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Infinite harmonic chain with heavy mass

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Infinite Harmonic Chain with Heavy Mass

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Abstract

Modelling a crystal with impurities we study an atomic chain of point masses with linear nearest neighbour interactions. We assume that the masses of the particles are normalised to 1, except for one heavy particle which has mass M. We investigate the macroscopic behaviour of such a system when M is large, and time and space are scaled accordingly. As main result we derive a PDE for the light particles that is coupled with an ODE for the heavy particle.

1 Introduction

In this paper we establish a micro-to-macro transition for an atomistic lattice system. Starting with a high-dimensional system of Hamiltonian ODEs we derive a reduced PDE model that describes the effective dynamics on large spatial and temporal scales. This kind of research has attracted a lot of attention over the last decades and the results cover both static and evolutionary problems. A lot of attention has been devoted to the nonlinear atomic chain

$$m(y)\ddot{u}(y,\tau) = V'(u(y+1,\tau) - u(y,\tau)) - V'(u(y,\tau) - u(y-1,\tau)) - W'(u(y,\tau)) \tag{1.1}$$

with nearest neighbour potential V and on-site potential W. Here $u(y,\tau) \in \mathbb{R}$ denotes the displacement at time τ of the y^{th}-atom from its rest position, and $m : \mathbb{Z} \to \mathbb{R}^+$ is the mass distribution. The literature on the macroscopic behaviour of (1.1) is quite large. Without any claim of completeness, we mention [18, 3] concerning the derivation and justification of the Korteweg de Vries (KdV) equation; [5] in which the nonlinear Schrödinger (nlS) equation emerges as a macroscopic description of modulated pulses; and [2, 1] in which Whitham's modulation theory is applied to FPU-like chains ($W \equiv 0$) in order to describe the macroscopic dynamics of strong microscopic oscillations. Finally, for discrete crystal models with harmonic interactions we quote [12] (but see also the more recent [6]), in which the macroscopic continuum limit is described in terms of linear wave equations and transport equations for the Wigner measure (see [9] and [4]).

The common feature of all the cited work is that the mass distribution is microscopically constant or at least periodic (for the case in which m varies on the macroscopic scale, we refer to [13]). On the contrary, here we are interested in the macroscopic behaviour of (1.1) with quadratic V and $W \equiv 0$ but with a mass distribution of the type

$$m(y) := 1 + (M-1)\delta(y), \tag{1.2}$$

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when the value of the heavy mass M becomes large. More precisely, we consider the lattice

$$m(y)\ddot{u}(y,\tau) = u(y+1,\tau) - 2u(y,\tau) + u(y-1,\tau) \tag{1.3}$$

with $y \in \mathbb{Z}$, $m(y)$ as in (1.2), and initial conditions

$$u(y,0) = u_0(y), \quad \dot{u}(y,0) = \dot{u}_0(y). \tag{1.4}$$

Then, by introducing the scaling parameter ε related to the heavy mass by $\varepsilon := \frac{1}{M}$, we study the macroscopic limit $\varepsilon \to 0$ of (1.3) using the *hyperbolic scaling.* That means the macroscopic time and the macroscopic (Lagrangian) space coordinate are given by $t := \varepsilon\tau$ and $x := \varepsilon y$, respectively, and the atomic distances are scaled by ε. We recall that other scalings are reasonable but describe different macroscopic regimes. For instance, the nlS equations corresponds to $t = \varepsilon^2\tau$ and $x = \varepsilon(y - c\tau)$, with c being the sound velocity, and the KdV equation relies on $t = \varepsilon^3\tau$ and $x = \varepsilon(y - c\tau)$.

The system (1.3) represents a crude, although rich of interesting behaviour, model for a monatomic crystal with an impurity. The problem of understanding how defects and impurities can influence the lattice vibration has a long story, both from the phenomenological and analytical point of view starting from the pioneering works [14] and [11]. Note that our system (1.3) has some similarities with the microscopic justification of the Brownian motion for lattice systems as in [15] and [16], and with the analysis of the Rayleigh gas in [17]. However, our work aims in a different direction as we concentrate on deterministic initial conditions and derive a continuum PDE governing the macroscopic evolution of the chain coupled with an ODE for the evolution of the heavy particle. More precisely, our macroscopic system consists of the usual wave equation for a macroscopic field $\mathcal{U}$ (related to the microscopic displacements u in a proper way) that holds for all $x \neq 0$, and describes the effective behaviour of the light particles. This PDE is strongly related to the heavy particle evolution by

$$\mathcal{U}(0,t) = \bar{u}(t) \quad \text{and} \quad \mathcal{U}_x(0^+,t) - \mathcal{U}_x(0^-,t) = \partial_t^2\bar{u}(t).$$

Here $\bar{u}$ is the macroscopic trajectory of heavy particle which evolves according to the first order ODE

$$\partial_t\bar{u} + 2\bar{u} = \bar{v}_0 + \bar{r},$$

where the constant $\bar{v}_0$ depends on the initial data. The forcing function $\bar{r} = \bar{r}(t)$ describes how the macroscopic evolution of the light particles affects the heavy particle, and can be computed from the initial data by solving a linear wave equation. The main effect of the light particles, however, is to decelerate the heavy particle via the term $2\bar{u}$.

It is interesting to note that the lattice (1.3) could be rewritten in the equivalent form

$$\ddot{u}(y,\tau) = u(y+1,\tau) - 2u(y,\tau) + u(y-1,\tau) - \frac{M-1}{M}\Phi(y)u(y,\tau), \tag{1.5}$$

where the potential function

$$\Phi(y) := \delta(y-1) - 2\delta(y) + \delta(y+1)$$

is supported only on the sites $-1, 0, 1$. The spectral properties of discrete Schrödinger operators of the type

$$-\Delta_d + \Phi(y), \tag{1.6}$$

where $\Delta_d u$ is the discrete Laplacian $\Delta_d u = u(y+1) - 2u(y) + u(y-1)$, have been recently determined in [7]. Using these results (but see also the former [8]) one can characterise the complete solution to the heavy-particle chain (1.3) for any fixed value of M. In this paper, however, we focus on the evolution of the heavy particle in the limit $\varepsilon \to 0$ and do not exploit the spectral properties of (1.6).

The paper is organised as follows. In Section 2 we introduce a rigorous mathematical framework for the micro-to-macro transition, and state our main results in Theorem 2.4. The proof of this theorem is contained in Section 3, and we conclude with some numerical simulations in Section 4.

2 Macroscopic behaviour of the system

The lattice (1.3) is a Hamiltonian system. In particular, the energy

$$\mathcal{E}(u, \dot{u}) = \mathcal{K}(\dot{u}) + \mathcal{P}(u) \tag{2.1}$$

given by

$$\mathcal{K}(\dot{u}) = \frac{1}{2}\sum_{y\in\mathbb{Z}} |\dot{u}(y)|^2 + \frac{M-1}{2}|\dot{u}_M|^2, \quad \mathcal{P}(u) = \frac{1}{2}\sum_{y\in\mathbb{Z}}(u(y+1) - u(y))^2. \tag{2.2}$$

is conserved during the evolution. Notice that we have outlined the contribution of the heavy mass in (2.2) by writing $u_M = u(0)$. For any $M > 0$ the system (1.3) is well–posed in the phase space $\mathcal{X} = \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$. That means, given an initial datum $(u(y, 0), \dot{u}(y, 0)) \in \mathcal{X}$, the equation (1.3) has unique solution $u \in C^2([0, +\infty); \mathcal{X})$.

For $M = 1$ the system (1.3) reduces to the harmonic chain and admits plane wave solutions

$$u(y, t) = e^{i(\omega t+\vartheta y)},$$

with frequency ω and wave vector $\vartheta \in \Omega = [-\pi, \pi]$, provided that ω satisfies the *dispersion relation*

$$\omega^2(\vartheta) = 2(1 - \cos(\vartheta)) = 4\sin^2(\theta/2). \tag{2.3}$$

Our subsequent analysis relies on both the discrete and the continuous Fourier transform. Recall, that for any $u \in \ell^2(\mathbb{Z})$ its discrete Fourier transform $\hat{u} = \mathcal{F}_{y\to\vartheta} u \in L^2(\Omega)$ is given by

$$\hat{u}(\vartheta) := \sum_{y\in\mathbb{Z}} e^{-i\vartheta y} u(y),$$

and the inversion formula reads

$$u(y) = \frac{1}{2\pi}\int_\Omega e^{iy\vartheta}\hat{u}(\vartheta)d\vartheta.$$

Applying the discrete Fourier transform to the lattice (1.3) we readily find

$$\ddot{\hat{u}}(\tau, \vartheta) + \frac{M-1}{2\pi}\int_\Omega \ddot{\hat{u}}(\tau, \vartheta)d\vartheta = -\omega^2(\vartheta)\hat{u}(\tau, \vartheta), \tag{2.4}$$

where ω is defined in (2.3).

Besides the discrete Fourier transform, we will also make an extensive use of the continuous Fourier transform $\mathcal{F}_{x\to\eta} : L^2(\mathbb{R}_x) \to L^2(\mathbb{R}_\eta)$ with

$$\hat{\mathcal{U}}(\eta) := \int_\mathbb{R} e^{-i\eta x}\mathcal{U}(x)dx, \qquad \mathcal{U}(x) = \frac{1}{2\pi}\int_\mathbb{R} e^{i\eta x}\hat{\mathcal{U}}(\eta)d\eta.$$

2.1 Passage to macroscopic time and space

In this section we consider large values for the mass M of the heavy particle and pass to the macroscopic scale. More precisely, we introduce the scaling parameter $\varepsilon := \frac{1}{M}$, and define the macroscopic time t and the macroscopic particle index x (and its dual variable η in the Fourier space) by

$$\begin{cases} \tau \in \mathbb{R} \rightsquigarrow t := \varepsilon\tau \in \mathbb{R}, \\ y \in \mathbb{Z} \rightsquigarrow x := \varepsilon y \in \mathbb{R}, \\ \vartheta \in \Omega \rightsquigarrow \eta := \frac{\theta}{\varepsilon} \in \frac{1}{\varepsilon}\Omega. \end{cases}$$

Following the scaling approach from [12], we introduce two operators relating the microscopic coordinates (ϑ and y) to the macroscopic ones (η and x). At first we define an operator $\mathcal{C}_\varepsilon : \ell^2(\mathbb{Z}) \to L^2(\mathbb{R}_\eta)$ by

$$\mathcal{C}_\varepsilon(f)(\eta) := \varepsilon^{1/2}\chi_\varepsilon(\eta)(\mathcal{F}_{y\to\vartheta}f)(\varepsilon\eta),$$

where $\chi_\varepsilon(\eta)$ denotes the characteristic function of the interval $\frac{1}{\varepsilon}\Omega$. Notice that the presence of the scaling factor $\varepsilon^{1/2}$ entails that $\mathcal{C}_\varepsilon$ is an isometry. Moreover, we introduce the operator $\mathcal{S}_\varepsilon : \ell^2(\mathbb{Z}) \to L^2(\mathbb{R}_x)$ by

$$f^\varepsilon(x) = (\mathcal{S}_\varepsilon f)(x) := \mathcal{F}^{-1}_{\eta\mapsto x}(\mathcal{C}_\varepsilon f)(x), \tag{2.5}$$

which is again an isometry. $\mathcal{S}_\varepsilon$ can be viewed as an interpolation operator between microscopic and macroscopic scale. In fact, the definition (2.5) implies

$$(\mathcal{S}_\varepsilon f)(x) = \left(\frac{1}{2\pi\varepsilon}\right)^{1/2} \sum_{y\in\mathbb{Z}} f(y)\mathrm{sinc}(\frac{x}{\varepsilon} - y), \quad x \in \mathbb{R},$$

for all $f \in \ell^2(\mathbb{Z})$ and all $x \in \mathbb{R}$, where $\mathrm{sinc} := \mathcal{F}^{-1}_{\eta\mapsto x}\chi_\Omega$.

We now implement this scaling machinery to reformulate the lattice system (1.3). First of all, given any solution u to (1.3) we define the macroscopic displacements $\mathcal{U}^\varepsilon$ and the macroscopic heavy particle trajectory u^ε_M by

$$\mathcal{U}^\varepsilon(x,t) := \varepsilon(\mathcal{S}_\varepsilon u)(x, t/\varepsilon), \tag{2.6}$$

$$u^\varepsilon_M(t) := \mathcal{U}^\varepsilon(0,t) = \frac{1}{2\pi}\int_{\mathbb{R}_\eta} \hat{\mathcal{U}}^\varepsilon(\eta,t)d\eta. \tag{2.7}$$

Correspondingly, the macroscopic time derivatives are given by

$$\begin{aligned} &\partial_t\mathcal{U}^\varepsilon(x,t) = (\mathcal{S}_\varepsilon\dot{u})(x,t/\varepsilon), \\ &\partial_t u^\varepsilon_M(t) = \partial_t\mathcal{U}^\varepsilon(0,t) = \frac{1}{2\pi}\int_{\mathbb{R}_\eta} \partial_t\hat{\mathcal{U}}^\varepsilon(\eta,t)d\eta, \end{aligned} \tag{2.8}$$

and using the definitions of $\mathcal{S}_\varepsilon$ and $\mathcal{C}_\varepsilon$ we find the relations for the Fourier transformed quantities. More precisely, we obtain

$$\begin{aligned} \hat{\mathcal{U}}^\varepsilon(\eta,t) &= (\mathcal{F}_{x\to\eta}\mathcal{U}^\varepsilon)(\eta,t) = \varepsilon\mathcal{F}_{x\to\eta}(\mathcal{S}_\varepsilon u)(\eta,t/\varepsilon) = \varepsilon(\mathcal{C}_\varepsilon u)(\eta,t/\varepsilon) \\ &= \varepsilon^{3/2}\chi_\varepsilon(\eta)\hat{u}(\varepsilon\eta,t/\varepsilon), \end{aligned}$$

and hence

$$\partial_t\hat{\mathcal{U}}^\varepsilon(\eta,t) = \sqrt{\varepsilon}\chi_\varepsilon(\eta)\hat{u}(\varepsilon\eta,t/\varepsilon).$$

For later use we state the scaling relations between $u_M^\varepsilon(t)$, $\partial_t u_M^\varepsilon(t)$ and their microscopic counterparts $u(0,t/\varepsilon)$ and $\dot u(0,t/\varepsilon)$. Exploiting the above definitions, we find

$$u_M^\varepsilon(t) = \frac{1}{2\pi}\int_{\mathbb{R}_\eta} \hat{\mathcal{U}}^\varepsilon(\eta,t)d\eta = \sqrt{\varepsilon}\frac{1}{2\pi}\int_\Omega \hat u(\vartheta,t/\varepsilon)d\vartheta = \varepsilon^{1/2}u(0,t/\varepsilon), \tag{2.9}$$

$$\partial_t u_M^\varepsilon(t) = \frac{1}{2\pi}\int_{\mathbb{R}_\eta} \partial_t\hat{\mathcal{U}}^\varepsilon(\eta,t)d\eta = \frac{1}{\sqrt{\varepsilon}}\frac{1}{2\pi}\int_\Omega \hat{\dot u}(\vartheta,t/\varepsilon)d\vartheta = \frac{1}{\sqrt{\varepsilon}}\dot u(0,t/\varepsilon). \tag{2.10}$$

Our next goal is to identify the evolution equations for the couple (2.6)–(2.7). Multiplying the Fourier transformed lattice equation (2.4) with $\varepsilon^{1/2}\chi_\varepsilon(\eta)$, and using $M = 1/\varepsilon$, we obtain

$$\partial_\tau^2(\mathcal{C}_\varepsilon u)(\eta,\tau) + \frac{1-\varepsilon}{2\pi\varepsilon}\chi_\varepsilon(\eta)\int_\Omega \varepsilon^{1/2}\partial_\tau^2\hat u(\vartheta,\tau)d\vartheta = -\omega^2(\varepsilon\eta)(\mathcal{C}_\varepsilon u)(\eta,\tau).$$

Notice that by the change of variables $\theta = \varepsilon\lambda$, the integral term in this equation can be written as

$$\frac{1-\varepsilon}{2\pi\varepsilon}\chi_\varepsilon(\eta)\int_\Omega \varepsilon^{1/2}\partial_\tau^2\hat u(\vartheta,\tau)d\vartheta = \varepsilon\frac{1-\varepsilon}{2\pi\varepsilon}\chi_\varepsilon(\eta)\int_{\mathbb{R}}\partial_\tau^2(\mathcal{C}_\varepsilon u)(\lambda,\tau)d\lambda.$$

Consequently, the couple $(\mathcal{U}^\varepsilon, u_M^\varepsilon)$ verifies

$$\partial_t^2\mathcal{U}^\varepsilon(x,t) + \frac{1-\varepsilon}{\varepsilon}a_\varepsilon(x)\partial_t^2 u_M^\varepsilon(t) + \mathcal{A}_\varepsilon\mathcal{U}^\varepsilon(x,t) = 0, \tag{2.11}$$

where the linear operator $\mathcal{A}_\varepsilon$ and the function a_ε are defined by

$$\mathcal{A}_\varepsilon v(x) := \frac{1}{\varepsilon^2}\mathcal{F}^{-1}_{\eta\to x}(\chi_\varepsilon(\cdot)\omega^2(\varepsilon\cdot)\hat v)(x), \quad a_\varepsilon(x) := \varepsilon\mathcal{F}^{-1}_{\eta\to x}(\chi_\varepsilon)(x). \tag{2.12}$$

In what follows we consider families of solutions, depending on the parameter ε, emanating from a family of initial data. The corresponding solutions to (1.3) will be then denoted by u^ε. Here are the assumptions on the initial conditions.

Assumptions on Initial Data 2.1. *Let $(u_0^\varepsilon, \dot u_0^\varepsilon)_{\varepsilon>0} \subset \ell^2(\mathbb{Z})\times\ell^2(\mathbb{Z})$ be a family of initial data with following properties: There exist constants $\bar v_0 \in \mathbb{R}$ and $C > 0$ such that*

$$\begin{aligned} \dot u_0^\varepsilon(0) &= \sqrt{\varepsilon}\bar v_0, \\ \varepsilon\|u_0^\varepsilon\|_{\ell^2(\mathbb{Z})} + \mathcal{E}(u_0^\varepsilon, \dot u_0^\varepsilon) &\le C, \end{aligned}$$

as well as functions $\mathcal{U}_0 \in H^1(\mathbb{R})$ and $\mathcal{V}_0 \in L^2(\mathbb{R})$ such that

$$\mathcal{U}_0^\varepsilon := \varepsilon\mathcal{S}_\varepsilon u_0^\varepsilon \rightharpoonup \mathcal{U}_0 \text{ and } \mathcal{V}_0^\varepsilon := \mathcal{S}_\varepsilon\dot u_0^\varepsilon \rightharpoonup \mathcal{V}_0$$

weakly in $H^1(\mathbb{R})$ and $L^2(\mathbb{R})$, respectively.

We collect the results of this section in the following Lemma. In particular, we prefer to work with the weak formulation of (2.11), because it turns out to be useful for the limit $\varepsilon \to 0$.

Lemma 2.2. *For any family of initial data as in Assumption 2.1 the functions $(\mathcal{U}^\varepsilon, u_M^\varepsilon)$ from (2.6) and (2.7) with $\mathcal{U}^\varepsilon : [0,+\infty) \to L^2(\mathbb{R})$ and $u_M^\varepsilon : [0,+\infty) \to \mathbb{R}$ verify,*

$$u_M^\varepsilon(t) = \frac{1}{2\pi}\int_{\mathbb{R}_\eta}\hat{\mathcal{U}}^\varepsilon(\eta,t)d\eta$$

and

$$\frac{1-\varepsilon}{\varepsilon}\int_{\mathbb{R}_x\times[0,+\infty)} u^\varepsilon_M(t)a_\varepsilon(x)\varphi_{tt}(x,t)dxdt+\int_{\mathbb{R}_x\times[0,+\infty)}\mathcal{U}^\varepsilon(x,t)\Big(\varphi_{tt}(x,t)+\mathcal{A}_\varepsilon\varphi(x,t)\Big)dxdt \tag{2.13}$$
$$=-\int_{\mathbb{R}_x}\mathcal{U}^\varepsilon_0(x)\varphi_t(x,0)dx+\int_{\mathbb{R}_x}\mathcal{V}^\varepsilon_0(x)\varphi(x,0)dx,$$

for any $\varphi\in C^2([0,+\infty);H^1(\mathbb{R}))$ *with bounded support.*

2.2 The main result

Before stating our main result, we introduce also the function

$$w^\varepsilon:[0,+\infty)\mapsto\ell^2(\mathbb{Z})$$

as the unique solution of the linear harmonic chain with equal masses and initial conditions identical to those for u^ε. More precisely, $w^\varepsilon=w^\varepsilon(y,t)$ is the unique solution to

$$\begin{cases}\ddot w^\varepsilon(y,t) &= w^\varepsilon(y+1,t)-2w^\varepsilon(y,t)+w^\varepsilon(y-1,t)\\ w^\varepsilon(y,0) &= u^\varepsilon_0,\\ \dot w^\varepsilon(y,0) &= \dot u^\varepsilon_0.\end{cases}$$

Then, we introduce the macroscopic analogon

$$\mathcal{W}^\varepsilon(x,t):=\varepsilon(\mathcal{S}_\varepsilon w^\varepsilon)(x,t/\varepsilon).$$

The main result on the harmonic chain is provided by [12, Theorem 4.2] and can be stated as follows.

Lemma 2.3. *Assumption 2.1 implies*

$$\left.\begin{array}{r}\mathcal{W}^\varepsilon(t)=\varepsilon\mathcal{S}_\varepsilon w^\varepsilon(t/\varepsilon)\rightharpoonup\mathcal{W}(t)\ \textit{in}\ H^1(\mathbb{R})\\ \partial_t\mathcal{W}^\varepsilon(t)=\mathcal{S}_\varepsilon\dot w^\varepsilon(t/\varepsilon)\rightharpoonup\partial_t\mathcal{W}(t)\ \textit{in}\ L^2(\mathbb{R})\end{array}\right\}\ \textit{as}\ \varepsilon\searrow 0 \tag{2.14}$$

for all $t\geq 0$. *Moreover,* $\mathcal{W}\in C^1_{loc}([0,+\infty);L^2(\mathbb{R}))\cap C^0_{loc}([0,+\infty);H^1(\mathbb{R}))$ *is the unique solution to*

$$\begin{cases}\mathcal{W}_{tt}-\Delta\mathcal{W}=0\ \textit{in}\ \ \textit{in}\ (H^1(\mathbb{R}))',\ \textit{and for a.a.}t\geq 0,\\ \mathcal{W}(x,0)=\mathcal{U}_0(x)\ \textit{a.e. in}\ \mathbb{R},\ \ \mathcal{W}_t(x,0)=\mathcal{V}_0(x)\ \textit{a.e. in}\ \mathbb{R}.\end{cases} \tag{2.15}$$

Here is the main result of this paper.

Theorem 2.4. *Under Assumption 2.1, there exists a unique couple* $(\bar u,\mathcal{U})$ *such that*

$$\left.\begin{array}{r}\mathcal{U}^\varepsilon(t)=\varepsilon\mathcal{S}_\varepsilon u^\varepsilon(t/\varepsilon)\rightharpoonup\mathcal{U}(t)\ \textit{in}\ H^1(\mathbb{R})\ \textit{for any}\ t\geq 0,\\ u^\varepsilon_M\to\bar u\ \textit{in}\ L^p_{loc}([0,+\infty)),\ \ 1\leq p<+\infty\end{array}\right\}\ \textit{as}\ \varepsilon\searrow 0.$$

Moreover, the couple $(\bar u,\mathcal{U})$ *is the unique solution to*

$$\begin{cases}\partial_t\bar u+2\bar u=\bar v_0+2\mathcal{W}(0,t)\ \textit{for all}\ t\geq 0,\bar u(0)=\mathcal{W}(0,0),\\ \displaystyle\int_{\mathbb{R}}\bar u(t)\langle\delta(\cdot),\varphi_{tt}(\cdot,t)\rangle dt+\int_{\mathbb{R}}\langle\mathcal{U}(\cdot,t),\varphi_{tt}(\cdot,t)-\Delta\varphi(\cdot,t)\rangle dt\\ \displaystyle\qquad\qquad=-\int_{\mathbb{R}}\mathcal{U}_0(x)\varphi_t(x,0)dx+\int_{\mathbb{R}}\mathcal{V}_0(x)\varphi(x,0)dx,\end{cases} \tag{2.16}$$

for all $\varphi\in C^2([0,+\infty);H^1(\mathbb{R}))$ *with bounded support and* $\mathcal{W}$ *as in Lemma 2.3.*

We proceed with some comments on the structure of the limit problem (2.16). First we mention that the equation for $\mathcal{U}$ is the weak formulation of the wave equation

$$\mathcal{U}_{tt}(x,t) - \Delta\mathcal{U}(x,t) = -\partial_t^2 \bar{u}(t)\delta(x), \tag{2.17}$$

and that $\mathcal{U}(\cdot,t) \in H^1(\mathbb{R})$ implies the continuity equation

$$\mathcal{U}(0^+,t) = \mathcal{U}(0^-,t).$$

Moreover, by construction we also have that $\bar{u}(t) \equiv \mathcal{U}(0,t)$ for any $t \geq 0$.

This fact is independent of the microscopic justification and can be proved by representing the solution to (2.17) by convolution with fundamental solution to the wave equation. We also notice that (2.17) is, at least for sufficiently regular initial conditions $\mathcal{U}_0$ and $\mathcal{V}_0$, equivalent to

$$\begin{cases} \partial_t^2 \bar{u}(t) = \mathcal{U}_x(0^+,t) - \mathcal{U}_x(0^-,t) \\ \mathcal{U}_{tt}(x,t) - \Delta\mathcal{U}(x,t) = 0 \text{ for } x > 0, \\ \mathcal{U}_{tt}(x,t) - \Delta\mathcal{U}(x,t) = 0 \text{ for } x < 0, \end{cases} \tag{2.18}$$

The coupling between the PDE and the ODE in (2.18) is interesting for it shows that the heavy particle causes a jump in the macroscopic strain $\mathcal{U}_{\S}$.

Finally, we discuss the interactions between the heavy particle and the 'background medium', which is made of the light particles. According to the ODE from (2.16), the medium decelerates the heavy particle due to the microscopic interactions, and the heavy mass drives the macroscopic evolution in the medium. However, if the initial value problem for $\mathcal{W}$ has a non-trivial solution, then there is a further macroscopic contribution of the medium to the evolution of the heavy mass. In particular, the medium can even accelerate the heavy particle, see for instance Example 2 in Section 4. In Corollary 2.5, we give a sufficient condition for the forcing term $\mathcal{W}(0,t)$ to vanish, so that the heavy mass decays exponentially to rest in this case.

Corollary 2.5. *If the initial data from Assumption 2.1 additionally satisfy*

$$\varepsilon\|u_0^\varepsilon\|_{\ell^1(\mathbb{Z})} + \|\dot{u}_0^\varepsilon\|_{\ell^1(\mathbb{Z})} \leq C$$

for some constant C independent of ε, then the forcing term $\mathcal{W}(0,t)$ in (2.16) vanishes.

Proof. We aim to show that the limits of the initial data vanish, that means $\mathcal{U}_0 \equiv 0$ and $\mathcal{V}_0 \equiv 0$, because this implies $\mathcal{W} \equiv 0$ thanks to the linear wave equation (2.15). To this end recall that

$$\int_{\mathbb{R}} (\mathcal{S}_\varepsilon \dot{u}^\varepsilon)(x)\varphi(x)dx = \varepsilon^{-1/2}\int_\Omega \hat{\dot{u}}^\varepsilon(\vartheta)\hat{\varphi}\Big(\frac{\vartheta}{\varepsilon}\Big)d\vartheta,$$

for any $\varphi \in L^2(\mathbb{R})$. Since $\dot{u}^\varepsilon$ is bounded in $\ell^1(\mathbb{Z})$, we find that $\hat{\dot{u}}^\varepsilon$ is bounded in $L^\infty(\Omega)$, which implies

$$\left|\int_{\mathbb{R}} (\mathcal{S}_\varepsilon \dot{u}^\varepsilon)(x)\varphi(x)dx\right| \leq C\int_\Omega \left|\hat{\varphi}\Big(\frac{\vartheta}{\varepsilon}\Big)\right| d\vartheta \leq \varepsilon C\|\hat{\varphi}\|_{L^1(\mathbb{R}_\eta)}.$$

for all test functions $\varphi \in \mathcal{S}(\mathbb{R}_\eta)$. From this we conclude $\mathcal{V}_0^\varepsilon = \mathcal{S}_\varepsilon \dot{u}^\varepsilon \to 0$ in $\mathcal{S}'(\mathbb{R}_x)$, and hence $\mathcal{V}_0 \equiv 0$. The proof of $\mathcal{U}_0 \equiv 0$ is analogous. ∎

3 Proof of the main result

The proof is organised as follows. In Section 3.1 we first derive some uniform (w.r.t. $\varepsilon > 0$) a priori estimates for $\mathcal{U}^\varepsilon, u_M^\varepsilon$ and $\partial_t u_M^\varepsilon$. These estimates, combined with some compactness arguments, entail the existence of a limit field $\mathcal{U}$ and a limit function $\bar{u}$. These limits are shown to satisfy the PDE in Section 3.2, and in Section 3.3 we establish the ODE for $\bar{u}$.

We give advice to the reader that with the same symbol C we will denote (possibly different) positive constants which can depend on the initial data but are independent of ε. Moreover, with a slight abuse of notation, we will indicate with the same symbol $\langle\cdot,\cdot\rangle$ a duality pairing, with respect to both the time and space variable. Moreover, we indicate with $\Delta = (\cdot)_{xx}$ the bounded linear operator acting from $H^1(\mathbb{R}) \to (H^1(\mathbb{R}))'$ such that

$$\langle -\Delta\mathcal{U}, \mathcal{V}\rangle := \int_{\mathbb{R}} \nabla\mathcal{U}(x)\cdot\nabla\mathcal{V}(x)dx, \quad \forall \mathcal{U},\mathcal{V}\in H^1(\mathbb{R}),$$

with $\nabla\mathcal{U} = \partial_x\mathcal{U}$.

3.1 Compactness results

Lemma 3.1. *There exists a constant $C > 0$ such that*

$$\frac{1}{2}\|\partial_t\mathcal{U}^\varepsilon(t)\|^2 + \frac{1}{2}\|\nabla\mathcal{U}^\varepsilon(t)\|^2 + \frac{1-\varepsilon}{2}|\partial_t u_M^\varepsilon(t)|^2 \le C \tag{3.1}$$

holds for all $t \ge 0$ and $\varepsilon > 0$.

Proof. Due to the choice of the scaling, the definitions (2.8) and (2.10), and the properties of the interpolation operator $\mathcal{S}_\varepsilon$ we find

$$\begin{aligned}\frac{1}{2}\int_{\mathbb{R}_x} |\partial_t\mathcal{U}^\varepsilon(x,t)|^2dx + \frac{1}{2}(1-\varepsilon)|\partial_t u_M^\varepsilon(t)|^2 + \frac{1}{2}\int_{\mathbb{R}_x}\mathcal{A}_\varepsilon\mathcal{U}^\varepsilon\cdot\mathcal{U}^\varepsilon(x,t)dx \\ = \mathcal{E}(u^\varepsilon,\dot{u}^\varepsilon)(t/\varepsilon) = \mathcal{E}(u^\varepsilon,\dot{u}^\varepsilon)(0),\end{aligned}$$

where the last equality comes from the conservation of energy, compare (2.1). Using the Plancherel Theorem and (2.12) we also obtain

$$\int_{\mathbb{R}}\mathcal{A}_\varepsilon\mathcal{U}^\varepsilon(x)\mathcal{U}^\varepsilon(x)dx = (2\pi)^{-1}\int_{\Omega_\varepsilon}\frac{1}{\varepsilon^2}\omega^2(\varepsilon\eta)|\hat{\mathcal{U}}^\varepsilon(\eta)|^2d\eta,$$

and thanks to $\omega(\theta)^2 \ge C\theta^2$ for all $\theta\in\Omega$ we find

$$\int_{\mathbb{R}}\mathcal{A}_\varepsilon\mathcal{U}^\varepsilon(x)\mathcal{U}^\varepsilon(x)dx \ge C\int_{\Omega_\varepsilon}\eta^2|\hat{\mathcal{U}}^\varepsilon(\eta)|^2d\eta = C\|\nabla\mathcal{U}^\varepsilon\|^2_{L^2(\mathbb{R})}.$$

This estimate completes the proof since the initial energy is bounded by assumption. ∎

Lemma 3.2. *We have*

$$|u_M^\varepsilon(t)| \le C(t+1), \quad |\partial_t u_M^\varepsilon(t)| \le C \tag{3.2}$$

for all for $t \ge 0$.

Proof. The energy estimate (3.1) gives

$$|\partial_t u^\varepsilon_M(t)| \le C,$$

end hence

$$|u^\varepsilon_M(t)| \le |u^\varepsilon_M(0)| + \int_0^t |\partial_t u^\varepsilon_M(s)| ds \le C(t+1).$$

∎

As an immediate corollary of the two Lemmata above, we obtain the following compactness result.

Corollary 3.3. *There exists a (not relabelled) subsequence of ε and two limit functions $(\mathcal{U}, \bar{u})$ with $\mathcal{U} \in W^{1,\infty}_{loc}\big([0,+\infty), L^2(\mathbb{R})\big) \cap L^\infty_{loc}\big([0,+\infty), H^1(\mathbb{R})\big)$ and $\bar{u} \in W^{1,\infty}(\mathbb{R})$ such that*

$$\mathcal{U}^\varepsilon(t) \rightharpoonup \mathcal{U}(t) \text{ in } H^1(\mathbb{R}) \text{ for all } t \ge 0, \tag{3.3}$$

$$u^\varepsilon_M \to \bar{u} \text{ in } L^p_{loc}(\mathbb{R}) \text{ for any } p \in [1, \infty). \tag{3.4}$$

Proof. Besides the estimates for $\partial_t \mathcal{U}^\varepsilon$, the energy bound (3.1) also implies that

$$\|\mathcal{U}^\varepsilon(t)\|_{L^2(\mathbb{R})} \le C(t+1) \tag{3.5}$$

for some C independent of t and ε. Thus, standard weak compactness results provide the existence of a limit function in $\mathcal{U}$ and of a (not relabelled) subsequence of $\varepsilon \searrow 0$ such that

$$\mathcal{U}^\varepsilon \overset{*}{\rightharpoonup} \mathcal{U} \text{ in } L^\infty_{loc}\big([0,+\infty); H^1(\mathbb{R})\big), \tag{3.6}$$

$$\partial_t \mathcal{U}^\varepsilon \overset{*}{\rightharpoonup} \partial_t \mathcal{U} \text{ in } L^\infty\big([0,+\infty); L^2(\mathbb{R})\big). \tag{3.7}$$

Moreover, a standard argument shows that (3.6) and (3.7) entail

$$\mathcal{U}^\varepsilon(t) \rightharpoonup \mathcal{U} \text{ in } H^1(\mathbb{R}) \text{ locally uniformly in } [0, +\infty).$$

Finally, the $W^{1,\infty}$-regularity and the convergence (3.4) follows from Lemma 3.2 and standard criterions for strong L^p-compactness. ∎

3.2 Wave equation for $\mathcal{U}$

Now we study the limits of the operator $\mathcal{A}_\varepsilon$ and the function $\frac{1}{\varepsilon} a_\varepsilon$.

Lemma 3.4. *For each $\psi \in H^1(\mathbb{R})$ we have*

$$\mathcal{A}_\varepsilon \psi \xrightarrow{\varepsilon \to 0} -\Delta \psi \text{ in } (H^1(\mathbb{R}))' \tag{3.8}$$

and

$$\int_{\mathbb{R}} a_\varepsilon(x) \psi(x) dx \xrightarrow{\varepsilon \to 0} \psi(0). \tag{3.9}$$

Proof. Using the Fourier transform, it is apparent that the convergence (3.8) is equivalent to

$$\lim_{\varepsilon \searrow 0} \int_{\mathbb{R}_\eta} (1 + |\eta|^2)^{-1} |\eta^2 - \chi_\varepsilon(\eta) \frac{1}{\varepsilon^2} \omega^2(\varepsilon\eta)|^2 |\hat{\psi}(\eta)|^2 d\eta = 0. \tag{3.10}$$

The functions

$$\eta \mapsto |\eta^2 - \chi_\varepsilon(\eta)\frac{1}{\varepsilon^2}\omega^2(\varepsilon\eta)|^2$$

are bounded by $C|\eta|^2$ and converge pointwise to 0 as $\varepsilon > 0$. Therefore, the Dominated Convergence Theorem applies to (3.10), where the dominant $(1+|\eta|^2)^{-1}|\eta|^2|\hat{\psi}|^2$ is integrable since $\psi \in H^1(\mathbb{R})$. Finally, (3.9) follows from

$$\begin{aligned}\lim_{\varepsilon\searrow 0}\int_{\mathbb{R}_x}\frac{1}{\varepsilon}a_\varepsilon(x)\psi(x)dx &= \lim_{\varepsilon\searrow 0}\frac{1}{2\pi}\int_{\mathbb{R}_\eta}\frac{1}{\varepsilon}\mathcal{F}_{x\to\eta}(a_\varepsilon)(\eta)\mathcal{F}_{x\to\eta}\psi(\eta)d\eta \\ &= \lim_{\varepsilon\searrow 0}\frac{1}{2\pi}\int_{\mathbb{R}_\eta}\chi_\varepsilon(\eta)\mathcal{F}_{x\to\eta}\psi(\eta)d\eta = \psi(0),\end{aligned}$$

and the proof is complete. ∎

Lemma 2.2 combined with Lemma 3.4 provides the evolution equation for $\mathcal{U}$ claimed in Theorem 2.4.

Corollary 3.5. *The couple $(\mathcal{U}, \bar{u})$ from Corollary 3.3 satisfies*

$$\begin{aligned}&\int_0^\infty \bar{u}(t)\langle\delta(\cdot), \varphi_{tt}(\cdot,t)\rangle dt + \int_0^\infty \langle\mathcal{U}(\cdot,t), \varphi_{tt}(\cdot,t) - \Delta\varphi(\cdot,t)\rangle dt \\ &= -\int_{\mathbb{R}}\mathcal{U}_0(x)\varphi_t(x,0)dx + \int_{\mathbb{R}}\mathcal{V}_0(x)\varphi(x,0)dx.\end{aligned}$$

for all $\varphi \in C_c^2([0,+\infty); H^1(\mathbb{R}))$ with bounded support.

Proof. Form Lemma 3.4 we conclude that

$$\langle\mathcal{U}^\varepsilon(\cdot,t), \varphi_{tt}(\cdot,t) + \mathcal{A}_\varepsilon\varphi(\cdot,t)\rangle \xrightarrow{\varepsilon\to 0} \langle\mathcal{U}(\cdot,t), \varphi_{tt}(\cdot,t) - \Delta\varphi(\cdot,t)\rangle,$$

and

$$\int_{\mathbb{R}_x} u_M^\varepsilon(t)\frac{1-\varepsilon}{\varepsilon}a_\varepsilon(x)\varphi_{tt}(x,t)dx \xrightarrow{\varepsilon\to 0} \bar{u}(t)\langle\delta(\cdot), \varphi_{tt}(\cdot,t)\rangle$$

holds pointwise in t. We combine these pointwise results with the a priori estimates (3.5), (3.2) and the convergence of the initial data, and we derive the desired result from (2.13) by means of the Dominated Convergence Theorem. ∎

3.3 Evolution of the heavy particle

In this section we derive the core of Theorem 2.4, that is the ODE for the heavy particle. At first we prove that the microscopic functions u_M^ε solve some integral equations involving the the zeroth order Bessel function, compare [19],

$$J_0(z) = \frac{1}{2\pi}\int_\Omega \cos(z\sin(\vartheta))d\vartheta.$$

Lemma 3.6. *For all $\varepsilon > 0$ the function $u_M^\varepsilon(t)$ satisfies*

$$u_M^\varepsilon(t) = \bar{v}_0\frac{1-\varepsilon}{2\pi}\int_\Omega\frac{\sin\Big(\omega(\vartheta)\frac{t}{\varepsilon}\Big)}{\omega(\vartheta)}d\vartheta - \int_0^t\frac{1-\varepsilon}{\varepsilon}J_0\Big(\frac{2(t-r)}{\varepsilon}\Big)\partial_r u_M^\varepsilon(r)dr + \mathcal{W}^\varepsilon(0,t), \tag{3.11}$$

with ω as in (2.3).

PROOF. ¿From the Fourier transformed lattice equation (2.4) and the definitions (2.6) and (2.7) we derive

$$\partial_t^2 \hat{\mathcal{U}}^\varepsilon(\eta,t) + \frac{1-\varepsilon}{2\pi}\chi_\varepsilon(\eta)\partial_t^2 u_M^\varepsilon(t) = -\frac{1}{\varepsilon^2}\omega^2(\varepsilon\eta)\hat{\mathcal{U}}^\varepsilon(\eta,t),$$

which is equivalent to the first order system

$$\partial_t \begin{pmatrix} \hat{\mathcal{U}}^\varepsilon(\eta,t) \\ \hat{\mathcal{V}}^\varepsilon(\eta,t) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\frac{1}{\varepsilon^2}\omega^2(\varepsilon\eta) & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathcal{U}}^\varepsilon(\eta,t) \\ \hat{\mathcal{V}}^\varepsilon(\eta,t) \end{pmatrix} + \begin{pmatrix} 0 \\ -(1-\varepsilon)\chi_\varepsilon(\eta)\partial_t^2 u_M^\varepsilon(t) \end{pmatrix}.$$

The solution to the corresponding homogeneous problem is given by the Green function

$$G^\varepsilon(\eta,t) = \begin{pmatrix} \cos\left(\omega(\varepsilon\eta)\frac{t}{\varepsilon}\right) & \varepsilon\frac{\sin\left(\omega(\varepsilon\eta)\frac{t}{\varepsilon}\right)}{\omega(\varepsilon\eta)} \\ -\omega(\varepsilon\eta)\frac{\sin\left(\omega(\varepsilon\eta)\frac{t}{\varepsilon}\right)}{\varepsilon} & \cos\left(\omega(\varepsilon\eta)\frac{t}{\varepsilon}\right) \end{pmatrix},$$

that is the exponential of t times the above 2×2 matrix. Next we represent $\hat{\mathcal{W}}^\varepsilon$ by G^ε, and use Duhamel's Principle to express $\hat{\mathcal{U}}^\varepsilon$ in terms of G^ε and $\partial_t^2 u_M^\varepsilon(t)$. Denoting the macroscopic Fourier initial data by $\hat{\mathcal{U}}_0^\varepsilon(\eta)$ and $\hat{\mathcal{V}}_0^\varepsilon(\eta)$ we thus find

$$\hat{\mathcal{W}}^\varepsilon(\eta,t) = \hat{\mathcal{U}}_0^\varepsilon(\eta)\cos\left(\omega(\varepsilon\eta)\frac{t}{\varepsilon}\right) + \varepsilon\hat{\mathcal{V}}_0^\varepsilon(\eta)\frac{\sin\left(\omega(\varepsilon\eta)\frac{t}{\varepsilon}\right)}{\omega(\varepsilon\eta)},$$

as well as

$$\hat{\mathcal{U}}^\varepsilon(\eta,t) = \hat{\mathcal{W}}^\varepsilon(\eta,t) - \int_0^t \varepsilon(1-\varepsilon)\chi_\varepsilon(\eta)\partial_r^2 u_M^\varepsilon(r)\frac{\sin\left(\omega(\varepsilon\eta)\frac{t-r}{\varepsilon}\right)}{\omega(\varepsilon\eta)}dr.$$

Finally, integrating the latter identity over $\displaystyle\frac{1}{2\pi}\int_{\mathbb{R}_\eta}$ and using integration by parts with respect to time (recall that $\partial_t u_M^\varepsilon(0) = \bar{v}_0$) we find the desired result. ∎

In order to identify the limit of (3.11), we use Laplace transform. More precisely, computing the Laplace transforms of both sides in (3.11) we obtain

$$f^\varepsilon(s) = \varepsilon\frac{1}{2\pi}\int_\Omega \frac{\bar{v}_0}{\varepsilon^2 s^2 + \omega^2(\vartheta)}d\vartheta - \frac{1-\varepsilon}{\varepsilon}\mathcal{J}^\varepsilon(s)sf^\varepsilon(s) + \mathfrak{W}_\varepsilon(s) + \frac{1-\varepsilon}{\varepsilon}\mathcal{J}^\varepsilon(s)u_M^\varepsilon(0),$$

where

$$f^\varepsilon := \mathcal{L}(u_M^\varepsilon), \quad \mathfrak{W}^\varepsilon := \mathcal{L}(\mathcal{W}^\varepsilon(0,\cdot)), \quad \mathcal{J}^\varepsilon = \mathcal{L}(J_0\left(\tfrac{2}{\varepsilon}\cdot\right)).$$

Notice that all these functions are well-defined on $\mathcal{M} = \{s\in\mathbb{C} \,:\, \mathrm{Re}(s) > 0\}$ and that

$$\mathcal{J}^\varepsilon(s) = \frac{\varepsilon}{\sqrt{4+\varepsilon^2 s^2}}.$$

Remark 3.7. *The convergence* (3.4) *is equivalent to $f^\varepsilon \to f := \mathcal{L}(\bar{u})$ uniformly on each compact set in $\mathcal{M}$.*

PROOF. In fact, if $(v_n)_n$ is a sequence of Laplace transformable distributions on $(0,\infty)$ such that $t\mapsto \exp^{-\lambda t} v_n(t)$ converges to $t\mapsto \exp^{-\lambda t} v(t)$ in $\mathcal{S}'\big((0,\infty)\big)$ for some $\lambda\in\mathbb{R}$, then $\mathcal{L}v_n \to \mathcal{L}v$ converge uniformly on each compact set in $\{s\in\mathbb{C} : \mathrm{Re} > \lambda\}$. ∎

Lemma 3.8. *The function f satisfies*

$$f(s) = \frac{\bar{v}_0}{2s} - \frac{1}{2} s f(s) + \mathfrak{W}(s) + \frac{1}{2}\mathcal{W}(0,0), \tag{3.12}$$

where $\mathfrak{W} = \mathcal{L}(\mathcal{W}0,\cdot)$. In particular, the function $\bar{u}$ from Corollary 3.3 is a solution to

$$\begin{cases} \partial_t \bar{u} + 2\bar{u} &= \bar{v}_0 + 2\mathcal{W}(0,t), \\ \bar{u}(0) &= \mathcal{W}(0,0) \end{cases} \tag{3.13}$$

Proof. A simple computations shows

$$\lim_{\varepsilon \searrow 0} \frac{1-\varepsilon}{\varepsilon} \mathcal{J}^\varepsilon(s) = \lim_{\varepsilon \searrow 0} (1-\varepsilon) \frac{1}{\sqrt{4+\varepsilon^2 s^2}} = \frac{1}{2},$$

where the convergence is uniformly on compact sets in $\mathcal{M}$, and hence we find

$$\lim_{\varepsilon \searrow 0} \frac{1-\varepsilon}{\varepsilon} \mathcal{J}^\varepsilon(s) s f^\varepsilon(s) = \frac{1}{2} s f(s) \text{ and } \lim_{\varepsilon \searrow 0} \frac{1-\varepsilon}{\varepsilon} \mathcal{J}^\varepsilon(s) u_M^\varepsilon(0) = \frac{1}{2}\mathcal{W}(0,0).$$

The convergence $\mathfrak{W}^\varepsilon \to \mathfrak{W}$ follows from the locally uniform convergence

$$\mathcal{W}^\varepsilon(0,t) = \langle \delta(\cdot), \mathcal{W}^\varepsilon(\cdot,t)\rangle \xrightarrow{\varepsilon \to 0} \mathcal{W}(0,t),$$

which holds thanks to (2.14). In order to finish the proof of (3.12) we use the identity

$$\frac{1}{2\pi} \int_\Omega \frac{1}{\varepsilon^2 s^2 + \omega^2(\vartheta)} d\vartheta = \frac{i}{2\pi} \int_{C_1(0)} \frac{1}{z^2 - \alpha_\varepsilon z + 1} dz, \tag{3.14}$$

with $\alpha_\varepsilon := \varepsilon^2 s^2 + 2$ and $C_1(0)$ being the unit disk in $\mathbb{C}$. The complex integral on the r.h.s. of (3.14) can be computed by means of the Residue Theorem. In fact, for each $s \in \mathcal{M}$ and $\varepsilon > 0$ the point $z_\varepsilon^- := \frac{1}{2}(\alpha_\varepsilon - \sqrt{\alpha_\varepsilon^2 - 4})$ belongs to the interior of $C_1(0)$ and is a simple pole of the integrand. Therefore, we find

$$\frac{1}{2\pi} \int_\Omega \frac{1}{\varepsilon^2 s^2 + \omega^2(\vartheta)} d\vartheta = \frac{1}{\sqrt{\alpha_\varepsilon^2 - 4}} = \frac{1}{\varepsilon s} \frac{1}{\sqrt{4+\varepsilon^2 s^2}},$$

and this implies

$$\varepsilon(1-\varepsilon) \frac{\bar{v}_0}{2\pi} \int_\Omega \frac{1}{\varepsilon^2 s^2 + \omega^2(\vartheta)} d\vartheta \xrightarrow{\varepsilon \to 0} \frac{\bar{v}_0}{2s}$$

locally uniformly in $\mathcal{M}$, and in turn (3.12). Finally, (3.12) is just the Laplace transform of the Cauchy problem (3.13) ∎

The proof of Theorem 2.4 now follows by combining Corollary 3.3, Corollary 3.5 and Lemma 3.8. In particular, the convergence of the whole sequence $(u_M^\varepsilon, \mathcal{U}^\varepsilon)$ to $(\bar{u}, \mathcal{U})$ follows from the uniqueness of the solution of the limit macroscopic problem (2.16).

4 Numerical simulations

We illustrate the results of Theorem 2.4 with numerical simulations for the two extreme situations, namely $v_0 \neq 0$ but $\mathcal{W}(0,t) = 0$, and $v_0 \equiv 0$ but $\mathcal{W}(0,t) \neq 0$.

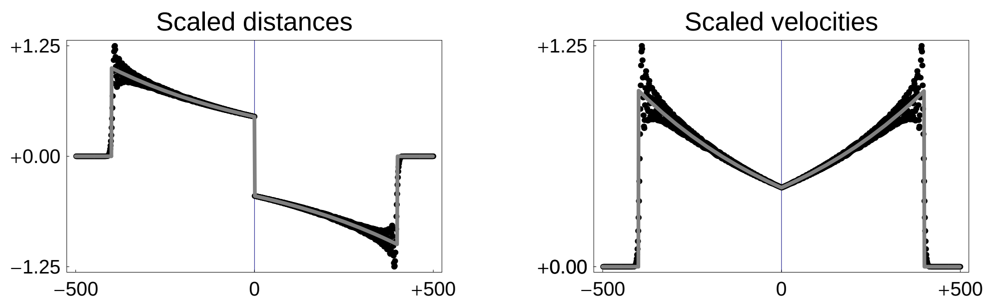

Figure 1: Example 1: Scaled snapshots of atomic distances and velocities at $\tau = 400$. The gray curves represent $\mathcal{U}_x$ and $\partial_t \mathcal{U}$ for the macroscopic solution (4.2).

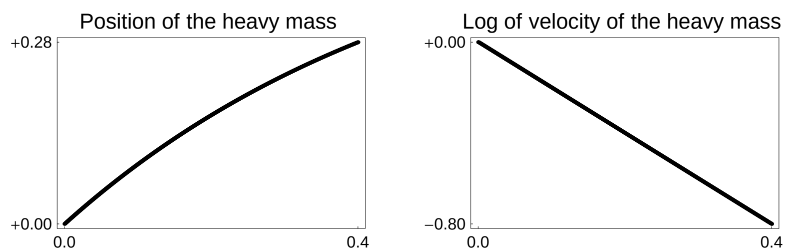

Figure 2: Example 1: Scaled position and velocity of the heavy particle against the macroscopic time t.

In the first example we study the lattice (1.3) with microscopic initial conditions

$$u(y,0) = 0, \qquad \dot{u}(y,0) = \sqrt{\varepsilon}\delta(y), \tag{4.1}$$

which give $\bar{v}_0 = 0$ and $\mathcal{U}_0 = \mathcal{V}_0 = 0$. The solution of the corresponding macroscopic problem can be computed from (2.17) by using the fundamental solution to the 1D wave equation, and turns out to be

$$\bar{u}(t) = \frac{1}{2}\left(1 - \exp\left(-2t\right)\right), \qquad \mathcal{U}(x,t) = \frac{1}{2}\chi_{\geq 0}(t - |x|)\Big(1 - \exp\left(-2(t - |x|)\right)\Big), \tag{4.2}$$

for all $x \in \mathbb{R}$ and $t \geq 0$. For the numerical simulation we choose $M = 1000$ ($\varepsilon = 0.001$), and solve the lattice equation for $N = 1001$ particles with Dirichlet boundary condition. This means $y = -500...500$ with $u(\pm 500, t) = 0$ for all $t \geq 0$.

The numerical results for the light particles are presented in Figure 1, which contains snapshots of the scaled atomic distances and velocities

$$\bar{r}^{\varepsilon}(y,\tau) := \frac{u^{\varepsilon}(y+1,\tau) - u^{\varepsilon}(y,\tau)}{\sqrt{\varepsilon}}, \quad \bar{v}^{\varepsilon}(y,\tau) := \frac{\dot{u}^{\varepsilon}(y,\tau)}{\sqrt{\varepsilon}}, \tag{4.3}$$

for fixed time $\tau = 400$, that means $t = 0.4$. According to Theorem 2.4, the scaled distances and velocities converge weakly as $\varepsilon \to 0$ to the macroscopic strain $\mathcal{U}_x$ and the macroscopic velocity $\mathcal{U}_t$, respectively, with $\mathcal{U}$ as in (4.2). Figure 2 illustrates the evolution of the heavy mass, and shows both

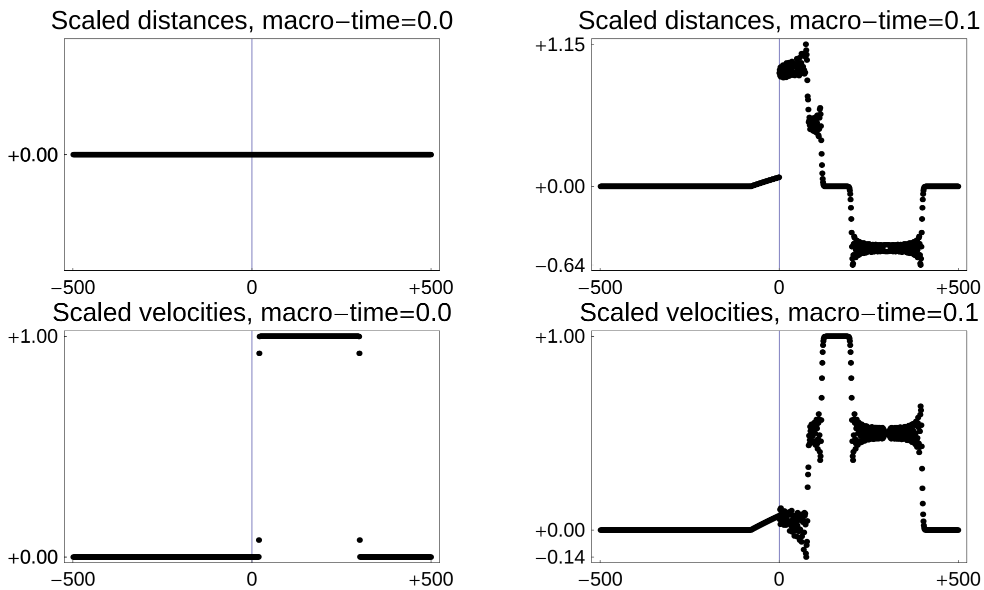

Figure 3: Example 2: Scaled snapshots of atomic distances and velocities at $\tau = 0.0$ and $\tau = 0.1$. The heavy mass is located at the vertical line.

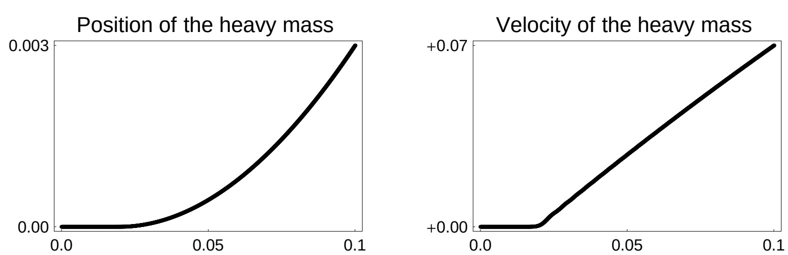

Figure 4: Scaled position and scaled velocity of the heavy particle against the macroscopic time for the second example.

$u_M^\varepsilon(t)$ and $\ln(\frac{d}{dt}u_M^\varepsilon(t))$ versus t. The velocity of the heavy mass decays exponentially with rate 2, and its acceleration coincides with the jump height in the macroscopic displacement at $x = 0$.

For the second example we impose the microscopic initial data

$$u_0(y) = 0, \quad \dot{u}_0(x) = \begin{cases} \sqrt{\varepsilon} & \text{for } 20 \le y \le 320, \\ 0 & \text{else,} \end{cases} \tag{4.4}$$

which correspond to

$$\bar{v}_0 = 0, \quad \mathcal{U}_0(x) = 0, \quad \mathcal{V}_0(x) = \chi_{[0.02,0.32]}(x), \tag{4.5}$$

and implies that the forcing function $\mathcal{W}(0,t)$ does not vanish identically. The numerical results for $M = 1000$ are presented in Figure 3 and Figure 4, and show that the medium of light particles accelerates the heavy mass.

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