On selection criteria for problems with moving inhomogeneities

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Abstract

We study mechanical problems with multiple solutions and introduce a thermodynamic framework to formulate two different selection criteria in terms of macroscopic energy productions and fluxes. Studying simple examples for lattice motion we then compare the implications for both resting and moving inhomogeneities.

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1 Introduction

The wave equation on $\mathbb{R}^3$ with a time-periodic source at the origin allows for a multitude of solutions. One way to single out a unique solution was proposed by Sommerfeld. His classic work [Som62] selects a unique solution based on boundary conditions and a so-called radiation condition. We discuss two central ingredients of his argument, based on the *macroscopic* characterisation of the forcing as a source and the *macroscopic* flow of energy, and investigate how these notions generalise to problems with moving inhomogeneities. Sommerfeld has a third ingredient to his argument, a *microscopic* radiation condition which is not investigated in detail here (one reason is that an extension to nonlinear systems is not at all obvious). Since we only focus on the first two ingredients of his argument, the selection criteria we formulate are *necessary* conditions for solutions that satisfy Sommerfeld's stipulations on production and energy flow as explained below; we show that they do not always single out a unique solution.

We present our exposition along two guiding examples of Fermi-Pasta-Ulam (FPU) chains of atoms. The governing equations are

$$\ddot{x}_j(t) = \Phi'(x_{j+1}(t) - x_j(t)) - \Phi'(x_j(t) - x_{j-1}(t)) + \zeta(t)\delta_{j0} \tag{1}$$

for every $j \in \mathbb{Z}$; this describes the motion of a one-dimensional chain of atoms $\{q_j\}_{j\in\mathbb{Z}}$ on the real line by the deformation $x_j \colon \mathbb{R} \to \mathbb{R}$, with $j \in \mathbb{Z}$ numbering the atoms, where the evolution is governed by Newton's law and neighbouring atoms are linked by springs.

The two cases we consider are (i) a chain with harmonic potential Φ and forcing ζ at the origin and (ii) a moving interface in a chain with bi-quadratic potential without forcing ($\zeta = 0$). These cases of a resting and a moving inhomogeneity behave quite differently. There is one commonly used approach due to Slepyan [Sle01], which establishes uniqueness for such problems via a causality principle which can be seen as a vanishing viscosity argument based on Sommerfeld's radiation condition. Our focus here is different, namely we aim to establish a framework for the analysis of energy flow and production

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terms that is applicable in a variety of situations, including the model examples discussed here. We show that the two notions put forward by Sommerfeld, source-sink nature respectively energy flux, no longer agree in the case of a moving inhomogeneity, unlike in the case considered by Sommerfeld.

Sommerfeld's radiation condition Sommerfeld's approach to radiation conditions is described in his book [Som62, §28], see also [Som49] and we thus just describe the gist of some key arguments. However, the discussion given in §3 for the case of a lattice model resembles the spatially continuous case very much, and we refer the reader to that section for a more detailed mathematical treatment.

Sommerfeld considers the wave equation on $\mathbb{R}^3$ with a temporally periodic forcing at the origin. A separation of variables ansatz leads to the Helmholtz equation with a source at the origin, thus an inhomogeneous equation. The corresponding homogeneous equation has nontrivial bounded kernel functions (in $\mathbb{R}^3$). Some kernel functions are excluded by *boundary conditions*, in Sommerfeld's case radially symmetric ones. This still does not single out a unique solution. In particular, there are two singular and decaying solutions $u^{\pm}$ to the inhomogeneous Helmholtz equation, which are well-defined outside the origin. Let $x^{\pm}$ be the corresponding solutions of the forced wave equation. The choice of the direction of time made in the separation of variables *ansatz* renders the corresponding solutions x^+ an *outwardly* radiating radial wave and x^- an *inwardly* radiating wave. In fact, x^+ describes a *source* solution to the forced wave equation, that means the forcing supplies energy to the system. On the contrary, x^- corresponds to a sink solution as the forcing deprives the system of energy.

Sommerfeld now introduces a *binary* choice, allowing only waves which propagate outwards and dismissing those which propagate inwards. This selection is necessary both for physical and mathematical reasons: mathematically, the choice is an integral part of the arguments leading to a unique fundamental solution of the forced wave equation, and physically the two solutions $x^{\pm}$ are qualitatively very different. In Sommerfeld's words [Som62],

> "Quellen sollen *Quellen*, nicht Senken der Energie sein." [Sources have to be *sources*, not sinks of the energy.] (SOM1)

We call this the *first formulation* of Sommerfeld's radiation condition. He then gives what we call the *second formulation*,

> "Die von den Quellen ausgestrahlte Energie muß sich ins Unendliche zerstreuen, *Energie darf nicht aus dem Unendlichen in die vorgeschriebenen Singularitäten des Feldes eingestrahlt werden*" [The energy radiated from the sources has to scatter to infinity, *energy must not be radiating from infinity into the prescribed singularities of the field*.] (SOM2)

As we noted before, characterising the involved solutions as sources or sinks is only one step along the path towards uniqueness for the forced oscillation problem. To ensure uniqueness one has finally to impose microscopic selection criteria as for instance the asymptotic radiation condition (20). Such conditions, however, are highly specific to the particular problem at hand, and will therefore not be investigated further. Instead we focus on the two former formulations which can in principle be generalised to more general problems.

Thermodynamic interpretation In §2 we establish a thermodynamic framework to analyse (SOM1) and (SOM2). The starting point are the microscopic conservation laws for mass, momentum, and energy. These laws can be derived from (1) even if Φ is nonlinear and converge to their macroscopic counterparts under the hyperbolic scaling of space and time. In the second step we then identify the macroscopic quantities that allow for a thermodynamic interpretation of Sommerfeld's radiation condition. In particular, we introduce the concept of *oscillatory energy*, identify the corresponding flux and production terms, and derive explicit expressions for these quantities in the aforementioned two special cases.

In §3 we apply the thermodynamic framework to the analogue of Sommerfeld's problem in harmonic chains and find that (SOM1) and (SOM2) are equivalent. Afterwards we study phase transition waves

in §4 and show that both conditions provide different selection criteria for moving inhomogeneities. While (SOM1) turns out to be equivalent to the usual entropy inequality, the implications of (SOM2) are very restrictive and depend strongly on the speed of the phase transition wave.

2 Macroscopic field equations in the presence of microscopic oscillations

Our approach to Sommerfeld's radiation condition in §3 and §4 is based on macroscopic balance laws that govern the effective dynamics of averaged quantities on large spatial and temporal scales. In this section we derive and discuss these balance laws and provide the atomistic expressions for all densities, fluxes and production terms. Our exposition is formal but we emphasise that all arguments can be made rigorous with Young measures, see [DH08, DHR06] and appendix A. For the sake of clarity we start with the conservation laws for the unforced FPU chain, (1) with $\zeta = 0$.

Microscopic conservation laws We can rewrite (1) with $\zeta = 0$ in terms of the atomic distances (discrete strain) $r_j := x_{j+1} - x_j$, and velocity $v_j := \dot{x}_j$ as first order equations

$$\dot{r}_j = v_{j+1} - v_j, \quad \dot{v}_j = \Phi'(r_j) - \Phi'(r_{j-1}), \tag{2}$$

which can be viewed as the discrete counterparts of the local conservation laws for mass and momentum in Lagrangian coordinates, see (6). Since the FPU chain is an autonomous Hamiltonian system with shift symmetry, we can also derive a local conservation law for the energy, namely

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\big(\tfrac{1}{2}v_j^2 + \Phi(r_{j-1})\big) = v_j\Phi'(r_j) - v_{j-1}\Phi'(r_{j-1}). \tag{3}$$

To characterize the thermodynamic properties of FPU chains we now derive a macroscopic description by applying the *hyperbolic scaling* of space and time. For a given scaling parameter $0 < \varepsilon \ll 1$, we define the *macroscopic time* τ and the *macroscopic particle index* ξ by

$$\tau = \varepsilon t, \quad \xi = \varepsilon j, \tag{4}$$

but we do *not* scale distances and velocities. We then regard the atomic data that correspond to a solution of (2) as functions that depend continuously on τ and are piecewise constant in ξ, that means we identify $r_j(t) = r_\varepsilon(\varepsilon t, \varepsilon j)$ and $v_j(t) = v_\varepsilon(\varepsilon t, \varepsilon j)$.

Of course, the functions r_ε and v_ε will, in general, be highly oscillatory with wave length of order ε and do not converge as $\varepsilon \to 0$ in a pointwise sense. However, as long as the solution to (2) is *bounded* we can assume, thanks to weak compactness, that for any *atomic observable* $\psi = \psi(r, v)$ the functions $\psi(r_\varepsilon, v_\varepsilon)$ converge weakly as $\varepsilon \to 0$, see Appendix A. The limit function $\langle\psi\rangle$ is then non-oscillatory and can be regarded as the *thermodynamic field* of ψ, that means $\langle\psi\rangle(\tau, \xi)$ gives the local mean value of ψ in the macroscopic point (τ, ξ).

Macroscopic conservation laws In the thermodynamic limit $\varepsilon \to 0$ the discrete conservation laws (2) and (3) transform into

$$\partial_\tau\langle r\rangle = \partial_\xi\langle v\rangle, \quad \partial_\tau\langle v\rangle = \partial_\xi\big\langle\Phi'(r)\big\rangle, \quad \partial_\tau\big\langle\tfrac{1}{2}v^2 + \Phi(r)\big\rangle = \partial_\xi\big\langle v\Phi'(r)\big\rangle. \tag{5}$$

These PDEs describe the local conservation laws for mass, momentum, and energy on the macroscopic scale and are well known within the thermodynamic theory of elastic bodies. In fact, they can be written as

$$\partial_\tau R - \partial_\xi V = 0, \quad \partial_\tau V + \partial_\xi P = 0, \quad \partial_\tau E + \partial_\xi F = 0, \tag{6}$$

with *macroscopic strain* $R = \langle r \rangle$, *macroscopic velocity* $V = \langle v \rangle$, *pressure* $P = -\big\langle \Phi'(r) \big\rangle$, *energy density* $E = \big\langle \frac{1}{2} v^2 + \Phi(r) \big\rangle$, and *energy flux* $F = -\big\langle v \Phi'(r) \big\rangle$. Moreover, splitting off the Galilean invariant part from both the energy density and the energy flux, we find

$$E = \tfrac{1}{2} V^2 + U, \quad F = VP + Q,$$

with *internal energy density* U and heat flux Q. It turns out that *radiation* in the sense of Sommerfeld precisely means energy transport via Q, see § 3, and therefore we call Q the *radiation flux*.

We emphasise that, in general, the conservation laws (6) do *not* constitute a closed system but must be accompanied by *closure relations*. Unfortunately, very little is known about the thermodynamic limit for most initial data and general interaction potentials. In some cases, however, it is possible to solve the closure problem. Below we show that all thermodynamic fields can be computed explicitly for (*i*) Sommerfeld's fundamental solution in forced harmonic chains, and (*ii*) phase transition waves in chains with bi-quadratic potential.

Oscillatory energy For our purposes it is convenient to introduce a split of the energy density E that accounts for the fact that the computations of local mean values and nonlinearities do not commute in the presence of oscillations. To obtain a precise measure for the strength of the oscillations we write

$$E = E_{\rm non} + E_{\rm osc}, \qquad E_{\rm non} = \tfrac{1}{2} V^2 + \Phi(R),$$

which means

$$E_{\rm non} = \tfrac{1}{2} \langle v \rangle^2 + \Phi\big(\langle r \rangle\big), \qquad E_{\rm osc} = \tfrac{1}{2} \big\langle \big(v - \langle v \rangle \big)^2 \big\rangle + \big\langle \Phi(r) - \Phi\big(\langle r \rangle\big) \big\rangle. \tag{7}$$

We refer to $E_{\rm osc}$ and $E_{\rm non}$ as oscillatory and non-oscillatory energy density, respectively, and emphasise that $E_{\rm osc}$ measures precisely the amount of macroscopic energy that is locally stored within the oscillations. From (5) and (7) we conclude that the partial energies are balanced by

$$\partial_\tau E_{\rm osc} + \partial_\xi Q = \Xi, \qquad \partial_\tau E_{\rm non} + \partial_\xi (PV) = -\Xi, \tag{8}$$

where the production

$$\Xi = -(P + \Phi'(R)) \partial_\xi V = \Big(\big\langle \Phi'(r) \big\rangle - \Phi'\big(\langle r \rangle\big) \Big) \partial_\xi \langle v \rangle,$$

describes how much non-oscillatory energy is transferred into oscillatory energy.

Thermodynamic fields for harmonic oscillations As a preparation for the discussion in §3 and §4 we now compute the thermodynamic fields for *travelling waves* in harmonic FPU chains. A travelling wave for FPU is an exact solution to (1) with $\zeta = 0$ that satisfies

$$r_j(t) = \mathcal{R}(j - c_{\rm ph} t), \quad v_j(t) = \mathcal{V}(j - c_{\rm ph} t) \tag{9}$$

for some *phase speed* $c_{\rm ph}$ and *profile functions* $\mathcal{R}$ and $\mathcal{V}$ that depend on the phase variable $\varphi = j - c_{\rm ph} t$. Travelling waves in FPU are determined by advance-delay-differential equations, see [FV99, DHM06, Her10], and describe fundamental *oscillatory patterns*. The thermodynamic fields for periodic or almost periodic travelling wave are independent of (τ, ξ) and can be computed by

$$\langle \psi \rangle := \frac{1}{2L} \int_{-L}^{L} \psi(\mathcal{R}(\varphi), \mathcal{V}(\varphi)) \, {\rm d}\varphi. \tag{10}$$

For a harmonic chain with interaction potential $\Phi(r) = \frac{1}{2} c_0^2 r^2 + d_1 r + d_0$, we immediately verify by Fourier transform that for prescribed $c_{\rm ph}$ with $0 < |c_{\rm ph}| < c_0$ travelling waves are given by

$$\mathcal{R}(\varphi) = R + \sum_{i=1}^{M} A_i \cos\left(\kappa_i \varphi + \kappa_i/2 + \eta_i\right), \qquad \mathcal{V}(\varphi) = V \mp c_0 \sum_{i=1}^{M} A_i \cos\left(\kappa_i \varphi + \eta_i\right), \tag{11}$$

with "−" and "+" for left and right moving waves, respectively, that means for $c_{\rm ph} < 0$ and $c_{\rm ph} > 0$, respectively. Here the wave numbers κ_i, $i = 1...M$, denote the positive solutions to $c_{\rm ph}^2 k^2 = \Omega(k)^2$, where $\Omega(k) = 2c_0 \sin(k/2)$ is the dispersion relation of the harmonic FPU chain. In particular, near sonic waves with $c_{\rm ph} \approx c_0$ have $M = 1$ and depend, up to phase shifts, on the four independent parameters R, V, $A = A_1$, and $\kappa = \kappa_1$.

The thermodynamic fields for harmonic travelling waves can easily be computed by (10) and (11). In fact, thanks to $\langle r \rangle = R$ and $\langle v \rangle = V$ we find

$$P = -c_0^2 R - d_1, \quad E_{\rm non} = \tfrac{1}{2} V^2 + \tfrac{1}{2} c_0^2 R^2 + d_1 R + d_0, \tag{12}$$

as well as

$$E_{\rm osc} = \tfrac{1}{2} c_0^2 A^2, \quad Q = \pm \Big(c_0 \sum_{i=1}^{M} \frac{A_i}{A} \cos(\kappa_i/2) \Big) E_{\rm osc} \tag{13}$$

with $A^2 = \sum_{i=1}^{M} A_i^2$. For periodic waves with $M = 1$ we therefore have $Q = c_{\rm gr} E_{\rm osc}$, where $c_{\rm gr} = \pm |\Omega'(\kappa)|$ is the *group speed*.

We emphasize that the thermodynamic computations presented above can be extended to superpositions of finitely many harmonic travelling waves, with obvious modifications. Since our aim is to analyse travelling waves, we do not spell out this extension. We also mention that a complete characterization of the energy transport in harmonic lattices can be derived in terms of Wigner-Husimi measures, see [Mie06].

Macroscopic description of forcing In order to generalise the formalism from above to forced FPU chains we assume, for simplicity, that the forcing acts only in the particle $j = 0$, see (1), and that ζ is periodic with

$$\zeta(t) = \zeta(t + t_{\rm per}), \qquad \int_0^{t_{\rm per}} \zeta(t)\, {\rm d}t = 0. \tag{14}$$

These conditions guarantee that the forcing does not contribute to the macroscopic conservation laws for mass $(2)_1$ and momentum $(2)_2$. The forcing, however, in general supplies some energy to the system, and hence the conservation law $(2)_3$ must be replaced by

$$\partial_\tau E + \partial_\xi F = \theta(\tau) \delta_0({\rm d}\xi). \tag{15}$$

The *macroscopic energy production* at $\xi = 0$ can be computed either as the jump of the macroscopic energy flux at $\xi = 0$ or by averaging the microscopic energy production. This reads

$$\theta(\tau) = F(\tau, 0+) - F(\tau, 0-) = \lim_{\delta \to 0} \lim_{\varepsilon \to 0} \frac{\varepsilon}{2\delta} \int_{(\tau-\delta)/\varepsilon}^{(\tau+\delta)/\varepsilon} v_0(t) \zeta(t)\, {\rm d}t. \tag{16}$$

3 The forced harmonic chain

Here we present the analogue to Sommerfeld's classical problem in harmonic FPU chains, that is the localised forced excitation problem

$$(\partial_t^2 - c_0^2 \Delta_1) x_j(t) = \zeta(t) \delta_j^0, \tag{17}$$

where Δ_1 denotes the discrete Laplacian $\Delta_1 x_j := x_{j+1} + x_{j-1} - 2x_j$. For simplicity we normalise the speed of sound to $c_0 = 1$ and assume that the chain is periodically forced at one of its eigenfrequencies σ with $0 < \sigma < 2$.

Explicit solutions via Helmholtz equation The separation of variables *ansatz* $x_j(t) = \mathrm{Re}(u_j e^{-\mathrm{i}\sigma t})$ transforms (17) into the discrete Helmholtz equation

$$\sigma^2 u_j + \Delta_1 u_j = \delta_0, \tag{18}$$

which can be solved by Fourier transform. There exist two *special solutions* u^+ and u^- defined by

$$u_j^{\pm} = \pm \frac{\exp(\pm \mathrm{i}\kappa |j|)}{\mathrm{i}2\Omega(\kappa)\Omega'(\kappa)},$$

where $\kappa = \kappa(\sigma)$ denotes the unique solution to

$$\sigma^2 = \Omega(k)^2, \qquad \Omega(k) = 2\sin(k/2), \qquad 0 < k < \pi.$$

Of course, the special solutions u^- and u^+ can be affinely combined and also superimposed by plane waves with wave number $\pm\kappa$, which are the kernel functions of the discrete Helmholtz operator. The general solution to (18) can therefore be parameterised by $\alpha, \beta \in \mathbb{C}$ as

$$u_j = u_j(\alpha, \beta) = u_j^+ + \alpha \exp(-i\kappa j) + \beta \exp(+i\kappa j). \tag{19}$$

Note that in particular $u_j^+ = u_j(0,0)$ and $u_j^- = u_j(\alpha^-, \beta^-)$ with $\alpha^- = \beta^- = -\big(\mathrm{i}2\Omega(\kappa)\Omega'(\kappa)\big)^{-1}$.

Sommerfeld's approach to the radiation condition can be viewed as the endeavour to remove the non-uniqueness and to single out a unique choice for α and β. To this end he introduces a microscopic selection criterion, whose analogue in FPU chains reads

$$\lim_{j\to+\infty} \Big(\frac{\mathrm{d}u_j}{\mathrm{d}j} - \mathrm{i}\kappa u_j\Big) = 0, \qquad \lim_{j\to-\infty} \Big(\frac{\mathrm{d}u_j}{\mathrm{d}j} + \mathrm{i}\kappa u_j\Big) = 0, \tag{20}$$

and implies that $\alpha = \beta = 0$ in (19). In particular, the microscopic radiation condition selects out u^+ but rules out u^-.

Macroscopic aspects of Sommerfeld's radiation condition We now show that the binary choice between u^- and u^+ can be understood in terms of purely macroscopic conditions on the production of oscillatory energy and the direction of the radiation fluxes. As remarked in §2, the thermodynamic framework can be extended to superpositions of harmonic waves. It is thus in principle possible to characterise all bounded solutions to (17), in particular kernel functions and their superpositions. The result of such an analysis is that the thermodynamic interpretation of (SOM1) and (SOM2) rejects superpositions of waves as long as their influx contribution exceeds the outward contribution. Thus, a half space of all bounded solutions is rejected, and a half-space accepted. We show this analysis here in detail for the two extreme cases corresponding to u_- and u_+. The analysis for the other solutions is, *mutatis mutandis*, analogous yet more complicated terms arise.

At first we notice that u^+ and u^- correspond to the real-valued displacements

$$x_j^{\pm}(t) = \pm \frac{\sin(\pm\kappa |j| - \sigma t)}{2\Omega(\kappa)\Omega'(\kappa)}.$$

Each of these solutions to (17) consists of two counter-propagating travelling waves that are glued together at $j = 0$, where the travelling waves propagate towards and away the inhomogeneity at $j = 0$ for x^+ and x^-, respectively. We also notice that x^+ and x^- transform into each other under time reversal, and that they define the atomic distances and velocities

$$v_j^{\pm}(t) = \mp A \cos(\pm\kappa |j| - \sigma t), \qquad r_j^{\pm}(t) = A \begin{cases} \cos(\pm\kappa j \pm \kappa/2 - \sigma t) & \text{for } j \geq 0, \\ \cos(\mp\kappa j \mp \kappa/2 - \sigma t) & \text{for } j < 0, \end{cases} \tag{21}$$

where the amplitude $A > 0$ is given by $1/A = 2\Omega'(\kappa) = 2\cos(\kappa/2)$.

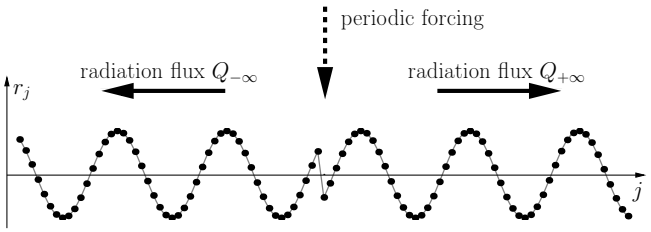

Figure 1: Sommerfeld's *source solution* for the FPU chain: The energy pumped in by the periodic forcing is radiated towards both $+\infty$ and $-\infty$. If time is reversed the source becomes a sink and the radiation fluxes on both sides change their sign.

The key observation towards the thermodynamic limit $\varepsilon \to 0$ is that both x^- and x_- converge to Young measures that are (i) independent of the macroscopic time $\tau = \varepsilon t$, (ii) constant for $\xi < 0$ and $\xi > 0$, where $\xi = \varepsilon j$ is the macroscopic particle index, and (iii) generated by periodic travelling waves. These assertions follow directly from (21) and the definition of Young measure convergence, see §2 and appendix A. They also imply that the macroscopic conservation laws (6) are trivially satisfied for $\xi \neq 0$.

Using (12) and (13) we now conclude that almost all thermodynamic fields are globally constant with

$$R = 0, \quad V = 0, \quad P = 0, \quad F = Q, \quad E_{\text{non}} = 0, \quad E = E_{\text{osc}}, \quad E_{\text{osc}} = \tfrac{1}{2}A^2,$$

but that the radiation flux Q is piecewise constant via $Q(\tau, \xi) = \pm\text{sign}(\xi)\Omega'(\kappa)E_{\text{osc}} =: Q_{\text{sgn}\,(\xi)\infty}$. The two values for Q are given by

$$Q_{-\infty} = \mp\tfrac{1}{4}A, \quad Q_{+\infty} = \pm\tfrac{1}{4}A,$$

and computing the macroscopic energy production by averaging, see (16), we find

$$\theta = -\frac{\sigma}{2\pi}\int_0^{2\pi/\sigma} v_0(t)\cos(\sigma t)\,\mathrm{d}t = \pm\frac{\sigma A}{2\pi}\int_0^{2\pi/\sigma}\cos(\sigma t)^2\,\mathrm{d}t = \pm\tfrac{1}{2}A.$$

Sommerfeld's first condition (SOM1) is naturally related to the sign of θ. For x^+ we have $\theta > 0$, so the forcing pumps in energy at $j = 0$ and the solution describes a *source* of the energy. The solution x^-, however, corresponds to a *sink* as $\theta < 0$ implies that energy flows out constantly at $j = 0$. Moreover, for the solutions at hand the balance of total energy reduces to

$$\theta = Q_{+\infty} - Q_{-\infty} = 2Q_{+\infty} = -2Q_{-\infty},$$

and implies that Sommerfeld's first and second formulation of the radiation condition are equivalent. Namely, (SOM2) stipulates that energy that is pumped in at $j = 0$ must be radiated away, and hence the radiation fluxes must point towards $\pm\infty$, see Fig. 1. Conversely, energy that is deprived from the system at $\xi = 0$ must be radiated in from $\pm\infty$, and we conclude that both (SOM1) and (SOM2) select out the solution x^+ but reject x^-.

4 Phase transition waves for a bi-quadratic FPU chain

We now consider travelling waves with a moving inhomogeneity and apply the selection criteria (SOM1) and (SOM2) to these waves. One motivation for studying this problem is that a constructive method to describe solution candidates has been worked out in great detail by [TV05]. We mention, however, two important caveats of our analysis: firstly, we assume the existence of subsonic travelling waves

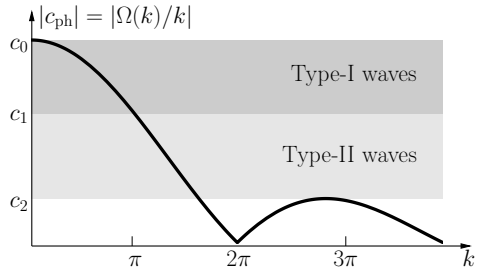

Figure 2: Phase transition waves with $|c_{\rm ph}| > c_2$ have periodic tails and come in two different types. Type-I waves have either $0 < c_{\rm gr} < c_{\rm ph}$ or $0 > c_{\rm gr} > c_{\rm ph}$, whereas Type-II waves correspond to either $c_{\rm gr} < 0 < c_{\rm ph}$ or $c_{\rm gr} > 0 > c_{\rm ph}$.

with a single inhomogeneity (interface). Guidance for the existence can be taken from [TV05]; yet existence is a subtle issue, and only for a small regime of subsonic velocities a rigorous existence proof exists [SZ09, SZ]; in particular it is worth to mention that there is a velocity regime where no travelling wave with a single interface can exist [SSZ]. Secondly, the selection criteria that result from the thermodynamic interpretation of (SOM1) and (SOM2) are *necessary* but not sufficient.

We study heteroclinic solutions to the travelling wave equation (9). To calculate the thermodynamic fluxes explicitly, we restrict our considerations to the piecewise quadratic potential

$$\Phi(r) = \tfrac{1}{2} \min\left\{(r-1)^2, (r+1)^2\right\}, \tag{22}$$

but mention that the arguments can, at least in principle, be generalised to genuinely nonlinear potentials as well. (The double-well nature of Φ describes the co-existence of different stable states and thus the possibility of interfaces between those states.)

The potential (22) is normalised to have unit sound speed, $c_0 = 1$. As illustrated in Fig. 2, there is a critical velocity $c_2 > 0$ such that for all with $c_{\rm ph}$ with $c_2 < |c_{\rm ph}| < 1$ there is a unique solution $\kappa > 0$ to

$$c_{\rm ph}^2 k^2 = \Omega^2(k), \quad \Omega(k) = 2\sin(k/2). \tag{23}$$

From now on we solely consider waves with $|c_{\rm ph}| > c_2$ because then the tails are periodic with unique wave number κ as chosen above. We therefore have

$$(\mathcal{R}, \mathcal{V})(\varphi) \xrightarrow{\varphi \to \pm\infty} (\mathcal{R}_{\pm\infty}, \mathcal{V}_{\pm\infty})(\varphi), \tag{24}$$

where both $(\mathcal{R}_{+\infty}, \mathcal{V}_{+\infty})$ and $(\mathcal{R}_{-\infty}, \mathcal{V}_{-\infty})$ are periodic travelling waves with phase speed $c_{\rm ph}$ and group speed $c_{\rm gr}$. To compute the thermodynamic fields explicitly, it is necessary that the asymptotic microscopic strains are confined to the harmonic wells. We thus require that both $\mathcal{R}_{-\infty}$ and $\mathcal{R}_{+\infty}$ have a definite sign. By symmetry we can assume that $\mathcal{R}_{\pm\infty}(\varphi) \gtrless 0$, and by shift invariance we can also assume that $\mathcal{R}(0) = 0$. Thus, the interface moves along $j = c_{\rm ph} t$ and $\xi = c_{\rm ph}\tau$ in the microscopic and macroscopic space-time coordinates, respectively. Notice, however, that we have not fixed the sign of $c_{\rm ph}$, so the wave travels from negative strain to positive strain for $c_{\rm ph} > 0$, and the other way around for $c_{\rm ph} < 0$.

Macroscopic constraints for phase transition waves Under the assumption that travelling waves with a single interface as described above exist and are asymptotically periodic in each well (possibly constant), all thermodynamic fields are constant on the left and on the right of the interface and are completely determined by the periodic tail oscillations in (24). The macroscopic conservation laws therefore reduce to jump conditions via $\partial_\tau \rightsquigarrow -c_{\rm ph}[\![\,]\!]$ and $\partial_\xi \rightsquigarrow [\![\,]\!]$, where the asymptotic jump and mean value of any thermodynamic field X are given by

$$[\![X]\!] = X_{+\infty} - X_{-\infty}, \quad \{X\} = \tfrac{1}{2}(X_{+\infty} + X_{-\infty}), \quad X_{\pm\infty} = \lim_{\xi \to \pm\infty} X(\tau, \xi).$$

In particular, the PDEs (6) transform into

$$c_{\rm ph}[\![R]\!] = -[\![V]\!], \quad c_{\rm ph}[\![V]\!] = [\![P]\!], \quad c_{\rm ph}[\![E_{\rm non} + E_{\rm osc}]\!] = [\![PV + Q]\!]. \tag{25}$$

We now express the values of all thermodynamic fields X in terms of $R_{\pm\infty}$, $V_{\pm\infty}$, $A_{\pm\infty}$, and the speeds $c_{\rm ph}$ and $c_{\rm gr}$. In this way, we recover well-known jump conditions and kinetic relations for phase transition waves [Tru82, Tru93]. The idea to compute thermodynamic quantities as averages of atomic observables is well established and can, for instance, be found in [TV05, SCC05]. The novel ingredient in our presentation is the reformulation in terms of oscillatory energy and radiation flux.

Due to the sign choice for $\mathcal{R}_{\pm\infty}$, we have $P_{\pm\infty} = -R_{\pm\infty} \pm 1$ and hence $[\![P]\!] = 2 - [\![R]\!]$, so the jump conditions for mass $(25)_1$ and momentum $(25)_2$ provide

$$[\![R]\!] = \frac{2}{1 - c_{\rm ph}^2}, \qquad [\![V]\!] = -\frac{2c_{\rm ph}}{1 - c_{\rm ph}^2}, \tag{26}$$

and therefore

$$[\![E_{\rm non}]\!] = 2\frac{c_{\rm ph}^2\,\{R\} - c_{\rm ph}\,\{V\}}{1 - c_{\rm ph}^2}, \qquad [\![PV]\!] = 2\frac{c_{\rm ph}\,\{R\} - c_{\rm ph}^2\,\{V\}}{1 - c_{\rm ph}^2}.$$

Using this and the formulae for $E_{\rm osc}$ and Q from (13), we then find

$$-c_{\rm ph}[\![E_{\rm non}]\!] + [\![PV]\!] = 2c_{\rm ph}\,\{R\}\,, \quad -c_{\rm ph}[\![E_{\rm osc}]\!] + [\![Q]\!] = (c_{\rm gr} - c_{\rm ph})[\![E_{\rm osc}]\!], \tag{27}$$

which is the analogue to (8). Consequently, the jump condition for the total energy $(25)_3$ enforces that the productions for oscillatory and non-oscillatory energy cancel via

$$\Xi = -2c_{\rm ph}\,\{R\} = (c_{\rm gr} - c_{\rm ph})[\![E_{\rm osc}]\!]. \tag{28}$$

This formula is important as it reveals that for phase transition waves there is no production of total energy but instead a steady transfer between the oscillatory and the non-oscillatory contributions of the energy. This transfer has power $-2\,\{R\}$ and drives the wave. More precisely, the *configurational force* Υ satisfies

$$c_{\rm ph}\Upsilon = -\Xi, \qquad \Upsilon := [\![\Phi(R)]\!] - \{\Phi'(R)\}\,[\![R]\!].$$

This is the *kinetic relation* and follows from (26) and (27) thanks to $[\![E_{\rm non}]\!] = [\![V]\!]\,\{V\} + [\![\Phi(R)]\!]$, $[\![PV]\!] = \{P\}\,[\![V]\!] + [\![P]\!]\,\{V\}$, and $P = -\Phi'(R)$. The production of oscillatory energy Ξ is the process commonly called dissipation.

We finally notice that time reversal changes the sign of $c_{\rm ph}$, $c_{\rm gr}$, Ξ, $V_{\pm\infty}$, $Q_{\pm\infty}$, but does not affect $R_{\pm\infty}$, $A_{\pm\infty}$, $E_{{\rm osc},\,\pm\infty}$, $E_{{\rm non},\,\pm\infty}$, $P_{\pm\infty}$, or Υ. We also observe that all thermodynamic fields are completely determined by

$$c_{\rm ph}, \quad A_{-\infty}, \quad A_{+\infty}, \quad \{V\}\,. \tag{29}$$

In fact, from (29) we compute κ and $c_{\rm gr}$ by (23) and set $[\![E_{\rm osc}]\!] = \frac{1}{2}[\![A^2]\!]$. Afterwards we solve $(26)_1$ and (28) for $R_{-\infty}$ and $R_{-\infty}$, which then allow us to compute $V_{-\infty}$ and $V_{+\infty}$ from $(26)_2$.

These jump conditions constitute *macroscopic constraints* which are *necessary* for the existence of a phase transition wave with speed $|c_{\rm ph}| \in (c_2, 1)$. However, it was proven in [SZ], that these conditions are also *sufficient*, at least for near sonic speeds with $0 < 1 - |c_{\rm ph}| \ll 1$. In conclusion, there exists a four-parameter family of phase transition waves, and it is natural to ask which of them are physically reasonable. Here selection criteria come naturally into the play.

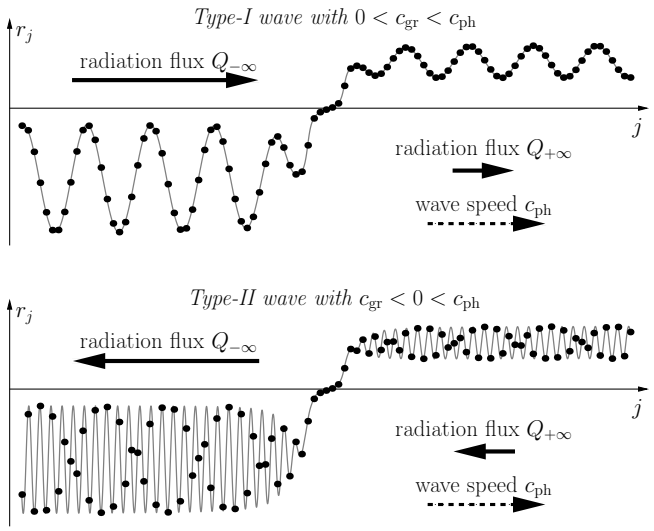

Figure 3: Phase transition waves are driven by a constant transfer between the oscillatory and the non-oscillatory energy and the radiation fluxes on both sides of the interface are proportional to the oscillatory energy and have the same sign. The cartoons illustrate the *source* solutions for so called type-I and type-II waves, which represent different order relation for the group velocity $c_{\rm gr}$ and the phase velocity $c_{\rm ph}$. If time is reversed, the interface becomes a sink of oscillatory energy and the radiation fluxes on both sides change their sign.

The macroscopic aspects of Sommerfeld's radiation conditions We first consider (SOM1). It is reasonable to require that the interface is a source rather than a sink of oscillatory energy, i.e., the production Ξ has to be non-negative

$$\Xi = (c_{\rm gr} - c_{\rm ph})[\![E_{\rm osc}]\!] \geq 0. \tag{30}$$

This inequality is *equivalent* to

$$c_{\rm ph}\Upsilon \geq 0, \tag{31}$$

which is the usual *entropy condition* for phase transition waves (see for example [TV05]). For all waves considered here, Condition (30) implies $E_{{\rm osc},\,+\infty} < E_{{\rm osc},\,-\infty}$ for waves moving to the right and $E_{{\rm osc},\,+\infty} > E_{{\rm osc},\,-\infty}$ for left-moving waves. In both cases we have $\Xi > 0$ if and only if the oscillations have smaller amplitude in front of the interface than behind the interface. (SOM1) select these solutions but rejects waves that travel from regions of low oscillations into regions of high oscillations. Note, however, that oscillations in front of the interface are not ruled out since it is only required that the wave propagates in direction of decreasing oscillations. This implies that there is still a four-parameter family of phase transition waves which satisfy (SOM1).

Sommerfeld's second formulation (SOM2), which stipulates that "energy is carried away from the interface", translates directly into a condition on the radiation flux. It requires, on both sides of the interface, that Q points away from the interface. This condition is very restrictive for phase transition waves with periodic tails because both $Q_{-\infty}$ and $Q_{+\infty}$ have the same sign as the group velocity, see (13). Thus (SOM2) can only be satisfied if there are no oscillations on one side of the interface. The precise implication depend on the sign of $c_{\rm gr}$, and therefore we distinguish between two types, see Figures 2 and 3. Type-I waves have $c_1 < |c_{\rm ph}| < 1$, where $c_1 := 2\Omega(\pi/2)/\pi$, and this implies $|c_{\rm gr}| < |c_{\rm ph}|$. Type-II waves correspond to $c_2 < |c_{\rm ph}| < c_1$, which means $\operatorname{sgn} c_{\rm gr} \neq \operatorname{sgn} c_{\rm ph}$.

For type-I waves, the radiation fluxes behind and in front the interface point towards and away from the interface, respectively. This is illustrated in Fig. 3, and holds regardless whether (30) is satisfied or not. Energy is therefore always radiated towards the interface, and the second formulation

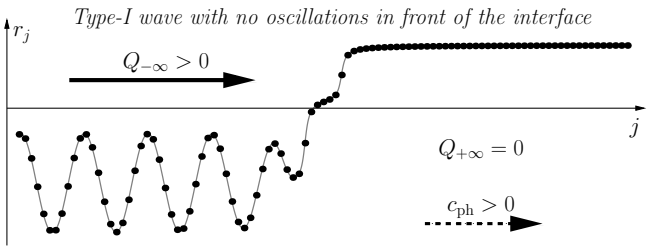

Figure 4: The *causality principle* only allows for phase transition waves that propagate into a region without oscillations.

of the radiation condition can only be satisfied if there are no oscillations behind the interface. Those waves, however, are usually regarded as unphysical as they violate (31). The only solution candidates that would accepted by both formulations have no oscillation, neither in front nor behind the interface; however, such waves do not exist for the potential (22).

The discussion is different for type-II waves. There is still radiation into the interface but now the radiation flux impinges from ahead. Therefore, both (SOM1) and (SOM2) are simultaneously fulfilled by solutions satisfying (31), namely II-waves that propagate into a region without oscillations, that means $E_{\rm osc,\,+\infty} = 0$ for right-moving $E_{\rm osc,\,-\infty} = 0$ for left-moving waves. From this we conclude that (SOM2) forbids type-I waves completely but allows for a two-parameter family of type-II waves.

Microscopic selection criteria Besides of macroscopic criteria as described above, there also exist microscopic selection rules for phase transition waves. These are far more restrictive and select out a two-parameter family of phase transition waves. For the sake of comparison we now summarise the main arguments about microscopic selection criteria for phase transition waves in bi-quadratic chains and refer to [TV05, CCS05] for more details. The key idea is that under the condition $\operatorname{sgn}\mathcal{R}(\varphi) = \operatorname{sgn}\varphi$ each phase transition waves is determined by the affine advance-delay-differential equation

$$c_{\rm ph}^2 \partial_\varphi^2 \mathcal{R} = \triangle\mathcal{R} - \triangle\operatorname{sgn}.$$

This equation can be regarded as the analogue to the inhomogeneous Helmholtz equation (18), and solutions can be represented by $\mathcal{R}(\varphi) = \operatorname{Re}(\mathcal{S}(\varphi))$ with

$$\mathcal{S}(\varphi) = -\frac{\mathrm{i}}{\pi}\int_\Gamma \frac{\Omega(k)^2 e^{+\mathrm{i}k\varphi}}{k\Omega^2(k) - c_{\rm ph}^2 k^3}\,\mathrm{d}k, \tag{32}$$

where Γ is an appropriately chosen contour in the complex plane. The microscopic selection criterion is based on the *causality principle* which chooses Γ to be the dented real axis that passes the origin $k = 0$ from below but the other real-valued poles $k = \pm\kappa$ of the integrand in (32) from above. Complex-valued calculus then provides the following expressions for the thermodynamic fields for a right moving wave

$$R_{\pm\infty} = \pm\frac{c_{\rm ph}}{1 - c_{\rm ph}^2} + \frac{c_{\rm ph}}{c_{\rm gr} - c_{\rm ph}}, \qquad A_{-\infty} = \frac{2c_{\rm ph}}{c_{\rm gr} - c_{\rm ph}}, \quad A_{+\infty} = 0,$$

with $[\![V]\!]$ as in (26), and therefore

$$[\![E_{\rm osc}]\!] = -\frac{2c_{\rm ph}^2}{(c_{\rm gr} - c_{\rm ph})^2} < 0, \qquad \Xi = \frac{2c_{\rm ph}^2}{c_{\rm ph} - c_{\rm gr}} > 0.$$

In particular, there exists a two-dimensional family of phase transition waves that is parameterised by the speed $c_{\rm ph}$ and the trivial parameter $\{V\}$. All these waves have no oscillations ahead the interface, see Figure 4, and (SOM1) is always satisfied. The validity of (SOM2) depends on the value of $c_{\rm gr}$, i.e., on whether the wave is of type-I or type-II.

Discussion This section shows that the case of a moving interface is different from that of a standing source as discussed in § 3: in the latter case, (SOM1) and (SOM2) are equivalent, but this is not true for the former case. For the moving interfaces considered in this section, the condition formulated in terms of sources and sinks, (SOM1), is equivalent to the entropy condition (31). The second formulation (SOM2) in terms of fluxes selects for type-I waves a solution that is constant *behind* the interface; this solution, however, is rejected by the entropy condition (31). Thus for moving interfaces, one has to distinguish between arguments that rely on the energy transport, as (SOM2), and arguments based on energy production, as (SOM1). Both conditions are only necessary. We stress again that this section is based on the assumption that there are single interface phase transition waves for the given potential Φ which are asymptotically periodic (possibly constant). This is proven only for a small parameter range of type-I waves [SZ09, SZ], and there is a nonexistence proof for single interface phase transition wave for a regime of lower velocities [SSZ].

A Appendix: Macroscopic conservation laws for FPU chains

Here we establish the thermodynamic limit for the forced FPU chain (1) provided that the forcing ζ satisfies (14). Our main goal is to show that the macroscopic balance laws for mass, momentum, and energy (see (5) and (15)) can be derived rigorously as follows:

1. The hyperbolic scaling transforms each *bounded* FPU solution into a family of *oscillatory* functions which depend on the macroscopic time τ and macroscopic Lagrangian space coordinate ξ.

2. This family of functions is compact in the sense of Young measures, and hence we can extract convergent subsequences. Along such a subsequence, the limit measure encodes the *local distribution functions* of the oscillatory data and hence the *local mean values* of atomic observables. These local mean values provide the *thermodynamic fields* and are, by construction, *non-oscillatory* functions in τ and ξ.

3. The FPU dynamics implies that the thermodynamic fields of each Young measure limit satisfy the macroscopic conservation laws of mass, momentum, and energy in a weak sense.

We now collect the mathematical tools for each of these step. We start with some basic facts about Young measures and refer the reader to [Bal89, Rou97, Val94, Tay97] for more details.

Let Ω be a domain in $\mathbb{R}^k$ and K be some convex and closed set in $\mathbb{R}^m$. A Young measure $\mu \in Y(\Omega;K)$ is a Ω-family of probability measures on K, that means a measurable map $\mu\colon y \in \Omega \to \mu(y,\mathrm{d}Q) \in Prob(K)$. Notice that each function $Q\colon \Omega \to K$ defines a trivial Young measure with $\mu(y,\mathrm{d}Q) = \delta_{Q(y)}(\mathrm{d}Q)$, where $\delta_{Q(y)}(\mathrm{d}Q)$ abbreviates the delta distribution in $Q(y)$.

Theorem 1 (Fundamental Theorem on Young Measures)**.** *Each family*

$$(Q_\varepsilon)_{0<\varepsilon\le 1} \subset L^\infty(\Omega;K)$$

is compact in the space of Young-measures $YM(\Omega;K)$. This means there exists a sequence $\varepsilon_n \to 0$ along with a limit measure $\mu \in YM(\Omega;K)$ such that

$$\psi(Q_{\varepsilon_n}) \xrightarrow{n\to\infty} \langle\psi\rangle \quad \textit{weakly}\star \textit{ in } L^\infty(\Omega), \tag{33}$$

for all observables $\psi \in C(K)$, where

$$\langle\psi\rangle(y) = \int_B \psi(Q)\mu(y,\mathrm{d}Q)$$

gives the local mean value of ψ in $y \in \Omega$.

Proof. See, for instance, [Tay97], Proposition 11.3 in Section 13.11. □

The convergence (33) is equivalent to

$$\int_\Omega \langle\psi\rangle(y)\phi(y)\,\mathrm{d}y = \lim_{n\to\infty}\int_\Omega \psi(Q_{\varepsilon_n}(y))\phi(y)\,\mathrm{d}y$$

for all test functions $\mu \in C_c^\infty(\Omega)$. Moreover, the subsequence converges strongly to some limit function Q_0 in $L^\infty(\Omega;K)$ if and only if the limit measure is trivial, $\mu(y,\mathrm{d}Q) = \delta_{Q_0(y)}(\mathrm{d}Q)$.

We now suppose that we are given a bounded solution to (1). As in §2, we regard the atomic distances $r_j = u_{j+1} - u_j$ and velocities $v_j = \dot{u}_j$ as the basic variables, i.e., we consider

$$Q_j(t) = (r_j(t), v_j(t)), \quad j \in \mathbb{Z}, \quad t \geq 0. \tag{34}$$

For a given scaling parameter $0 < \varepsilon \leq 1$ we introduce τ and ξ by (4), so the macroscopic Lagrangian space-time coordinate is given by

$$\Omega = \{(\tau,\xi)\ :\ \tau > 0,\ \xi \in \mathbb{R}\}.$$

Moreover, we identify (34) with piecewise constant functions on Ω as follows

$$Q_\varepsilon(\varepsilon t, \varepsilon j + \eta) = Q_j(t) \quad \text{ for every } t \geq 0,\ j \in \mathbb{Z},\ |\eta| \leq \tfrac{1}{2}. \tag{35}$$

By assumption, we have $(Q_\varepsilon)_{0<\varepsilon\leq 1} \subset L^\infty(\Omega;K)$ for some ball $K \subset \mathbb{R}^2$, and Theorem 1 provides at least one subsequence that converges to some limit measure $\mu \in YM(\Omega;K)$. Moreover, for each atomistic observable ψ we can compute the corresponding thermodynamic field via

$$\big\langle\psi(r,v)\big\rangle(\tau,\xi) = \int_{\mathbb{R}^2} \psi(r,v)\mu(\tau,\xi,\,\mathrm{d}r\mathrm{d}v).$$

We are now able to state and prove the main result on the thermodynamic limit of forced FPU chains. It is a direct consequence of the discrete conservation laws derived from FPU, the notion of Young-measure convergence, and the properties of distributional derivatives.

Theorem 2 (Macroscopic conservation laws for FPU)**.** *The thermodynamic fields of each Young measure limit μ of* (1) *satisfies the conservation laws* (5) *within the following domains in the sense of distributions: The laws for mass* $(5)_1$ *and momentum* $(5)_2$ *hold for Ω. The conservation of energy* $(5)_3$ *holds for Ω if $\zeta \equiv 0$, and otherwise at least for $\tilde{\Omega} = \Omega \setminus \{\xi = 0\}$.*

Proof. Within this proof we write $Q_\varepsilon(\tau,\xi) = \big(r_\varepsilon(\tau,\xi), v_\varepsilon(\tau,\xi)\big)$. The equation of motion (1) combined with the scaling rules (4) and (35), implies the following discrete conservation laws

$$\partial_\tau r_\varepsilon - \nabla_{+\varepsilon} v_\varepsilon = 0, \tag{36}$$

$$\partial_\tau v_\varepsilon - \nabla_{-\varepsilon}\Phi'(r_\varepsilon) = \zeta(\tau/\varepsilon)\chi_\varepsilon(\xi), \tag{37}$$

$$\partial_\tau\big(\tfrac{1}{2}v_\varepsilon^2 + \Phi(r_\varepsilon) - \varepsilon\nabla_{-\varepsilon}\Phi(r_\varepsilon)\big) - \nabla_{-\varepsilon}\big(v_\varepsilon\Phi'(r_\varepsilon)\big) = \zeta(\tau/\varepsilon)v_0(\tau/\varepsilon)\chi_\varepsilon(\xi) \tag{38}$$

for all $\tau > 0$ and almost all $\xi \in \mathbb{R}$, where the discrete differential operators $\nabla_{\pm\varepsilon}$ and the scaled cut off function χ_ε are given by

$$(\nabla_{\pm\varepsilon} f)(\tau,\xi) = \frac{\pm f(\tau,\xi\pm\varepsilon) \mp f(\tau,\xi)}{\varepsilon}, \qquad \chi_\varepsilon(\xi) = \frac{\chi_{\{|\xi|<\varepsilon/2\}}(\xi)}{\varepsilon}.$$

We now multiply (36) with a test function $\mu \in C_c^\infty(\Omega)$ and integrate with respect to both τ and ξ. Using integration by parts and expansions with respect to ε we then find

$$\int_\Omega r_\varepsilon\partial_\tau\mu - v_\varepsilon\partial_\xi\mu\,\mathrm{d}\tau\mathrm{d}\xi = O(\varepsilon),$$

and the limit $\varepsilon \to 0$ provides $(5)_1$ in the sense of distributions. Similarly, and using that (14) implies

$$\int_\Omega \zeta(\tau/\varepsilon)\chi_\varepsilon(\xi)\mu(\tau,\xi)\,\mathrm{d}\tau\mathrm{d}\xi = \varepsilon\int_0^\infty \zeta(t)\mu(\varepsilon t,0)\,\mathrm{d}t + O(\varepsilon) = O(\varepsilon),$$

we derive $(5)_2$ from (37). Finally, the assertions about the energy conservation follow from (38), where for $\zeta \neq 0$ we assume that all test functions μ are compactly supported in $\tilde{\Omega}$. □

Since the energy is conserved in $\tilde{\Omega}$ we can balance the energy in the whole domain Ω via (15).

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