\; U(r,\,k,\,S)$	$\mathrm{d}U \;=\; \omega\,\mathrm{d}S \;-\; p\,\mathrm{d}r \;-\; g\,\mathrm{d}k$

For illustration we display the Equations of State for two simple cases. For the harmonic potential

$$\Phi(d) \;=\; c_0 + c_1\,d + \frac{c_2}{2}\,d^2, \tag{2.13}$$

there result the dispersion relation

$$\omega(k) \;=\; \sqrt{c_2}\,\sin\left(\pi k\right)/\pi \tag{2.14}$$

and

$$W(r,\,k,\,\gamma) \;=\; c_0 + c_1 r + \frac{1}{2}c_2 r^2 + \omega(k)^2\gamma \tag{2.15}$$

or, equivalently,

$$U(r,\,k,\,S) \;=\; c_0 + c_1 r + \frac{1}{2}c_2 r^2 + \omega(k)S. \tag{2.16}$$

Another example is the hard-sphere model of the atomic chain, which corresponds to

$$\Phi(d) \;=\; \begin{cases} 0 & \text{for } d \geq 0, \\ +\infty & \text{for } d < 0. \end{cases} \tag{2.17}$$

Although this potential is not smooth, the notion of traveling waves may be extended to this model. There result the following Equations of State

$$U(r,\, k,\, S) = \frac{1}{2}\frac{S^2}{r^2}k(1-k). \tag{2.18}$$

We mention that for both examples not only the Equations of States are known, but even explicit expressions for the traveling waves are available, see [DHM04, Her04]). Moreover, for both examples the modulation equations (2.9) may be derived rigorously (again [DHM04, Her04]).

2.3 Existence of traveling waves

In this section we summarize the variational approach to the existence problem, because it is closely related to our first approximation scheme. This variational approach was introduced by Filip and Venakides in [FV99]. However, the approach is restricted to convex atomic interaction potentials Φ. In order to simplify some technical arguments, we will assume, that the convex interaction potential Φ satisfies the following regularity assumptions.

Assumption 2.1

1. *Φ is smooth (at least C^2) and it is defined on the whole real axis,*
2. *the second derivative of Φ satisfies*

$$0 < m \leq \Phi'' \leq M < \infty. \tag{2.19}$$

where m and M are two constants.

These assumptions implies, that the operator

$$\partial\Phi \;:\; L^2([0,\,1]) \to L^2([0,\,1]), \quad \text{with} \quad (\partial\Phi\mathbb{V})(\varphi) \;:=\; \Phi'(\mathbb{V}(\varphi)) \tag{2.20}$$

is well defined, Lipschitz continuous and strongly monotone, i.e.

$$m \,\|\,\mathbb{V}_2 - \mathbb{V}_1\,\|^2 \leq \langle \partial\Phi(\mathbb{V}_2) - \partial\Phi(\mathbb{V}_1),\, \mathbb{V}_2 - \mathbb{V}_1\rangle \;\leq\; M \,\|\,\mathbb{V}_2 - \mathbb{V}_1\,\|^2 \,. \tag{2.21}$$

Here, $\langle\cdot,\,\cdot\rangle$ and $\|\cdot\|$ denote the usual scalar product and the usual norm in $L^2([0,\,1])$, respectively. For fixed $k \in (0,\,1)$ let A_k and $\hat{A}_k$ be two integral operators defined by

$$(A_k\mathbb{V})(\varphi) := \int\limits_{\varphi-k/2}^{\varphi+k/2} \mathbb{V}(\varphi')\,\mathrm{d}\varphi', \quad \hat{A}_k\mathbb{V} := A_k\mathbb{V} - k\int\limits_0^1 \mathbb{V}(\varphi')\,\mathrm{d}\varphi'. \tag{2.22}$$

The first observation of Filip and Venakides regards the difference differential equations (1.5), which can be transformed into an integral equation containing only

the traveling velocity wave $\mathbb{V}$ as the unknown quantity. In our notations, this integral equation reads

$$\omega^2\,\mathbb{V} = \hat{A}_k\,\partial\Phi\Big(r + \hat{A}_k\mathbb{V}\Big). \tag{2.23}$$

The corresponding traveling distance wave $\mathbb{R}$ then follows from

$$\mathbb{R} = \hat{A}_k\mathbb{V}. \tag{2.24}$$

This reformulation of (1.5) provides a very elegant approach to the existence problem. Again following [FV99], we define (for fixed r and $k \in (0,\,1)$) a functional $\mathcal{W}$ on $L^2([0,\,1])$ as follows

$$\mathcal{W}(r,\,k,\,\mathbb{V}) \;:=\; \int_0^1 \Phi\Big(r + \hat{A}_k\mathbb{V}(\varphi)\Big)\,\mathrm{d}\varphi. \tag{2.25}$$

Now we are able to prove existence of traveling waves as solutions of the following optimization problem.

Problem 2.2 *For fixed r, $k \in (0,\,1)$ and $\gamma > 0$ we maximize the functional*

$$\mathbb{V} \in L^2([0,\,1]) \;\;\rightarrow\;\; \mathcal{W}(r,\,k,\,\mathbb{V}) \tag{2.26}$$

under the constraint $\mathbb{V} \in H_\gamma$, where

$$H_\gamma \;:=\; \Big\{\mathbb{V} \in L^2([0,\,1]) \;:\; \frac{1}{2}\int_0^1 \mathbb{V}(\varphi)^2\,\mathrm{d}\varphi \le \gamma\Big\}. \tag{2.27}$$

Theorem 2.3 *For every r, all $k \in (0,\,1)$ and arbitrary $\gamma > 0$ there exists a maximizer $\tilde{\mathbb{V}}$ of Problem 2.2, such that*

1. *$\tilde{\mathbb{V}}$ is element of the boundary of H_γ, i.e.*

$$\frac{1}{2}\int_0^1 \tilde{\mathbb{V}}(\varphi)^2\,\mathrm{d}\varphi \;=\; \gamma. \tag{2.28}$$

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

$$\tilde{\omega}^2\tilde{\mathbb{V}} = \hat{A}_k\,\partial\Phi\Big(r + \hat{A}_k\tilde{\mathbb{V}}\Big). \tag{2.29}$$

Sketch of the proof. Since the operator $\hat{A}_k$ is compact, the convex functional (2.26) is continuous with respect to the weak topology in $L^2([0,\,1])$. Knowing this, we maximize an continuous functional on the compact set H_γ (compact in the weak topology), which provides existence of a maximizer. Since the functional is convex, the maximizer cannot be an inner point of H_γ. □

We proceed with two remarks.

1. There is no uniqueness result, neither for the maximizer nor for the LAGRANGE multiplier.

2. The equation of state is formally given by

$$W(r,\,k,\,\gamma) \;=\; \mathcal{W}\Big(r,\,k,\,\gamma,\,\tilde{\mathbb{V}}(r,\,k,\,\gamma)\Big). \tag{2.30}$$

   For fixed $(r,\,k,\,\gamma)$ the profile $\tilde{\mathbb{V}}(r,\,k,\,\gamma)$ is a maximizer from Theorem 2.3.

In the next section we derive an approximation scheme for traveling waves, which is closely related to Problem 2.2. For this reason we summarize some important properties of the functional $\mathcal{W}$.

Lemma 2.4 *Let $\mathbb{V}_1$ and $\mathbb{V}_2$ be two function in $L^2([0,\,1])$, and let W_1, W_2 be defined by $W_i = \mathcal{W}(r,\,k,\,\mathbb{V}_i)$, $i = 1,\,2$. Then there holds*

$$W_2 - W_1 \;\geq\; \langle \partial_{\mathbb{V}} \mathcal{W}(r,\,k,\,\mathbb{V}_1),\,\mathbb{V}_2 - \mathbb{V}_1 \rangle \,+\, \frac{m}{2}\,\|\,\hat{A}_k\mathbb{V}_2 - \hat{A}_k\mathbb{V}_1\,\|^2\,. \tag{2.31}$$

Furthermore, any $\mathbb{V} \in L^2([0,\,1])$ satisfies

$$\mathcal{W}(r,\,k,\,\mathbb{V}) \;\geq\; \frac{m}{2}\,\|\,\hat{A}_k\mathbb{V}\,\|^2 \,+\mathcal{W}(r,\,k,\,0) \tag{2.32}$$

as well as

$$\begin{aligned} 0 \;&\leq\; \mathcal{W}(r,\,k,\,\mathbb{V}) - \mathcal{W}(r,\,k,\,0) + \frac{m}{2}\,\|\,\hat{A}_k\mathbb{V}\,\|^2 \\ &\leq\; \langle \partial_{\mathbb{V}}\,\mathcal{W}(r,\,k,\,\mathbb{V}),\,\mathbb{V}\rangle\;. \end{aligned} \tag{2.33}$$

Here, $\partial_{\mathbb{V}}\,\mathcal{W}(r,\,k,\,\mathbb{V})$ denotes the GATEAUX*-derivative of $\mathcal{W}$ with respect to $\mathbb{V}$.*

Sketch of the proof. The estimate (2.31) follows from the convexity of $\mathcal{W}$ (with respect to $\mathbb{V}$) by applying standard methods of convex analysis. (2.32) and (2.33) then follow from (2.31) by setting $\mathbb{V}_2 = \mathbb{V}$, $\mathbb{V}_1 = 0$ and $\mathbb{V}_1 = \mathbb{V}$, $\mathbb{V}_2 = 0$, respectively. □

3 Approximation Schemes

3.1 γ-Scheme

We now derive the γ-scheme which can be considered as a direct approximation of the optimization problem 2.2. For simplicity we shall assume that the interaction potential satisfies the regularity assumption 2.1.

Scheme 3.1 *Let $k \in (0,\, 1)$, $\gamma > 0$ and r be given, and let $\mathbb{V}_0 \in H_\gamma$ be an arbitrary initial datum with $\hat{A}_k \mathbb{V}_0 \neq 0$. Then we define inductively two sequences*

$$(n \mapsto \mathbb{V}_n) \subset H_\gamma \quad \textit{and} \quad (n \mapsto \omega_n) > 0 \tag{3.1}$$

by the following iteration step

$$\mathbb{V}_{n+1} = f_n \mathbb{Z}_n, \quad \omega_{n+1} = \frac{1}{\sqrt{f_n}}, \tag{3.2}$$

where

$$\mathbb{Z}_n = \partial_{\mathbb{V}} \mathcal{W}(r,\, k,\, \mathbb{V}_n), \quad f_n = \frac{\sqrt{2\gamma}}{\| Z_n \|}. \tag{3.3}$$

Note that the scheme 3.1 is well defined as long as $\| \mathbb{Z}_n \| > 0$. Furthermore, for all n we have

$$\frac{1}{2} \| \mathbb{V}_n \|^2 = \gamma \quad \text{and} \quad \omega_{n+1}^2 \mathbb{V}_{n+1} = \mathbb{Z}_n = \hat{A}_k \partial \Phi \Big(r + \hat{A}_k \mathbb{V}_n \Big). \tag{3.4}$$

This approximation scheme for traveling waves was described by Filip and Venakides in [FV99]. However, they did not prove any convergence or compactness result for this scheme.

Theorem 3.2 *The scheme 3.1 is well defined and has the following properties.*

1. *The sequence*

$$n \;\mapsto\; W_n \;:=\; \mathcal{W}(r,\, k,\, \mathbb{V}_n) \tag{3.5}$$

increases monotonously with

$$W_n > W_0 > \Phi(r). \tag{3.6}$$

2. *The sequence $n \mapsto \omega_n$ is strictly positive and bounded.*

3. *The sequence $n \mapsto (\mathbb{V}_n,\, \omega_n)$ is compact in $H_\gamma \times \mathbb{R}_+$.*

4. *Let* $(\mathbb{V},\, \omega)$ *be an accumulation point of the sequence* $n \mapsto (\mathbb{V}_n,\, \omega_n)$. *Then,* $\mathbb{V}$ *is a traveling velocity wave with frequency* ω. *Furthermore,* $\mathbb{V}$ *is an element of the boundary of* H_γ.

Proof.

1. In what follows we write $\mathcal{W}(\mathbb{V})$ instead of $\mathcal{W}(r,\, k,\, \mathbb{V})$. Lemma 2.4 yields

$$\begin{aligned} W_{n+1} - W_n &= \frac{m}{2} \,\|\, \hat{A}_k \mathbb{V}_{n+1} - \hat{A}_k \mathbb{V}_n \,\|^2 + \langle \partial_{\mathbb{V}} \mathcal{W}(\mathbb{V}_n),\, \mathbb{V}_{n+1} - \mathbb{V}_n \rangle \\ &= \frac{m}{2} \,\|\, \hat{A}_k \mathbb{V}_{n+1} - \hat{A}_k \mathbb{V}_n \,\|^2 + \omega_{n+1}^2 \,\langle \mathbb{V}_{n+1},\, \mathbb{V}_{n+1} - \mathbb{V}_n \rangle \\ &\geq \frac{m}{2} \,\|\, \hat{A}_k \mathbb{V}_{n+1} - \hat{A}_k \mathbb{V}_n \,\|^2 + \\ &\quad \omega_{n+1}^2 \big(\|\, \mathbb{V}_{n+1} \,\|^2 - \|\, \mathbb{V}_{n+1} \,\| \|\, \mathbb{V}_n \,\| \big) \\ &\geq \frac{m}{2} \,\|\, \hat{A}_k \mathbb{V}_{n+1} - \hat{A}_k \mathbb{V}_n \,\|^2 + \omega_{n+1}^2 (2\gamma - 2\gamma) \\ &\geq \frac{m}{2} \,\|\, \hat{A}_k \mathbb{V}_{n+1} - \hat{A}_k \mathbb{V}_n \,\|^2 \geq\, 0. \end{aligned} \tag{3.7}$$

   This estimate implies the monotonicity of the sequence $n \mapsto W_n$. Due to $\hat{A}_k \mathbb{V}_0 \neq 0$ and since (2.32) there holds $W_0 > \mathcal{W}(0) = \Phi(r)$.

2. Let us assume that there is an integer n with $\mathbb{Z}_n = 0$. ¿From (2.33) we then conclude

$$0 \geq W_n - \mathcal{W}(0) + \frac{m}{2} \,\|\, \hat{A}_k \mathbb{V}_n \,\|^2 \geq 0. \tag{3.8}$$

   However, this estimate contradicts $W_n \geq W_0 > \mathcal{W}(0)$, and thus the scheme is well defined. Since $\mathbb{V}_n \in H_\gamma$ and because the operator $\partial_{\mathbb{V}} \mathcal{W}$ is bounded, the sequence $n \mapsto \mathbb{Z}_n$ is bounded. We conclude

$$\omega_{n+1}^4 2\gamma \;= \|\, \mathbb{Z}_n \,\|^2 <\; \infty, \tag{3.9}$$

   and therefore $\omega_{n+1} < \infty$.

3. The sequence $n \mapsto W_n$ is convergent, because it is monotonously increasing and, according to Theorem 2.3, also bounded. From (3.7) there follows

$$\lim_{n \to \infty} \left(\hat{A}_k \mathbb{V}_{n+1} - \hat{A}_k \mathbb{V}_n \right) \;=\; 0. \tag{3.10}$$

   The continuity of $\partial\Phi$ and $\hat{A}_k$ now implies

$$\lim_{n \to \infty} (\mathbb{Z}_{n+1} - \mathbb{Z}_n) \;=\; 0. \tag{3.11}$$

   Together with (3.4) we obtain

$$\lim_{n \to \infty} \left(\omega_{n+1}^2 \mathbb{V}_{n+1} - \omega_n^2 \mathbb{V}_n \right) \;=\; 0. \tag{3.12}$$

Equations (3.4) and (3.12) imply

$$\lim_{n\to\infty} \left(\omega_n^2 \mathbb{V}_n - \mathbb{Z}_n\right) = \lim_{n\to\infty} \left(\omega_n^2 \mathbb{V}_n - \omega_{n+1}^2 \mathbb{V}_{n+1}\right) = 0. \tag{3.13}$$

Furthermore, from (2.33) there follows

$$\langle \mathbb{Z}_n,\, \mathbb{V}_n \rangle \;\; \geq \;\; \frac{m}{2} \,\| \hat{A}_k \mathbb{V}_n \|^2 \,. \tag{3.14}$$

4. Next we prove by contradiction that $n \mapsto \omega_n$ is uniformly positive. Let $j \mapsto \omega_{n_j}$ a subsequence which converges to 0. With (3.13) there then follows

$$\lim_{j\to\infty} \left\langle \mathbb{Z}_{n_j},\, \mathbb{V}_{n_j} \right\rangle \,=\, \lim_{j\to\infty} \omega_{n_j}^2 \,\| \mathbb{V}_{n_j} \|^2 = 0, \tag{3.15}$$

and (3.14) implies

$$\lim_{j\to\infty} \hat{A}_k \mathbb{V}_{n_j} = 0 \quad \text{and} \quad \lim_{j\to\infty} W_{n_j} = \mathcal{W}(r,\, k,\, \gamma,\, 0) = \Phi(r),$$

which contradicts (3.6)

5. Since H_γ is weakly compact, we can extract subsequences $j \mapsto n_j$, such that the sequence $j \mapsto \mathbb{V}_{n_j}$ converges weakly to a limit $\mathbb{V}_\infty \in H_\gamma$. Passing to another subsequence may assume that $j \mapsto \omega_{n_j}$ converges to $\omega_\infty > 0$. Since the operator $\partial_{\mathbb{V}} \mathcal{W}$ is compact, there holds in the sense of strong convergence

$$\lim_{j\to\infty} \mathbb{Z}_{n_j} \;=\; \partial_{\mathbb{V}} \mathcal{W}(\mathbb{V}_\infty) \;=:\; \mathbb{Z}_\infty. \tag{3.16}$$

Furthermore, we find

$$\mathbb{V}_{n_j} \;\; = \;\; \frac{\mathbb{Z}_{n_j}}{\omega_{n_j}^2} + \frac{\omega_{n_j}^2 \mathbb{V}_{n_j} - \mathbb{Z}_{n_j}}{\omega_{n_j}^2}. \tag{3.17}$$

The convergence results (3.13) and (3.16) now imply the strong convergence

$$\lim_{j\to\infty} \mathbb{V}_{n_j} \;\; = \;\; \frac{\mathbb{Z}_\infty}{\omega_\infty^2}, \tag{3.18}$$

as well as

$$\omega_\infty^2 \mathbb{V}_\infty \;\; = \;\; \partial_{\mathbb{V}} \mathcal{W}(\mathbb{V}_\infty). \tag{3.19}$$

In particular, $\| \mathbb{V}_\infty \|^2 = 2\gamma$.

□

We conclude this section with some remarks.

1. We are not able to prove, that the scheme 3.1 converges, i.e. that there is exactly one accumulation point. However, numerical simulations indicate convergence.

2. Let $(\mathbb{V}_1, \omega_1)$ and $(\mathbb{V}_2, \omega_2)$ be two accumulation points. Then there holds

$$\mathcal{W}(r, k, \mathbb{V}_1) \;=\; \mathcal{W}(r, k, \mathbb{V}_2). \tag{3.20}$$

3. The set of accumulation points may depend on $\mathbb{V}_0$.

4. It is easy to show, that the the cone

$$H_{\mathrm{sym}} \;:=\; \left\{\mathbb{V} \in L^2([0, 1]) \;:\; \mathbb{V}\left(\frac{1}{2} - \cdot\right) = \mathbb{V}\left(\frac{1}{2} + \cdot\right) \text{ a.e.}\right\}.$$

   is invariant under the action of the operators $\partial\Phi$ and $\hat{A}_k$. Thus, if we choose the initial datum $\mathbb{V}_0$ as an element in H_{sym}, the whole sequence $n \mapsto \mathbb{V}_n$ remains in H_{sym}. Since H_{sym} is closed, we have proved the existence of traveling velocity waves within H_{sym}.

3.2 S-Scheme and T-Scheme

The scheme 3.1 allows the numerical computation of traveling wave profiles as well as of the corresponding equation of state $W = W(r, k, \gamma)$. However, sometimes it is more convenient (cf. the discussion in Section 2.2 and the applications in [DH05]) to replace the parameter γ by the entropy S or by the temperature T. For this reason we present some modifications of scheme 3.1 which allow to prescribe either S or T. Unfortunately we could not derive any convergence or compactness result for these schemes. However, numerical experiments indicate that the modified schemes converge, at least for reasonable initial data.

Scheme 3.3 *Let (r, k, S) or (r, k, T) be given and let $\mathbb{V}_0 \in L^2([0, 1])$ be an arbitrary initial datum with $\hat{A}_k\mathbb{V}_0 \neq 0$. Furthermore, let the parameter $\lambda \in (0, 1)$ be fixed. Then we define inductively two sequences $(n \mapsto \mathbb{V}_n) \subset L^2([0, 1])$ and $(n \mapsto \omega_n) > 0$ by*

$$\mathbb{V}_{n+1} = \lambda f_n \mathbb{Z}_n + (1 - \lambda)\mathbb{V}_n, \quad \omega_{n+1} = \frac{1}{\sqrt{f_n}}, \quad \mathbb{Z}_n = \hat{A}_k\, \partial\Phi\Big(r + \hat{A}_k\mathbb{V}_n\Big). \tag{3.21}$$

Here, f_n is given either by $f_n = S^{2/3} \parallel Z_n \parallel^{-4/3}$ (if S is prescribed) or by $f_n = T\parallel Z_n\parallel^{-2}$ (if T is prescribed).

Note that the schemes 3.1 and 3.3 are quite similar; they differ mainly in the computation rule for f_n. Furthermore, in 3.3 we introduced the additional parameter λ, which improves the convergence in numerical simulations. Applications of the scheme 3.3 may be found in [Her04] and [DH05].

4 Numerical Simulations

The scheme 3.1 can be applied to the TODA-potential (1.3), although it does not satisfy the condition (2.19) of the regularity assumption 2.1. However, there holds an a-priori estimate for the traveling distance wave $\mathbb{R} = \hat{A}_k \mathbb{V}$, namely

$$\|\mathbb{R}\|_\infty \leq \sqrt{2\gamma} =: \mu_\gamma. \tag{4.1}$$

In particular, for fixed γ_0 we may change the potential outside the interval $[-\mu_{\gamma_0}, +\mu_{\gamma_0}]$, so that the modified potential satisfies all regularity assumptions. The estimate (4.1) guaranties, that all traveling waves with $\gamma \leq \gamma_0$ can be calculated by means of the modified potential. The TODA potential has the advantage, that the parameter r can be eliminated explicitly. In particular, since

$$\mathcal{W}(r,\, k,\, \gamma;\, \mathbb{V}) \quad = \quad \exp(1-r)\mathcal{W}(1,\, k,\, \gamma;\, \mathbb{V}) + r - 1, \tag{4.2}$$

we can restrict all considerations to $r = 1$.

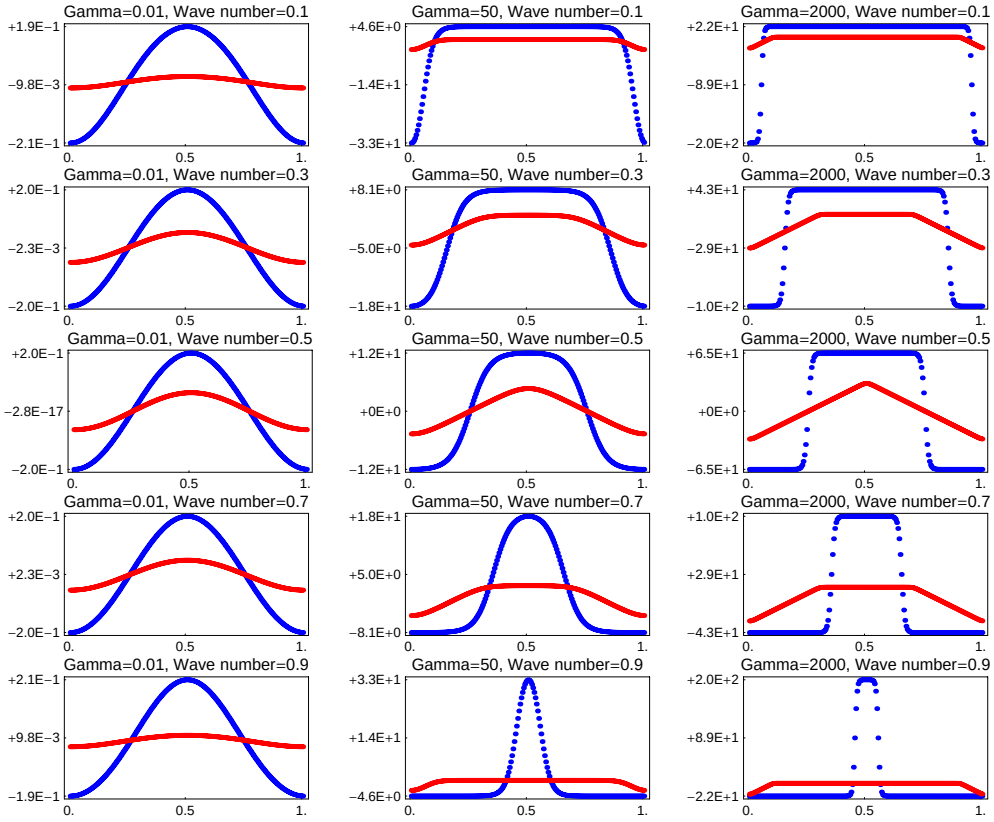

Figure 2: The profile functions $\mathbb{V}$ (blue) and $\mathbb{R}$ (red), depicted over $\varphi \in [0,\, 1]$, for $r = 1$ and for different values of γ and k. The atomic interaction potential Φ is the TODA-Potential.

Since the schemes 3.1 and 3.3 are not discrete in the phase variable φ, we shall briefly describe how they can be implemented. We divide the unit interval into $2M$

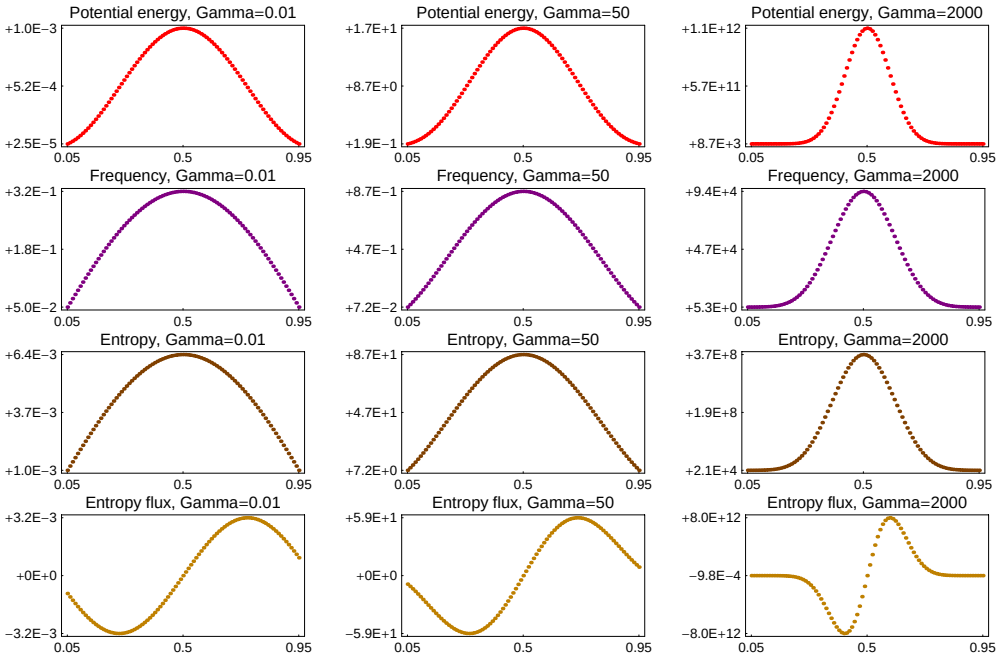

Figure 3: Potential energy W, frequency ω, entropy density S and entropy flux g, all depicted over $k \in [0,\, 1]$, for $r = 1$ and for different values of γ.

subintervals with equal length $\delta = 1/(2M)$, and approximate any 1-periodic function $\mathbb{V}$ by a $2M$-dimensional vector $V = (V_i)_{i=1\ldots 2M}$ with norm

$$\| V \|_\delta^2 \;=\; \delta \sum_{j=1}^{2M} V_j^2. \tag{4.3}$$

Furthermore, for the sake of simplicity we restrict to wave numbers k which can be written as $k = 2K/2M$ for $K \in \{1,\, ...,\, M\}$. The operators $\partial\Phi$ and $\hat{A}_k$ then can be approximated as follows

$$\big(\partial\Phi^{(\delta)}(r+V)\big)_i \;=\; \Phi'(r+V_i), \tag{4.4}$$

$$\Big(\hat{A}_k^{(\delta)} V\Big)_i \;=\; \delta \sum_{j=i-K}^{i+K-1} \frac{V_j + V_{j+1}}{2} - k\delta \sum_{j=1}^{2M} V_j. \tag{4.5}$$

The fully discretized versions of the schemes 3.1 and 3.3, as well as the corresponding analog of Theorem 3.2, can now be derived immediately. In our simulations we always use $M = 600$.

Figure 2 shows for different values of γ and k the profile functions $\mathbb{V}$ and $\mathbb{R}$ as functions of φ, where all computations rely on the γ-scheme 3.1. In Figure 3 we have plot, for different values of γ, various thermodynamic quantities as functions of k. For small γ (in our example $\gamma = 0.01$) the nonlinear potential may be approximated by a quadratic one

$$\Phi\Big(1 + \hat{A}_k \mathbb{V}\Big) \;\approx\; \Phi(1) + \Phi'(1)\hat{A}_k\mathbb{V} + \frac{1}{2}\Phi''(1)\Big(\hat{A}_k\mathbb{V}\Big)^2 \;=\; 1 + \frac{1}{2}\Big(\hat{A}_k\mathbb{V}\Big)^2 \tag{4.6}$$

Consequently, all profile functions are close to sine-functions and the dispersion relation may be approximated by the harmonic one, see (2.14). The data for moderate γ, here $\gamma = 50$, reveal for $\mathbb{V}$ and $\mathbb{R}$ a strong dependence on k. For very large γ the shape of the profile $\mathbb{V}$ is close to a piecewise constant function with two jump discontinuities. A similar asymptotic behavior for traveling waves of the LENNARD-JONES-Potential was proved in [FM02].

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