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Variational evolution of one-dimensional Lennard-Jones systems

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1 Introduction

Scope of this paper is twofold: on one hand we continue the study of Lennard-Jones systems from the standpoint of variational principles, on the other hand these allow to provide a non-trivial example within the theory of minimizing movements. In a one-dimensional static setting, Lennard-Jones systems have been shown to be equivalent to energies of Fracture Mechanics using the notion of equivalence by Γ-convergence [8, 9]. Here we prove that this equivalence also holds as gradient-flow type dynamics are concerned. Within the theory of minimizing movements, the scaled Lennard-Jones energies we consider are an example of a sequence of non-convex functionals for which Γ-convergence and gradient-flow dynamics commute.

We start by briefly recalling the minimizing-movement scheme. Typically, we are given an 'energy functional' F, defined on a space X, whose (local) minimizers provide the stable configurations of the system. As an answer to the problem of modeling the evolution from a given initial state u^0, in [11] (see also [1, 5]) a general scheme is proposed, based on an iterative-minimization process. More precisely, in the particular case in which X is a Hilbert space, we fix a 'time step' $\tau > 0$ and consider the sequence $(u^k_\tau)_k$ recursively defined by letting $u^0_\tau = u^0$ and u^k_τ $(k \geq 1)$ be a minimizer of the penalized functional

$$v \mapsto F(v) + \frac{1}{2\tau}\|v - u^{k-1}_\tau\|^2_X\,; \tag{1.1}$$

the last term tends to constrain the minimizer u^k_τ on a $O(\tau)$-neighbourhood of u^{k-1}_τ, thus giving a X-continuous trajectory in the limit. We interpret u^k_τ as the state of the system at discrete times $t = k\tau$. Let $u_\tau\colon [0, +\infty) \to X$ be its piecewise-constant extension for all positive times: $u_\tau(t) = u^{\lfloor t/\tau\rfloor}_\tau$; a function $u\colon [0, +\infty) \to X$ is a *minimizing movement* for F from u^0 if u is the pointwise limit of a (sub)sequence (u_{τ_n}). As a standard example we mention the case $X = L^2(\Omega)$, with Ω an open subset of $\mathbb{R}^n$, and $F(u) = \int_\Omega |\nabla u|^2\,\mathrm{d}x$ on the Sobolev space $H^1(\Omega)$, extended with value $+\infty$ otherwise; it turns out that the

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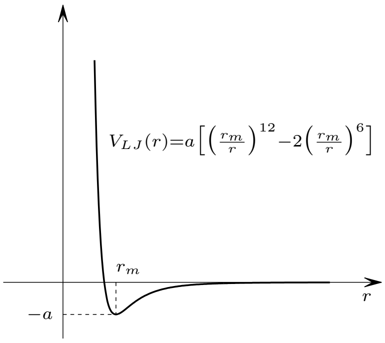
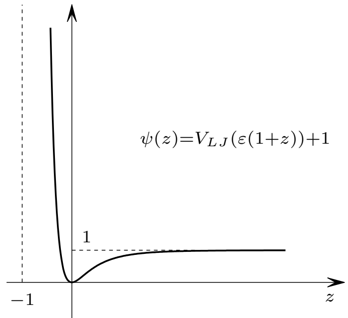


(a) Potential of Lennard-Jones type



(b) A possible function ψ in the definition of F_ε (here $\varepsilon = r_m$ and $a = 1$)

Figure 1 - Potentials of Lennard-Jones type

evolution of an initial datum u^0 is given by the (weak) solution of the heat equation $u_t = \Delta_x u$ with initial condition $u(\cdot, 0) = u^0$ and Neumann boundary conditions.

Consider now the case of an energy F_ε which depends on a small parameter ε, and assume that we know its limit F as $\varepsilon \to 0$ (technically, the Γ-limit in a suitable topology). We cannot expect that the evolution of the system from an initial state, driven by the functional F_ε according to the scheme above, is close to the evolution ruled by the limit F: indeed two different limit processes are involved ($\varepsilon \to 0$ and $\tau \to 0$), that do not commute. In general then we have a *minimizing movement along the sequence* F_ε that does depend on the particular ε-τ regime (see [7] Section 8). It is particularly noteworthy when we can uniquely characterize the limit, independently of the choice of the specific infinitesimal sequences ε_n and τ_n: if this is the case, we say that Γ-convergence *commutes* with the minimizing movements method. A simple condition which guarantees that the two procedures commute is the convexity of the functionals F_ε (see [7] Section 11.1 and [4]): as a heuristic motivation, consider that, in the convex case, the constraint expressed, for each ε, by the penalization term in (1.1) does not match with the existence of a nearby local minimizer other than the global one.

In this paper we focus the attention on a well-known family of non-convex energies defined through a Lennard-Jones potential, and prove the validity of this commutativity property. More precisely, we consider the family $(F_\varepsilon)_{\varepsilon>0}$ of functionals defined on the set of functions $u\colon [0,1] \cap \varepsilon\mathbb{Z} \to \mathbb{R}$ by (see (2.4))

$$(1.2) \qquad F_\varepsilon(u) = \sum_{i=0}^{N_\varepsilon - 1} \psi\left(\frac{u_{i+1} - u_i}{\sqrt{\varepsilon}}\right), \qquad (u_i := u(i\varepsilon),\ N_\varepsilon := \lfloor 1/\varepsilon \rfloor),$$

where $\psi\colon (-1, +\infty) \to \mathbb{R}$ is, up to a translation, a convex-concave potential of Lennard-Jones type with minimum in 0 (see Figure 1(b)). We refer to the next section for the motivation of the ε-scaling considered here, which leads to the prototypical free-discontinuity functional, namely the Mumford-Shah functional

(or Griffith fracture energy)

$$F(u) = \frac{1}{2}\psi''(0)\int_0^1 |u'|^2\,\mathrm{d}x + a\#S(u),$$

with an increasing-jump condition $u^+ > u^-$, where $a = \lim_{z\to+\infty}\psi(z)$. It is known that the minimizing-movement scheme can be applied to the functional F giving the heat equation with Neumann boundary conditions on the jump set (and on the boundary), with the constraint that $S(u(t))$ is decreasing (see, e.g., [7] Example 7.3).

For every $\varepsilon, \tau > 0$ we can define the discrete evolution $(u^k_{\varepsilon,\tau})_k$ from an initial datum, driven by the functional F_ε according to the scheme (1.1). As above, we denote by $u_{\varepsilon,\tau}$ its piecewise-constant extension for all positive times: $u_{\varepsilon,\tau}(t) = u^{\lfloor t/\tau\rfloor}_{\varepsilon,\tau}$. In Section 3 we prove a compactness result for sequences $\big(u_{\varepsilon_n,\tau_n}\big)$ and in Section 4 we characterize the *minimizing movement along* F_{ε_n} (with time step τ_n); namely, we prove that all limit points of $\big(u_{\varepsilon_n,\tau_n}\big)$ are weak solutions of the heat equation, independently of the particular sequences (ε_n) and (τ_n), with fixed jump set, hence obtaining the minimizing movement for the Mumford-Shah functional. Note that a similar commutativity result between Γ-convergence and gradient flow has been obtained for Ginzburg-Landau energies [13].

It must be noted that part of the results are obtained under the technical assumption $\tau << \varepsilon^2$. An assumption on the relation between ε and τ seems in contrast with the scope of the paper, as commutability between Γ-convergence and minimizing movements is concerned. It must hence be noted that a general result (see [7] Section 8.2) ensures that for ε small enough with respect to τ the minimizing movement along the sequence F_ε does converge to a minimizing movement for the limit F. Hence, a smallness requirement on τ seems only a technical assumption.

2 Setting of the problem and preliminary results

Function spaces. Let $I = (a, b)$ be a bounded open interval. We denote by $W^{k,p}(I)$ and $H^k(I) := W^{k,2}(I)$ the standard Sobolev spaces on I. Moreover, we say that a function $u\colon I \to \mathbb{R}$ is *piecewise-*$W^{1,p}(I)$ if there exist $a = x_0 < x_1 < \ldots < x_{m+1} = b$ such that

$$u \in W^{1,p}(x_k, x_{k+1}) \quad \text{for every } k = 0, \ldots, m. \tag{2.1}$$

It is well known that, considering the continuous representative of u in each interval, the limits

$$u^+(x_k) := \lim_{x\to x_k^+} u(x), \qquad u^-(x_k) := \lim_{x\to x_k^-} u(x)$$

exist and are finite. The minimal set $\{x_1, \ldots, x_m\}$ for which (2.1) holds coincides with the *discontinuity set* $S(u)$ of the function u.

If $u \in BV(I)$, i.e. u is a function with *bounded variation* in I, then its distributional derivative Du is a measure which can be written as

$$Du = u'\mathrm{d}x + D^s u, \tag{2.2}$$

for a suitable function $u' \in L^1(I)$ and with $D^s u$ singular with respect to the Lebesgue measure $\mathrm{d}x$. It is well known that if $u \in BV(I)$ then the unilateral (approximate) limits $u^{\pm}(x)$ exist and are finite for every $x \in I$.

A relevant subspace of $BV(I)$ is the space $SBV(I)$ (*special* functions with bounded variation) determined by the condition that $D^s u$ is concentrated on the set $S(u)$ of discontinuity points of u (i.e., the points where $u^{\pm}$ are different). In this case,

$$D^s u = (u^+ - u^-)\mathrm{d}\mathscr{H}^0 \llcorner S(u),$$

(here $\mathscr{H}^0$ denotes the counting measure) and we refer to $D^s u$ as the *jump* part $D^j u$ of the derivative Du. It turns out that u is piecewise-$W^{1,p}(I)$ if and only if $u \in SBV(I)$, the set $S(u)$ is finite and $u' \in L^p(I)$. In this case, the density u' in the decomposition (2.2) is nothing but the usual weak derivative of u as a Sobolev function in each interval of the partition determined by $S(u)$. A crucial property of this space is given by the following compactness and closure results (see [3], Th. 4.8 and Th. 4.7, where the general n-dimensional setting is considered; see also [6], Thm 7.3, for the one-dimensional case).

Theorem 2.1 *Let (u_n) be an equibounded sequence of piecewise-$H^1(I)$ functions, with*

$$\sup_n \Big(\int_a^b |u_n'(x)|^2 \, \mathrm{d}x + \# S(u_n) \Big) < +\infty.$$

Then there exist a subsequence (u_{n_k}) and a piecewise-$H^1(I)$ function u such that

$$u_{n_k} \to u, \quad u_{n_k}' \rightharpoonup u' \quad \text{in } L^2(a,b).$$

Moreover, $D^j u_{n_k} \rightharpoonup D^j u$ weakly* in the sense of measures.

For a function $u = u(x,t)$ depending on both a space and a time variable, if $u(\cdot,t)$ is piecewise-$H^1(I)$ we denote by $u_x(\cdot,t)$ the (density of the absolutely continuous part of the) derivative of $u(\cdot,t)$.

Since in this paper we do not make use of any technical result about Γ-convergence, we refer the interested reader to [6] and [10] for a thorough presentation. In view of the arguments displayed in the next subparagraph, we only need to recall that the main feature of Γ-convergence for a sequence of functionals is that, under mild compactness assumptions, it leads to the convergence of minima and minimizers.

Lennard-Jones potentials. Consider a one-dimensional array of particles whose mutual interactions can be described by a nearest-neighbour scheme ruled by a *potential of Lennard-Jones type*, i.e.:

$$V_{LJ}(r) = 4a \left[\Big(\frac{\sigma}{r}\Big)^{12} - \Big(\frac{\sigma}{r}\Big)^{6} \right] = a \left[\Big(\frac{r_m}{r}\Big)^{12} - 2\Big(\frac{r_m}{r}\Big)^{6} \right],$$

where: r denotes the distance between the particles, a is the depth of the potential well and $r_m = 2^{1/6}\sigma$ is the distance at which the minimum is attained (see Figure 1(a)). These parameters can be adjusted according to experimental data.

Assume a reference configuration in which the coordinates of the particles form the set $[0,1] \cap \varepsilon\mathbb{Z}$, where we choose the space step $\varepsilon = r_m$. A configuration

w is a function $w\colon [0,1]\cap\varepsilon\mathbb{Z}\to\mathbb{R}$; we denote the value $w(i\varepsilon)$ simply by w_i. Then the energy corresponding to w is given by

$$\sum_{i=0}^{N_\varepsilon-1} V_{LJ}(w_{i+1}-w_i)\,,$$

with the constraint that $w_{i+1}>w_i$. The effective configurations under given boundary data are obtained by minimizing this energy. In terms of the displacement $v=w-id$, and making the difference quotient $(v_{i+1}-v_i)/\varepsilon$ explicit, each term of the sum can be written as $V_{LJ}\big(\varepsilon(1+\frac{v_{i+1}-v_i}{\varepsilon})\big)$. Since the minimizers are not affected by the addition of a constant in the energy, we equivalently consider the following functional, whose absolute minimum is zero:

$$E_\varepsilon(v)=\sum_{i=0}^{N_\varepsilon-1}\psi\Big(\frac{v_{i+1}-v_i}{\varepsilon}\Big)\,,$$

where $\psi(t)=V_{LJ}(\varepsilon(1+t))+a$ (independent of ε): see Figure 1(b)).

When ε is small, the minimizers of E_ε can be qualitatively described by means of the minimizers of the Γ-limit functional for $\varepsilon\to 0$. In order to have the same functional domain for E_ε independently of ε, we consider each function $v\colon [0,1]\cap\varepsilon\mathbb{Z}\to\mathbb{R}$ as a function in $L^1(0,1)$, defined by $v(x)=v(\lfloor x/\varepsilon\rfloor)$. Then it turns out (see [6], Theorem 11.7) that the Γ-limit of (E_ε) with respect to the L^1-convergence is given by

$$E(v)=\begin{cases} a\,\#S(v) & \text{if } v \text{ is piecewise constant on } (0,1)\\ & \quad\text{and } v^+>v^- \text{ on } S(v),\\ +\infty & \text{otherwise.}\end{cases}$$

A more refined analysis of the displacement v (i.e. of the “correction” term with respect to the identity) can be obtained by suitably rescaling the state variable, so as to obtain a non-trivial limit. By letting $v=\sqrt{\varepsilon}u$ we get the functionals:

$$F_\varepsilon(u)=\sum_{i=0}^{N_\varepsilon-1}\psi\Big(\frac{u_{i+1}-u_i}{\sqrt{\varepsilon}}\Big).$$

In [8] (see also [9]) it is proved that as a Γ-limit we get the well-known Mumford-Shah functional

$$F(u)=\frac{1}{2}\psi''(0)\int_0^1|u'|^2\,\mathrm{d}x+a\,\#S(u),$$

with the constraint $u^+>u^-$. Note that, in terms of the variable u, the initial configuration w can be written as $w=id+\sqrt{\varepsilon}u$.

In this paper we focus on the relationship between the asymptotic bahaviour of F_ε as $\varepsilon\to 0$ and the methods of *minimizing movements* described below.

Setting of the problem and first results. Let $\varepsilon>0$ be given. If u is a function $[0,1]\cap\varepsilon\mathbb{Z}\to\mathbb{R}$, we denote the value $u(i\varepsilon)$ simply by u_i; therefore, we often write u as an indexed family $(u_i)_{i=0,1,\dots,N_\varepsilon}$ where $N_\varepsilon=\lfloor 1/\varepsilon\rfloor$. By u we will also denote the piecewise-constant extension defined by $u(x)=u_i$ with $i=\lfloor x/\varepsilon\rfloor$. The $L^p(0,1)$ norms of u are defined taking this extension into account.

Let $\psi\colon(-1,+\infty)\to[0,+\infty)$ be a C^1 function satisfying the following conditions (see the model example in Figure 1(b)):

A1) there exists $z_0 > 0$ such that ψ is C^3 and convex in $(-1, z_0)$ and is concave in $(z_0, +\infty)$;

A2) $\lim_{z\to -1^+} \psi(z) = +\infty, \qquad \lim_{z\to +\infty} \psi(z) = 1.$

A3) $\psi(0) = 0$, $\psi'(0) = 0$ and $\psi''(0) > 0$.

Remark 2.2 As regards the smoothness assumptions about ψ, we point out that the requirement that ψ is globally C^1 is needed to deduce the optimality conditions in the form of Proposition 2.9, while the assumption that ψ is C^3 on $(-1, z_0)$ is used in the proof of Theorem 3.4; otherwise, C^2 suffices.

Note, in particular, that the stated conditions imply that ψ is monotone on each of the intervals $(-1, 0]$ and $[0, +\infty)$; moreover, 0 is a minimum point and there exists a constant $\nu > 0$ such that

$$\psi(z) \geq \nu z^2 \qquad \text{for } z \leq z_0. \tag{2.3}$$

On the space of discrete functions $u\colon [0,1] \cap \varepsilon\mathbb{Z} \to \mathbb{R}$ we consider the functionals

$$F_\varepsilon(u) = \begin{cases} \displaystyle\sum_{i=0}^{N_\varepsilon - 1} \psi\Big(\frac{u_{i+1} - u_i}{\sqrt{\varepsilon}}\Big) & \text{if } u_{i+1} - u_i > -\sqrt{\varepsilon} \text{ for all } i \\ +\infty & \text{otherwise.} \end{cases} \tag{2.4}$$

It will be useful to express F_ε in an "integral form" with explicit dependence on the difference quotient:

$$F_\varepsilon(u) = \begin{cases} \displaystyle\sum_{i=0}^{N_\varepsilon - 1} \varepsilon\, \varphi_\varepsilon\Big(\frac{u_{i+1} - u_i}{\varepsilon}\Big) & \text{if } u_{i+1} - u_i > -\sqrt{\varepsilon} \text{ for all } i \\ +\infty & \text{otherwise,} \end{cases} \tag{2.5}$$

where

$$\varphi_\varepsilon(z) = \frac{1}{\varepsilon}\psi(\sqrt{\varepsilon} z). \tag{2.6}$$

Thus $\varphi_\varepsilon\colon (-1/\sqrt{\varepsilon}, +\infty) \to [0, +\infty)$.

For a function $u\colon [0,1] \cap \varepsilon\mathbb{Z} \to \mathbb{R}$ a key role will be played by the "singular set" of the points i where the discrete gradient $(u_{i+1} - u_i)/\varepsilon$ exceeds the threshold given by the inflection point of ψ. More precisely, we define

$$I_\varepsilon^+(u) = \Big\{ i \in \mathbb{Z} : \quad 0 \leq i \leq N_\varepsilon - 1, \ \frac{u_{i+1} - u_i}{\varepsilon} > \frac{z_0}{\sqrt{\varepsilon}} \Big\}. \tag{2.7}$$

For future reference we state the following lemma.

Lemma 2.3 *Let $u\colon [0,1] \cap \varepsilon\mathbb{Z} \to \mathbb{R}$ with $F_\varepsilon(u) < +\infty$. Then*

a) $\# I_\varepsilon^+(u) \leq \dfrac{1}{\nu z_0^2} F_\varepsilon(u)$;

b) if $\zeta_0 \in (-1, 0)$ is such that $\psi(\zeta_0) \geq F_\varepsilon(u)$, then $\dfrac{u_{i+1} - u_i}{\varepsilon} > \dfrac{\zeta_0}{\sqrt{\varepsilon}}$ for every $i = 0, \dots, N_\varepsilon - 1$.

Proof. Estimate (a) immediately follows from (2.3), since

$$F_\varepsilon(u) \geq \sum_{i \in I_\varepsilon^+(u)} \nu z_0^2 = \nu z_0^2 \# I_\varepsilon^+(u).$$

As for (b), for every i we have

$$\psi\Big(\sqrt{\varepsilon}\frac{u_{i+1}-u_i}{\varepsilon}\Big) \leq F_\varepsilon(u) \leq \psi(\zeta_0),$$

and we conclude by the monotonicity of ψ in $(-1,0]$. □

For any given $u\colon [0,1]\cap\varepsilon\mathbb{Z} \to \mathbb{R}$ we define the extension $\hat{u}$ on $[0,1]$ obtained by linear interpolation outside the set $\varepsilon I_\varepsilon^+(u)$:

(2.8)
$$\hat{u}(x) = \begin{cases} u_i & \text{if } i := \lfloor x/\varepsilon \rfloor \in I_\varepsilon^+(u) \text{ or } i = N_\varepsilon \\ (1-\lambda)u_i + \lambda u_{i+1} & \text{otherwise (here, } i := \lfloor x/\varepsilon\rfloor \text{ and } \lambda = x/\varepsilon - \lfloor x/\varepsilon \rfloor). \end{cases}$$

Remark 2.4 *a*) The extension $\hat{u}$ is right-continuous and

$$i\varepsilon \in S(\hat{u}) \quad \text{if and only if} \quad i-1 \in I_\varepsilon^+(u).$$

Note that $\hat{u}^+(x) - \hat{u}^-(x) > 0$ for every $x \in S(\hat{u})$.

b) Recalling that by u we also denote the piecewise-constant function $[0,1] \to \mathbb{R}$ defined by $u(x) = u_i$ with $i = \lfloor x/\varepsilon \rfloor$, we have

$$|\hat{u}(x) - u(x)| \leq z_0\sqrt{\varepsilon} \qquad \text{for every } x \in [0,1]. \tag{2.9}$$

An important compactness property for the extensions $\hat{u}$ is given by the following lemma.

Lemma 2.5 *Let (ε_n) be a positive infinitesimal sequence and let (v_n) be an equibounded sequence of functions $[0,1]\cap\varepsilon_n\mathbb{Z} \to \mathbb{R}$ such that*

$$F_{\varepsilon_n}(v_n) \leq M$$

for some constant M. Let $\hat{v}_n$ be the extensions introduced according to (2.8). Then

$$\int_0^1 |\hat{v}_n'(x)|^2 \,\mathrm{d}x + \# S(\hat{v}_n) \leq \frac{M}{\nu \min(z_0^2, 1)}. \tag{2.10}$$

In particular, up to a subsequence, there exists a piecewise-$H^1(0,1)$ function v such that

$$\hat{v}_n \to v, \quad \hat{v}_n' \rightharpoonup v' \quad \text{in } L^2(0,1).$$

Moreover, $D^j\hat{v}_n \rightharpoonup D^j v$ weakly in the sense of measures.*

Proof. We have:

$$\begin{aligned}
M \geq F_{\varepsilon_n}(v_n) &= \sum_{i \notin I^+_{\varepsilon_n}(v_n)} \varepsilon_n \varphi_{\varepsilon_n}\left(\frac{(v_n)_{i+1}-(v_n)_i}{\varepsilon_n}\right) \\
&\quad + \sum_{i \in I^+_{\varepsilon_n}(v_n)} \varepsilon_n \varphi_{\varepsilon_n}\left(\frac{(v_n)_{i+1}-(v_n)_i}{\varepsilon_n}\right) \\
&\geq \nu \sum_{i \notin I^+_{\varepsilon_n}(v_n)} \varepsilon_n \left(\frac{(v_n)_{i+1}-(v_n)_i}{\varepsilon_n}\right)^2 + \nu z_0^2 \,\# I^+_{\varepsilon_n}(v_n) \\
&\geq \nu \min(z_0^2, 1)\left[\int_0^1 |\hat{v}_n'(x)|^2 \,\mathrm{d}x + \# S(\hat{v}_n)\right].
\end{aligned}$$

We conclude by applying Theorem 2.1. $\square$

Remark 2.6 By the uniform estimate (2.9), the $L^p(0,1)$ convergence of $(\hat{v}_n)$ is equivalent to the $L^p(0,1)$ convergence of the piecewise-constant functions v_n.

Lemma 2.7 *Let (v_n) and v be as in Lemma 2.5. Then*

a) $v^+ - v^- > 0$ on $S(v)$;

b) up to a subsequence, (v_n) satisfies the following property: for every $\overline{x} \in S(v)$ there exists a sequence (x^n) with

$$x^n \in S(\hat{v}_n) \quad \textit{and} \quad \lim_{n\to\infty}\big(\hat{v}_n^+(x^n) - \hat{v}_n^-(x^n)\big) > 0.$$

Proof. a) Since $D^j \hat{v}_n$ are positive measures which weakly* converge to $D^j v$, this latter is a positive measure, too.

b) Let $\overline{x} \in S(v)$ and let V be an open neighborhood of $\overline{x}$ such that $S(v) \cap \overline{V} = \{\overline{x}\}$. By the weak* convergence of the measures $D^j \hat{v}_n$ to $D^j v$ on V, we have (see, e.g., [3], Prop. 1.62) $D^j v(V) = \lim_{n\to\infty} D^j \hat{v}_n(V)$, i.e.:

$$v^+(\overline{x}) - v^-(\overline{x}) = \lim_{n\to\infty} \sum_{x \in S(\hat{v}_n)\cap V} \big(\hat{v}_n^+(x) - \hat{v}_n^-(x)\big). \tag{2.11}$$

By estimate (2.10) for every $n \in \mathbb{N}$, we can define $x_1^n, \ldots, x_m^n$, with m independent of n, such that

$$S(\hat{v}_n) \subseteq \{x_i^n : \ i = 1, \ldots, m\}.$$

Up to a subsequence we can assume that every sequence $(x_i^n)_n$ converges to a point in $[0,1]$: denote by S this set of points. It turns out that $S \cap V \neq \emptyset$, otherwise $v^+(\overline{x}) - v^-(\overline{x}) = 0$ by (2.11). By the arbitrariness of V we must have $\overline{x} \in S$. Hence, we can choose V such that $V \cap S = \{\overline{x}\}$. From (2.11) it follows that there exists a sequence $(x_i^n)_n$ converging to $\overline{x}$ such that

$$x_i^n \in S(\hat{v}_n), \quad \text{and} \quad \limsup_{n\to\infty}\big(\hat{v}_n^+(x_i^n) - \hat{v}_n^-(x_i^n)\big) > 0,$$

otherwise $v^+(\overline{x}) - v^-(\overline{x}) = 0$. $\square$

Minimizing movements along F_ε. As mentioned in the introduction, we apply the method of the minimizing movements to the functionals F_ε, but we allow the spatial-discretization parameter ε to vary as the time-discretization step goes to zero.

For each $\varepsilon > 0$ let $u^0_\varepsilon \colon [0,1] \cap \varepsilon\mathbb{Z} \to \mathbb{R}$ be a given function and let $\tau > 0$ be fixed. We recursively define a sequence $u^k := u^k_{\varepsilon,\tau}$ ($k \in \mathbb{N}$) of real-valued functions on $[0,1] \cap \varepsilon\mathbb{Z}$, by requiring that u^0 is the initial datum u^0_ε just fixed, while for any $k \geq 1$, the function u^k is a minimizer of

$$G^k_{\varepsilon,\tau}(v) := F_\varepsilon(v) + \frac{1}{2\tau}\sum_{i=0}^{N_\varepsilon} \varepsilon |v_i - u_i^{k-1}|^2 \,, \tag{2.12}$$

with respect to all functions $v \colon [0,1]\cap\varepsilon\mathbb{Z} \to \mathbb{R}$. We state some easy consequences of this definition.

Proposition 2.8 *For every $k \in \mathbb{N}$ the following properties hold:*

a) $F_\varepsilon(u^k) \leq F_\varepsilon(u^{k-1})$,

b) $\displaystyle\sum_{i=0}^{N_\varepsilon} \varepsilon |u^k_i - u^{k-1}_i|^2 \leq 2\tau\big[F_\varepsilon(u^{k-1}) - F_\varepsilon(u^k)\big]$,

c) $\|u^k\|_\infty \leq \|u^{k-1}\|_\infty \leq \|u^0_\varepsilon\|_\infty$.

Proof. The minimality of u^k with respect to the test function $v = u^{k-1}$, implies that

$$F_\varepsilon(u^k) + \frac{1}{2\tau}\sum_{i=0}^{N_\varepsilon} \varepsilon |u^k_i - u^{k-1}_i|^2 \leq F_\varepsilon(u^{k-1}).$$

From this inequality, (a) and (b) follow immediately.

Moreover, if $M := \|u^{k-1}\|_\infty$, then for every u we have

$$G^k_{\varepsilon,\tau}((u \wedge M) \vee (-M)) \leq G^k_{\varepsilon,\tau}(u).$$

Therefore $\|u^k\|_\infty \leq \|u^{k-1}\|_\infty$. □

Since u^k is a solution of a minimum problem in finite dimension we get the classical optimality conditions.

Proposition 2.9 *Let u^k be defined recursively by* (2.12) *Then, the following equations hold:*

$$-\varphi'_\varepsilon\left(\frac{u^k_1 - u^k_0}{\varepsilon}\right) + \frac{\varepsilon}{\tau}(u^k_0 - u^{k-1}_0) = 0$$

$$\varphi'_\varepsilon\left(\frac{u^k_i - u^k_{i-1}}{\varepsilon}\right) - \varphi'_\varepsilon\left(\frac{u^k_{i+1} - u^k_i}{\varepsilon}\right) + \frac{\varepsilon}{\tau}(u^k_i - u^{k-1}_i) = 0 \qquad (0 < i < N_\varepsilon)$$

$$\varphi'_\varepsilon\left(\frac{u^k_{N_\varepsilon} - u^k_{N_\varepsilon - 1}}{\varepsilon}\right) + \frac{\varepsilon}{\tau}(u^k_{N_\varepsilon} - u^{k-1}_{N_\varepsilon}) = 0.$$

For any given $\varepsilon > 0$ and $\tau > 0$ and for every $k \in \mathbb{N}$ we interpret the values $(u^k_{\varepsilon,\tau})_i$ (for $i = 0, \dots, N_\varepsilon$) as the discrete evolution, at the time $t = k\tau$, of the initial (discrete) datum $u^0_\varepsilon \colon [0,1] \cap \varepsilon\mathbb{Z} \to \mathbb{R}$. The goal is to detect the limit evolution as $\varepsilon, \tau \to 0$.

Remark 2.10 The optimality conditions in the proposition above easily suggest the form of the evolution equation satisfied by a possible limit function u. Indeed, by dividing the i-th equation by ε and applying the mean-value theorem to $\varphi'_\varepsilon(z) = \psi'(\sqrt{\varepsilon} z)/\sqrt{\varepsilon}$, we get

$$\frac{u^k_i - u^{k-1}_i}{\tau} = \psi''(\sqrt{\varepsilon}\xi)\frac{u^k_{i+1} - 2u^k_i + u^k_{i-1}}{\varepsilon^2},$$

where ξ is a suitable value between the two difference quotients. Hence, in the limit we obtain

$$u_t = \psi''(0)u_{xx}$$

at the points in which u is twice differentiable (see Theorem 4.1).

On the initial datum u^0_ε we make the following assumptions:

$B1)$ $(u^0_\varepsilon)_\varepsilon$ is an equibounded set of functions $[0,1] \cap \varepsilon\mathbb{Z} \to \mathbb{R}$; i.e., we have $\sup\{(u^0_\varepsilon)_i : 0 \le i \le N_\varepsilon,\ \varepsilon > 0\} < +\infty$;

$B2)$ there exists $M > 0$ such that $F_\varepsilon(u^0_\varepsilon) \le M$ for every $\varepsilon > 0$.

With in view the analysis of the limit, as $\varepsilon, \tau \to 0$, of the discrete evolutions $(u^k_{\varepsilon,\tau})_k$ defined in the previous section, we introduce the piecewise-constant spatial-time extension $u_{\varepsilon,\tau}$ of these values to $[0,1] \times [0, +\infty)$ by defining

$$\begin{aligned} &u_{\varepsilon,\tau} \colon [0,1] \times [0, +\infty) \to \mathbb{R}, \\ &u_{\varepsilon,\tau}(x,t) = \big(u^k_{\varepsilon,\tau}\big)_i \quad \text{with } k = \lfloor t/\tau \rfloor \text{ and } i = \lfloor x/\varepsilon \rfloor. \end{aligned} \tag{2.13}$$

In the following section we give a compactness result (Theorem 3.2) for the family $u_{\varepsilon,\tau}$ as $\varepsilon, \tau \to 0$.

3 Compactness

The compactness result contained in Theorem 3.2 follows a standard line in the theory of minimizing movements (see [1], [2] and [7]). In Theorem 3.4 we prove a regularity result for the limit function.

Proposition 3.1 *For any $s, t \ge 0$, with $s < t$, we have*

$$\|u_{\varepsilon,\tau}(\cdot,t) - u_{\varepsilon,\tau}(\cdot,s)\|_2 \le \big(2F_\varepsilon(u^0_\varepsilon)\big)^{1/2}\sqrt{t - s + \tau}.$$

Proof. Let $x \in [0,1]$ and $0 \le s < t$ be fixed; set $h = \lfloor s/\tau \rfloor$ and $k = \lfloor t/\tau \rfloor$. For every i it turns out that:

$$\begin{aligned} \left|\left(u^k_{\varepsilon,\tau}\right)_i - \left(u^h_{\varepsilon,\tau}\right)_i\right| &\le \sum_{j=h}^{k-1} \left|\left(u^{j+1}_{\varepsilon,\tau}\right)_i - \left(u^j_{\varepsilon,\tau}\right)_i\right| \\ &\le \sqrt{k-h}\sqrt{\sum_{j=h}^{k-1} \left|\left(u^{j+1}_{\varepsilon,\tau}\right)_i - \left(u^j_{\varepsilon,\tau}\right)_i\right|^2}\,. \end{aligned}$$

Therefore, by Proposition 2.8, we have

$$\begin{aligned} \sum_{i=0}^{N_\varepsilon} \varepsilon\left|\left(u^k_{\varepsilon,\tau}\right)_i - \left(u^h_{\varepsilon,\tau}\right)_i\right|^2 &\le (k-h)\sum_{i=0}^{N_\varepsilon}\sum_{j=h}^{k-1} \varepsilon\left|\left(u^{j+1}_{\varepsilon,\tau}\right)_i - \left(u^j_{\varepsilon,\tau}\right)_i\right|^2 \\ &\le 2\tau(k-h)\sum_{j=h}^{k-1}\left(F_\varepsilon(u^j_{\varepsilon,\tau}) - F_\varepsilon(u^{j+1}_{\varepsilon,\tau})\right) \\ &\le 2\tau(k-h)\left(F_\varepsilon(u^h_{\varepsilon,\tau}) - F_\varepsilon(u^k_{\varepsilon,\tau})\right) \le 2(t-s+\tau)F_\varepsilon(u^0_\varepsilon). \quad \square \end{aligned}$$

Theorem 3.2 *Under the assumptions* $(B1)$ *and* $(B2)$, *let* (ε_n) *and* (τ_n) *be positive infinitesimal sequences, and let* $v_n = u_{\varepsilon_n,\tau_n}$ *be the piecewise-constant functions defined in* (2.13). *For every* $t \ge 0$ *denote by* $\hat{v}_n(\cdot,t)$ *the piecewise-affine extension of* $v_n(\cdot,t)$ *according to* (2.8). *Then there exist a subsequence (not relabelled) of* (v_n) *and a function* $u \in C^{1/2}([0,+\infty);L^2(0,1))$ *such that*

$$v_n \to u, \quad \hat{v}_n \to u \quad \text{in } L^\infty([0,T];L^2(0,1)) \text{ and a.e. in } (0,1)\times(0,T)$$

for every $T \ge 0$. *Moreover, for every* $t \ge 0$,

$$\begin{aligned} &u(\cdot,t) \text{ is piecewise-}H^1(0,1) \\ &(\hat{v}_n)_x(\cdot,t) \rightharpoonup u_x(\cdot,t) \quad \text{in } L^2(0,1). \end{aligned}$$

Finally, every $\overline{x} \in S\big(u(\cdot,t)\big)$ *can be approximated by jump points of* $\hat{v}_n(\cdot,t)$ *as in Lemma* 2.7(*b*).

Proof. Let $t \ge 0$ be fixed. By Proposition 2.8(a) we have that $F_{\varepsilon_n}\big(v_n(\cdot,t)\big)$ is a bounded sequence. Thus, we can apply Lemma 2.5 to the functions $v_n(\cdot,t)$: the sequence $(\hat{v}_n(\cdot,t))_n$ is pre-compact with respect to the $L^2(0,1)$ convergence; moreover, the limit is piecewise-$H^1(0,1)$, and we have weak-L^2 convergence of $(\hat{v}_n)_x(\cdot,t)$. Note that, by the uniform estimate (2.9), the $L^2(0,1)$ (or a.e.) convergence of $(\hat{v}_n)$ is equivalent to the corresponding convergence of (v_n).

By a diagonalization argument we can assume that, up to a subsequence, $\hat{v}_n(\cdot,t)$ converge in $L^2(0,1)$ for every $t \in \mathbb{Q}^+$: let $u(\cdot,t)$ be the limit function. The estimate in Proposition 3.1 allows to get the $L^2(0,1)$ convergence for every $t \ge 0$ (hence, $u(\cdot,t)$ is well defined for every $t \ge 0$). Moreover

$$\|u(\cdot,t) - u(\cdot,s)\|_2 \le C\sqrt{t-s}, \tag{3.1}$$

for any $s,t \ge 0$, with $s < t$ and for a suitable constant C, independent of s and t. Thus $u \in C^{1/2}([0,+\infty);L^2(0,1))$. Furthermore, by the uniqueness of the L^2 limit, the compactness result of Theorem 2.1 guarantees that $u(\cdot,t)$ is piecewise-$H^1(0,1)$ and that $(\hat{v}_n)_x(\cdot,t)$ weakly converges to $u_x(\cdot,t)$ in $L^2(0,1)$ for every $t \geq 0$.

We now prove the convergence of (v_n) to u in $L^\infty([0,T];L^2(0,1))$ (from which the analogous convergence of $(\hat{v}_n)$ follows as well). Let $T > 0$ be fixed. For any given $S \in \mathbb{N}$, define $t_j = jT/S$ for $j = 0,\ldots,S$; then, for every $t \in [0,T]$ there exists $j = 0,\ldots,S-1$ with $t_j \leq t \leq t_{j+1}$. By Proposition 3.1 and estimate (3.1), we have:

$$\begin{aligned}\|v_n(\cdot,t) - u(\cdot,t)\|_2 &\leq \|v_n(\cdot,t) - v_n(\cdot,t_j)\|_2 + \|v_n(\cdot,t_j) - u(\cdot,t_j)\|_2 \\ &\qquad + \|u(\cdot,t_j) - u(\cdot,t)\|_2 \\ &\leq 2C\sqrt{t - t_j + \tau_n} + \|v_n(\cdot,t_j) - u(\cdot,t_j)\|_2 \,.\end{aligned}$$

Fix $\sigma > 0$ and let $n_\sigma \in \mathbb{N}$ be such that

$$\|v_n(\cdot,t_j) - u(\cdot,t_j)\|_2 \leq \sigma \quad \text{for every } n \geq n_\sigma \text{ and } j = 0,\ldots,S-1.$$

Then

$$\sup_{t\in[0,T]} \|v_n(\cdot,t) - u(\cdot,t)\|_2 \leq 2C\sqrt{(T/S) + \tau_n} + \sigma \qquad \text{for every } n \geq n_\sigma,$$

and this yields

$$\limsup_{n\to+\infty} \sup_{t\in[0,T]} \|v_n(\cdot,t) - u(\cdot,t)\|_2 \leq 2C\sqrt{(T/S)} + \sigma.$$

By the arbitrariness of S and σ we deduce the convergence in $L^\infty([0,T];L^2(0,1))$. In particular, we have the convergence in $L^2((0,1)\times(0,T))$, and hence the convergence a.e. (up to a subsequence).

Finally, if $\overline{x} \in S\big(u(\cdot,t)\big)$ then we can apply Lemma 2.7 (b) to the sequence $v_n = v_n(\cdot,t)$. $\square$

Remark 3.3 The weak-$L^2(0,1)$ convergence of the sections $(\hat{v}_n)_x(\cdot,t)$ and their uniform boundedness in $L^2(0,1)$ (see Lemma 2.5) allow to deduce the weak-$L^2\big((0,1)\times(0,T)\big)$ convergence of $(\hat{v}_n)_x$.

Theorem 3.4 *Let $v_n = u_{\varepsilon_n,\tau_n}$ be a sequence converging to a function u as in Theorem 3.2. Then $u_x(\cdot,t) \in H^1(0,1)$ for a.e. $t \geq 0$. Moreover, for a.e. $t \geq 0$, we have $u_x(0,t) = u_x(1,t) = 0$ and $u_x(\cdot,t) = 0$ on $S\big(u(\cdot,t)\big)$.*

For future reference it is useful to isolate from the proof a technical lemma.

Let $v_n = u_{\varepsilon_n,\tau_n}$ be a sequence converging to u according to Theorem 3.2. In the sequel we will drop the index n and simply write ε and τ in place of ε_n and τ_n. By (2.13) we have

$$v_n(x,t) = \big(u^k_{\varepsilon,\tau}\big)_i \quad \text{with } k = \lfloor t/\tau \rfloor \text{ and } i = \lfloor x/\varepsilon \rfloor. \tag{3.2}$$

We extend this definition by setting

$$\big(u^k_{\varepsilon,\tau}\big)_i = \begin{cases} \big(u^k_{\varepsilon,\tau}\big)_0 & \text{if } i \in \mathbb{Z},\, i < 0, \\ \big(u^k_{\varepsilon,\tau}\big)_{N_\varepsilon} & \text{if } i \in \mathbb{Z},\, i > N_\varepsilon\,. \end{cases}$$

Thus, for every $x \in \mathbb{R}$ and $t \geq 0$ we can define the piecewise-constant function

$$w_n(x,t) = \varphi_\varepsilon'\Big(\frac{(u^k_{\varepsilon,\tau})_{i+1} - (u^k_{\varepsilon,\tau})_i}{\varepsilon}\Big), \qquad \text{with} \quad \begin{array}{c} i = \lfloor x/\varepsilon \rfloor \\ k = \lfloor t/\tau \rfloor. \end{array} \tag{3.3}$$

Lemma 3.5 *For every $t \geq 0$*

$$w_n(\cdot,t) \rightharpoonup \psi''(0) u_x(\cdot,t) \qquad \text{in } L^2(0,1).$$

Moreover, the sequence (w_n) is bounded in $L^1\big((0,1)\times(0,T)\big)$ for every $T > 0$.

Proof. Let $t \geq 0$ be fixed. Denote by χ_n the characteristic function of the set $\bigcup_{i \in I^+_\varepsilon} \varepsilon[i,i+1)$, where $I^+_\varepsilon = I^+_\varepsilon\big(v_n(\cdot,t)\big)$. Consider the decomposition

$$w_n(\cdot,t) = \chi_n w_n(\cdot,t) + (1-\chi_n) w_n(\cdot,t).$$

By Lemma 2.3 and the decreasing monotonicity of $F_\varepsilon(u^k)$ with respect to k (see Lemma 2.8), it turns out that

$$\begin{aligned} \int_0^1 |\chi_n w_n(x,t)|^2 \, \mathrm{d}x &= \sum_{i \in I^+_\varepsilon} \varepsilon |w_n(i\varepsilon,t)|^2 \\ &\leq \varepsilon(\# I^+_\varepsilon)\varphi_\varepsilon'\Big(\frac{z_0}{\sqrt{\varepsilon}}\Big)^2 \leq \frac{M}{\nu z_0^2}\psi'(z_0)^2 \,, \end{aligned}$$

so that $\big(\chi_n w_n(\cdot,t)\big)$ is bounded in $L^2(0,1)$. By the same argument we get

$$\int_0^1 |\chi_n w_n(x,t)| \, \mathrm{d}x \leq \varepsilon(\# I^+_\varepsilon)\varphi_\varepsilon'\Big(\frac{z_0}{\sqrt{\varepsilon}}\Big) \leq \sqrt{\varepsilon}\frac{M}{\nu z_0^2}\psi'(z_0) \to 0 \tag{3.4}$$

as $n \to +\infty$. We conclude that $\chi_n w_n(\cdot,t) \rightharpoonup 0$ weakly in $L^2(0,1)$.

Let us now consider $(1-\chi_n)w_n(\cdot,t)$. Note that, in the notation of (3.3), if $i \notin I^+_\varepsilon$ and $x \in [i\varepsilon,(i+1)\varepsilon)$ we have

$$\frac{(u^k_{\varepsilon,\tau})_{i+1} - (u^k_{\varepsilon,\tau})_i}{\varepsilon} = (\hat{v}_n)_x(x,t),$$

where $\hat{v}_n(\cdot,t)$ is the extension of $v_n(\cdot,t)$ according to (2.8). If we take into account that $(\hat{v}_n)_x(x,t) = 0$ in $\big(i\varepsilon,(i+1)\varepsilon\big)$ if $i \in I^+_\varepsilon$, then

$$(1-\chi_n)w_n(\cdot,t) = \varphi_\varepsilon'\big((\hat{v}_n)_x(\cdot,t)\big).$$

Consider now the Taylor expansion of φ_ε' at 0; for every $x \in [i\varepsilon,(i+1)\varepsilon)$, with $i \notin I^+_\varepsilon$, we have

$$\varphi_\varepsilon'\big((\hat{v}_n)_x(x,t)\big) = \varphi_\varepsilon'(0) + \varphi_\varepsilon''(0)(\hat{v}_n)_x(x,t) + \frac{1}{2}\varphi_\varepsilon'''(\xi_n)\big((\hat{v}_n)_x(x,t)\big)^2$$

with ξ_n between 0 and $(\hat{v}_n)_x(x,t)$; hence,

$$\varphi_\varepsilon'\big((\hat{v}_n)_x(x,t)\big) = \psi''(0)(\hat{v}_n)_x(x,t) + \frac{1}{2}\sqrt{\varepsilon} r_n\big((\hat{v}_n)_x(x,t)\big)^2 \tag{3.5}$$

with $r_n = \psi'''(\sqrt{\varepsilon}\xi_n)$. From Lemma 2.3 we deduce that

$$\frac{\zeta_0}{\sqrt{\varepsilon}} < (\hat{v}_n)_x(x,t) \leq \frac{z_0}{\sqrt{\varepsilon}}$$

where $\zeta_0 \in (-1,0)$ is such that $\psi(\zeta_0) \geq M$. Then (r_n) is a bounded sequence.

Note that (3.5) holds for $i \in I_\varepsilon^+$, too, with $r_n = 0$ as a possibile choice (indeed $(\hat{v}_n)_x(x,t) = 0$ for such indices).

By a similar argument, through a first-order expansion, we get the equi-boundedness of the L^2-norms of $\varphi'_\varepsilon\big((\hat{v}_n)_x(\cdot,t)\big)$, hence the weak convergence of the left-hand side of (3.5). Now we can deduce the weak-L^2 convergence of $w_n(\cdot,t)$ by the weak-L^2 convergence of $(\hat{v}_n)_x(\cdot,t)$ to $u(\cdot,t)$, which implies the weak-L^1 convergence of the right-hand side of (3.5).

Finally, by (3.4) and (3.5) we get the boundedness of the L^1 norms of w_n in $(0,1)\times(0,T)$, for every $T > 0$. □

Proof of Theorem 3.4. By Proposition 2.8

$$\sum_{i=0}^{N_\varepsilon} \varepsilon \big| \big(u^k_{\varepsilon,\tau}\big)_i - \big(u^{k-1}_{\varepsilon,\tau}\big)_i \big|^2 \leq 2\tau \big[F_\varepsilon\big(u^{k-1}_{\varepsilon,\tau}\big) - F_\varepsilon\big(u^k_{\varepsilon,\tau}\big)\big].$$

Let $T > 0$ be fixed, and $M_\tau = \lfloor T/\tau \rfloor$. Then

$$\sum_{k=1}^{M_\tau}\sum_{i=0}^{N_\varepsilon} \tau\varepsilon \big| \big(u^k_{\varepsilon,\tau}\big)_i - \big(u^{k-1}_{\varepsilon,\tau}\big)_i \big|^2 \leq 2\tau^2 F_\varepsilon(u^0_\varepsilon) \leq 2\tau^2 M$$

(where M is given in assumption $(B2)$). By Proposition 2.9 and the extension, defined above, of $\big(u^k_{\varepsilon,\tau}\big)_i$ for $i < 0$ and $i > N_\varepsilon$, this estimate can be written as

$$\sum_{k=1}^{M_\tau} \tau \sum_{i\in\mathbb{Z}} \varepsilon\tau^2 \left[\varepsilon^{-1}\left(\varphi'_\varepsilon\Big(\frac{(u^k_{\varepsilon,\tau})_{i+1} - (u^k_{\varepsilon,\tau})_i}{\varepsilon}\Big) - \varphi'_\varepsilon\Big(\frac{(u^k_{\varepsilon,\tau})_i - (u^k_{\varepsilon,\tau})_{i-1}}{\varepsilon}\Big)\right)\right]^2 \leq 2\tau^2 M\,.$$

Let $\tilde{w}_n(\cdot,t)$ be the function obtained as the piecewise-affine extension of the values $w_n(\cdot,t)$ on the nodes $\varepsilon\mathbb{Z}$. By the previous estimate we have

$$\sum_{k=1}^{M_\tau} \tau \int_{\mathbb{R}} \big[(\tilde{w}_n)_x(x,k\tau)\big]^2 \,\mathrm{d}x \leq 2M,$$

and therefore, for every $\delta > 0$ and $\tau < \delta$:

$$\int_\delta^T \mathrm{d}t \int_{\mathbb{R}} \big[(\tilde{w}_n)_x(x,t)\big]^2 \,\mathrm{d}x \leq 2M.$$

By Fatou's Lemma

$$\int_\delta^T \Big(\liminf_{n\to+\infty} \int_{\mathbb{R}} \big[(\tilde{w}_n)_x(x,t)\big]^2 \,\mathrm{d}x\Big)\,\mathrm{d}t \leq 2M. \tag{3.6}$$

We deduce that

$$\liminf_{n\to+\infty} \int_{\mathbb{R}} \big[(\tilde{w}_n)_x(x,t)\big]^2 \,\mathrm{d}x < +\infty \qquad \text{for a.e. } t > 0.$$

We now fix t satisfying this condition; then, we can assume that, up to a subsequence,

$$\int_{\mathbb{R}} \big[(\tilde{w}_n)_x(x,t)\big]^2 \,\mathrm{d}x \leq C \tag{3.7}$$

for a suitable constant C independent of n.

The functions $w_n(\cdot,t)$ in (3.3) take the value 0 outside the interval $[0,\varepsilon N_\varepsilon]$. Therefore, the weak convergence stated in Lemma 3.5 yields

$$w_n(\cdot,t) \rightharpoonup w(\cdot,t) := \begin{cases} \psi''(0)\,u_x(\cdot,t) & \text{in } (0,1), \\ 0 & \text{otherwise in } \mathbb{R} \end{cases} \qquad \text{in } L^2(\mathbb{R}).$$

By (3.7) this implies the weak convergence in $L^2(\mathbb{R})$ of the piecewise-affine functions $\tilde{w}_n(\cdot,t)$. Indeed, $\sum_i \varepsilon \big|w_n\big((i+1)\varepsilon,t\big) - w_n(i\varepsilon,t)\big|^2 \leq \varepsilon^2 C$. Thus

$$\tilde{w}_n(\cdot,t) \rightharpoonup w(\cdot,t) \qquad \text{in } L^2(\mathbb{R}). \tag{3.8}$$

At this point we have proved that for a.e. $t \geq 0$ both (3.7) and (3.8) hold, up to a subsequence possibly depending on t. Therefore, for any open interval $J \supset [0,1]$ we have $w \in H^1(J)$; in particular, $u_x(\cdot,t) \in H^1(0,1)$ and $u_x(0,t) = u_x(1,t) = 0$ for a.e. $t \geq 0$. Moreover, for such values of t, by the compact injection of $H^1(0,1)$ into $C([0,1])$, we deduce that

$$\tilde{w}_n(\cdot,t) \to \psi''(0)u_x(\cdot,t) \quad \text{in } C([0,1]).$$

Let $\overline{x}$ be a jump point of $u(\cdot,t)$; on account of Lemma 2.7(b) we can assume that there exist a sequence (x^n) converging to $\overline{x}$ and a value $\gamma > 0$ such that for every n

$$x^n \in S\big(\hat{v}_n(\cdot,t)\big), \qquad \hat{v}_n^+(x^n,t) - \hat{v}_n^-(x^n,t) \geq \gamma > 0.$$

Recall that x^n can be expressed as $i_n\varepsilon$, for a suitable i_n. By Remark 2.4(a), $x^n = i_n\varepsilon \in S\big(\hat{v}_n(\cdot,t)\big)$ if and only if $i_n - 1 \in I_\varepsilon^+\big(\hat{v}_n(\cdot,t)\big)$. Then

$$\begin{aligned} \tilde{w}_n\big((i_n-1)\varepsilon,t\big) = w_n\big((i_n-1)\varepsilon,t\big) &= \varphi_\varepsilon'\Big(\frac{\hat{v}_n^+(x^n,t) - \hat{v}_n^-(x^n,t)}{\varepsilon}\Big) \\ &\leq \varphi_\varepsilon'\Big(\frac{\gamma}{\varepsilon}\Big) = \frac{1}{\sqrt{\varepsilon}}\psi'\Big(\frac{\gamma}{\sqrt{\varepsilon}}\Big). \end{aligned}$$

Note now that $\lim_{z\to+\infty} z\psi'(z) = 0$; indeed, for every $z \geq 2z_0$ there exists a value $\xi_z \in (z/2, z)$ such that

$$\frac{\psi(z) - \psi(z/2)}{z/2} = \psi'(\xi_z) \geq \psi'(z) \geq 0,$$

from which $0 \leq z\psi'(z) \leq 2\big(\psi(z) - \psi(z/2)\big) \to 0$ as $z \to +\infty$. Therefore,

$$\lim_{n\to+\infty} \tilde{w}_n((i_n-1)\varepsilon,t) = 0,$$

and the uniform convergence of $\tilde{w}_n(\cdot,t)$ to $\psi''(0)u_x(\cdot,t)$ imply that $u_x(\overline{x},t) = 0$. $\square$

4 Limit equation and evolution of the singular set.

Limit equation. Assume that $(u_\varepsilon^0)_{\varepsilon>0}$ is an indexed family of functions satisfying conditions $(B1)$ and $(B2)$ and converging a.e. (as piecewise-constant functions) to a function u^0. By the estimate of Lemma 2.5 we have that u^0 is piecewise-$H^1(0,1)$. For any fixed time step τ let $u_{\varepsilon,\tau}$ be the discrete evolution of the initial datum u^0_ε as in (2.13).

Theorem 4.1 *Let $v_n = u_{\varepsilon_n,\tau_n}$ be a sequence converging to a function u as in Theorem 3.2 (thus $u_x(\cdot,t) \in H^1(0,1)$ for a.e. $t \geq 0$ by Theorem 3.4). Then*

$$u_t = \psi''(0)(u_x)_x$$

in the distributional sense in $(0,1)\times(0,+\infty)$, and

$$\begin{aligned} &u(\cdot,0) = u^0 \quad \text{a.e. in } (0,1);\\ &u_x(\cdot,t) = 0 \quad \text{on } S\big(u(\cdot,t)\big)\cup\{0,1\} \text{ for a.e. } t \geq 0. \end{aligned}$$

Proof. As above, we will drop the index n and simply write ε and τ in place of ε_n and τ_n.

Taking Theorem 3.2 and Theorem 3.4 into account, we only have to prove that u satisfies the equation $u_t = \psi''(0)(u_x)_x$ in the distributional sense and that $u(\cdot,0) = u^0$. Note that $u(\cdot,0)$ is well defined since $u \in C^{1/2}([0,+\infty);L^2(0,1))$. As to the latter, we have:

$$\begin{aligned} \|u(\cdot,0)-u^0\|_{L^2(0,1)} &\leq \|u(\cdot,0)-u_{\varepsilon,\tau}(\cdot,0)\|_2 + \|u_{\varepsilon,\tau}(\cdot,0)-u^0\|_2\\ &= \|u(\cdot,0)-u_{\varepsilon,\tau}(\cdot,0)\|_2 + \|u^0_\varepsilon - u^0\|_2\,. \end{aligned}$$

Both terms on the right-hand side tend to 0 since for every $T > 0$ we have $u_{\varepsilon,\tau} \to u$ in $L^\infty\big([0,T];L^2(0,1)\big)$ (see Theorem 3.2), and (u^0_ε) is an equibounded sequence converging a.e. to u^0.

We now address the evolution equation. Fix $T > 0$ and let $M_\tau = \lfloor T/\tau \rfloor$. Let $\phi \in C^\infty_c\big((0,1)\times(0,T)\big)$ be fixed, and define

$$\phi^k_i = \phi(i\varepsilon, k\tau) \qquad \text{with } k,i \in \mathbb{Z}.$$

Recall the summation by parts formula:

$$\sum_{j=0}^{l-1} a_j(b_{j+1}-b_j) = a_l b_l - a_0 b_0 - \sum_{j=0}^{l-1}(a_{j+1}-a_j)b_{j+1}\,.$$

Then ($l = M_\tau$) we have:

$$\begin{aligned} A := &\sum_{i=0}^{N_\varepsilon}\sum_{k=0}^{M_\tau-1} \varepsilon\tau(u^k_{\varepsilon,\tau})_i \,\frac{\phi^{k+1}_i-\phi^k_i}{\tau}\\ &= \varepsilon\sum_{i=0}^{N_\varepsilon}\left[(u^{M_\tau}_{\varepsilon,\tau})_i\phi^{M_\tau}_i - (u^0_{\varepsilon,\tau})_i\phi^0_i - \sum_{k=0}^{M_\tau-1}\left((u^{k+1}_{\varepsilon,\tau})_i-(u^k_{\varepsilon,\tau})_i\right)\phi^{k+1}_i\right]. \end{aligned}$$

Since ϕ has compact support in $(0,1)\times(0,T)$ we have $\phi^0_i = \phi^k_0 = 0$ and, for ε and τ sufficiently small we can assume that $\phi^{M_\tau}_i = \phi^k_{N_\varepsilon} = 0$.

The optimality conditions now yield:

$$A = -\tau\sum_{i=0}^{N_\varepsilon}\sum_{k=0}^{M_\tau-1}\left[\varphi'_\varepsilon\left(\frac{(u^{k+1}_{\varepsilon,\tau})_{i+1}-(u^{k+1}_{\varepsilon,\tau})_i}{\varepsilon}\right) - \varphi'_\varepsilon\left(\frac{(u^{k+1}_{\varepsilon,\tau})_i-(u^{k+1}_{\varepsilon,\tau})_{i-1}}{\varepsilon}\right)\right]\phi^{k+1}_i.$$

Apply again the summation by parts formula, with

$$a_j = \phi_j^{k+1}, \qquad b_j = \varphi_\varepsilon'\left(\frac{(u_{\varepsilon,\tau}^{k+1})_j - (u_{\varepsilon,\tau}^{k+1})_{j-1}}{\varepsilon}\right);$$

then

$$A = \tau \sum_{i=0}^{N_\varepsilon} \sum_{k=0}^{M_\tau - 1} (\phi_{i+1}^{k+1} - \phi_i^{k+1}) \varphi_\varepsilon'\left(\frac{(u_{\varepsilon,\tau}^{k+1})_{i+1} - (u_{\varepsilon,\tau}^{k+1})_i}{\varepsilon}\right).$$

We conclude that

$$\begin{aligned} &\sum_{i=0}^{N_\varepsilon} \sum_{k=0}^{M_\tau - 1} \varepsilon\tau (u_{\varepsilon,\tau}^k)_i \, \frac{\phi_i^{k+1} - \phi_i^k}{\tau} \\ &\qquad = \sum_{i=0}^{N_\varepsilon} \sum_{k=0}^{M_\tau - 1} \varepsilon\tau \, \frac{\phi_{i+1}^{k+1} - \phi_i^{k+1}}{\varepsilon} \, \varphi_\varepsilon'\left(\frac{(u_{\varepsilon,\tau}^{k+1})_{i+1} - (u_{\varepsilon,\tau}^{k+1})_i}{\varepsilon}\right). \end{aligned} \tag{4.1}$$

Let now $\phi_{\varepsilon,\tau}^{(0,1)}$ and $\phi_{\varepsilon,\tau}^{(1,0)}$ be the piecewise-constant functions on $\mathbb{R}^2$ defined by

$$\phi_{\varepsilon,\tau}^{(0,1)}(x,t) = \frac{\phi_i^{k+1} - \phi_i^k}{\tau}, \quad \phi_{\varepsilon,\tau}^{(1,0)}(x,t) = \frac{\phi_{i+1}^k - \phi_i^k}{\varepsilon}$$

where $i = \lfloor x/\varepsilon \rfloor$ and $k = \lfloor t/\tau \rfloor$. Then, we can write the left-hand side of (4.1) in the following form (as $\phi = 0$ in a neighborhood of $\partial([0,1] \times [0,T])$):

$$\int_0^1 \int_0^T u_{\varepsilon,\tau}(x,t) \phi_{\varepsilon,\tau}^{(0,1)}(x,t) \, \mathrm{d}x\mathrm{d}t.$$

In the limit as $n \to +\infty$ we get

$$\int_0^1 \int_0^T u(x,t) \frac{\partial \phi}{\partial t}(x,t) \, \mathrm{d}x\mathrm{d}t.$$

We now examine the right-hand side of (4.1). By means of the functions w_n introduced in equation (3.3), this term can be written as

$$\int_0^1 \mathrm{d}x \int_0^T \phi_{\varepsilon,\tau}^{(1,0)}(x,t) w_n(x,t) \, \mathrm{d}t.$$

By Lemma 3.5, in the limit as $n \to +\infty$ we get

$$\psi''(0) \int_0^1 \mathrm{d}t \int_0^T \frac{\partial \phi}{\partial x} \frac{\partial u}{\partial x} \, \mathrm{d}x\,,$$

which concludes the proof. □

Evolution of the singular set. Let $u_{\varepsilon,\tau}^k$ $(k = 0, 1, 2, \dots)$ be the discrete evolution of the initial datum u_ε^0 as introduced in Section 2 through the minimization of the functional in (2.12). In what follows we analyse the evolution of the singular set $I_\varepsilon^+(u_{\varepsilon,\tau}^k)$ (see (2.7)) with respect to the index k. The key tool will be estimate (4.3) below and the subsequent lemma, which are a discrete version of the argument applied in [12] (Lemma 4.10 and Proposition 4.11); this will require a condition on the ratio τ/ε^2.

We simply write u_i^k in place of $\left(u^k_{\varepsilon,\tau}\right)_i$. Fix $0 \le i < N_\varepsilon$ and define

$$v^k := \frac{u^k_{i+1} - u^k_i}{\varepsilon}$$

(for the sake of simplicity we do not write the dependence of v_i^k on i). If $0 < i < N_\varepsilon - 1$, then by the optimality conditions in Proposition 2.9 we have

$$\begin{aligned} v^{k+1} - v^k &= \frac{1}{\varepsilon}\left(u^{k+1}_{i+1} - u^{k+1}_i - u^k_{i+1} + u^k_i\right) \\ &= \frac{1}{\varepsilon}(u^{k+1}_{i+1} - u^k_{i+1}) - \frac{1}{\varepsilon}(u^{k+1}_i - u^k_i) \\ &= \frac{\tau}{\varepsilon^2}\left[\varphi'_\varepsilon\left(\frac{u^{k+1}_{i+2} - u^{k+1}_{i+1}}{\varepsilon}\right) + \varphi'_\varepsilon\left(\frac{u^{k+1}_i - u^{k+1}_{i-1}}{\varepsilon}\right) - 2\varphi'_\varepsilon\left(\frac{u^{k+1}_{i+1} - u^{k+1}_i}{\varepsilon}\right)\right]. \end{aligned}$$

Hence,

$$\begin{aligned} (v^{k+1} - v^k) &+ 2\frac{\tau}{\varepsilon^2}\varphi'_\varepsilon\left(\frac{u^{k+1}_{i+1} - u^{k+1}_i}{\varepsilon}\right) \\ &= \frac{\tau}{\varepsilon^2}\left[\varphi'_\varepsilon\left(\frac{u^{k+1}_{i+2} - u^{k+1}_{i+1}}{\varepsilon}\right) + \varphi'_\varepsilon\left(\frac{u^{k+1}_i - u^{k+1}_{i-1}}{\varepsilon}\right)\right], \end{aligned} \tag{4.2}$$

and

$$(v^{k+1} - v^k) + 2\frac{\tau}{\varepsilon^2}\varphi'_\varepsilon\left(\frac{u^{k+1}_{i+1} - u^{k+1}_i}{\varepsilon}\right) \le 2\frac{\tau}{\varepsilon^2}\max\varphi'_\varepsilon.$$

We introduce the function

$$g(z) = 2\frac{\tau}{\varepsilon^2}\varphi'_\varepsilon(z).$$

Then, the previous inequality can be re-written in the form

$$(v^{k+1} - v^k) + g\big(v^{k+1}\big) \le \max g. \tag{4.3}$$

Note that in case $i = 0$ or $i = N_\varepsilon - 1$, only one of the two terms on the right-hand side of equation (4.2) remains. Since $\max\varphi'_\varepsilon$ is positive, estimate (4.3) still holds unchanged for $i = 0$ and $i = N_\varepsilon - 1$.

Lemma 4.2 *Let $g\colon \mathbb{R} \to \mathbb{R}$ be a Lipschitz function with Lipschitz constant $L < 1$. Let $(a_k)_{k\ge0}$ be a sequence of real numbers, and let $C \in \mathbb{R}$ be such that*

$$a_{k+1} - a_k + g(a_{k+1}) \le g(C) \qquad \text{for every } k.$$

Then

$$a_0 \le C \quad \Rightarrow \quad \big(a_k \le C \quad \text{for every } k\big).$$

Proof. If we set $\tilde a_k = a_k - C$ e $\tilde g(z) = g(C+z) - g(C)$ then we can argue with $C = 0$ and $g(0) = 0$. Therefore, for every k

$$a_{k+1} - a_k \le -g(a_{k+1}) \le L|a_{k+1}|.$$

The inequality $a_k \le 0$ now yields

$$a_{k+1} \le L|a_{k+1}|,$$

hence $a_{k+1} \leq 0$ if $L < 1$. $\square$

We would like to apply the previous lemma with $C = z_0/\sqrt{\varepsilon}$, i.e. with the maximizer of g. The Lipschitz constant of g involves the second derivative $\varphi''_\varepsilon(z) = \psi''(\sqrt{\varepsilon}z)$. Now recall the boundedness of $\big(F_\varepsilon(u^0_\varepsilon)\big)_\varepsilon$ (see assumption $(B2)$), hence the uniform boundedness of $F_\varepsilon(u^k_{\varepsilon,\tau})$ with respect to ε, τ and k by Proposition 2.8. Thus, if $\zeta_0 \in (-1, 0)$ is such that $\psi(\zeta_0) > M$, then (see Lemma 2.3)

$$\frac{u^k_{j+1} - u^k_j}{\varepsilon} > \frac{\zeta_0}{\sqrt{\varepsilon}} \quad \text{for every } k \in \mathbb{N} \text{ and } j = 0, \dots, N_\varepsilon - 1.$$

Therefore, the relevant domain for the function g in (4.3) is $[\zeta_0/\sqrt{\varepsilon}, +\infty)$. Hence, we meet the requirement that the Lipschitz constant of g is less than 1 if

$$2\frac{\tau}{\varepsilon^2} \max_{[\zeta_0, +\infty)} \psi'' < 1. \tag{4.4}$$

The application of Lemma 4.2 to the sequence (v_k) now gives the following result.

Proposition 4.3 *If condition* (4.4) *holds, then*

$$I^+_\varepsilon(u^{k+1}_{\varepsilon,\tau}) \subseteq I^+_\varepsilon(u^k_{\varepsilon,\tau})$$

for every $k \geq 0$.

By the estimate of Lemma 2.5 we have $u^0_\varepsilon \in SBV(0, 1)$, and we can define m points $x^\varepsilon_1 \leq x^\varepsilon_2 \leq \dots \leq x^\varepsilon_m$ (not necessarily distinct, and with m independent of ε), such that for every $\varepsilon > 0$ we have

$$I^+_\varepsilon(u^0_\varepsilon) \subseteq \{x^\varepsilon_j : \ j = 1, \dots, m\}.$$

Therefore, up to a subsequence, we can assume that

$$\lim_{\varepsilon \to 0} x^\varepsilon_j = x_j \qquad \text{for every } j = 1, \dots, m. \tag{4.5}$$

Denote by S this set of limit points.

Since, for every $t \geq 0$, each jump point of $u(\cdot, t)$ is the limit of a sequence of jump points of the piecewise-linear functions $\hat{v}_n(\cdot, t)$ (see Theorem 3.2), if (4.4) holds then, by Proposition 4.3

$$S\big(u(\cdot, t)\big) \subseteq S \qquad \text{for every } t \geq 0.$$

Taking into account this condition and Theorem 4.1, we characterize the limit motion as the heat equation with Neumann boundary conditions on $(0, 1) \setminus S(u^0)$; that is, the same as the minimzing movement of the Mumford-Shah energy as described in [7] Section 8.3. This characterization is valid until the first collision time, for which $\#S\big(u(\cdot, t^+)\big) < \#S\big(u(\cdot, t^-)\big) = \#(S(u^0))$.

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