

Upscaling of dislocation walls in finite domains

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We wish to understand the macroscopic plastic behaviour of metals by upscaling the micro-mechanics of dislocations. We consider a highly simplified dislocation network, which allows our discrete model to be a one dimensional particle system, in which the interactions between the particles (dislocation walls) are singular and non-local. As a first step towards treating realistic geometries, we focus on finite-size effects rather than considering an infinite domain as typically discussed in the literature. We derive effective equations for the dislocation density by means of Γ -convergence on the space of probability measures. Our analysis yields a classification of macroscopic models, in which the size of the domain plays a key role.

Key words: Plasticity; Multiscale; Straight edge-dislocations; Discrete-to-continuum limit; Γ -convergence; 74Q05, 74C05, 82B21, 49J45, 82D35

1 Introduction

Dislocations in metals are curve-like defects in the atomic lattice of the metal. Typical metals have many dislocations (as much as 1000 km of dislocation curve in a cubic millimetre [25, p. 20]), and their collective motion is the microscopic mechanism behind macroscopic *permanent* or *plastic* deformation.

At scales of millimetres or more, plastic deformation is well described by continuum-level theories (see e.g. [4, Ch. 6]); at scales of 1–100 μm , however, the specimen size, material grain size, and dislocation distribution scales become comparable, and these high-level theories break down. At these smaller scales, *crystal plasticity* models attempt to capture the interaction between dislocations and grain boundaries by including additional degrees of freedom representing dislocation densities.

Although more detailed, such (meso-scale) crystal-plasticity models depend on closing the Bogoliubov–Born–Green–Kirkwood–Yvon hierarchy of multi-point correlation functions at the two-point or three-point correlation levels. Current methods commonly postulate a *closure assumption* involving certain averages, and estimate these averages from the statistics of smaller-scale models. see for instance [6, 7, 18, 27, 35, 37].

While this statistical approach makes sense from a practical point of view, the question remains whether discrete models of dislocations could not be scaled up rigorously, without *ad hoc* closure assumptions—although possibly in a simpler setup. Such a rigorous upscaling has been performed, for instance, for the case of parallel dislocations *on a single slip plane*, represented by a ‘queue’ of points on the real line [11–13, 15, 19], for arbitrary planar dislocations [2, 26], for arbitrary collections of parallel dislocations [5, 14, 29], and even for the scale of atoms to individual dislocations [1, 24].

However, these upscaling techniques fail to capture one of the more intriguing aspects of interacting dislocations: the cancellation that takes place in *pile-ups* of edge dislocations at grain boundaries. Roy *et al.* pointed out [31] that the stresses in such pile-ups are very sensitive to the local stacking of the dislocations, leading to incorrect predictions if the averaging is not done correctly. This may also be the reason why there are multiple, mutually contradicting dislocation-density models in the literature (e.g. [10, 17, 18]).

Sparked by this observation, Scardia *et al.* analyzed the structure of pile-ups in detail [16, 32], and showed that five different regimes exist, depending on a local aspect ratio (see also [20, 22, 34] for an analysis of one of these regimes using formal asymptotics). We describe the results of [16, 32] in detail below.

The authors of [16, 32] made several simplifying assumptions, one of which is to allow the dislocations to move in a half-infinite domain. Since dislocation-density models aim to describe the cases where grain size and pile-up width are comparable, a finite domain bounded by grain boundaries on both sides is more natural. In this paper, we therefore generalize the results of [16, 32] by considering any finite length for the domain in which the dislocations are situated. This brings us to our main research question:

How do finite domains change the results from [16, 32]?

After introducing our discrete model (Section 1.1), we describe the upscaling procedure in Section 1.2. Then we state Theorem 1.1 - our main result - and how to interpret it from a practical point of view.

1.1 Setting of the discrete energy

Inspired by [31], we consider the dislocations to be arranged equidistantly in $n + 1$ vertical walls of dislocations, which are assumed to be infinitely long. Figure 1 shows a schematic picture of this configuration.

In the steady state, we obtain the positions of the dislocation walls, denoted by $\tilde{x}_1 \leq \tilde{x}_2 \leq \dots \leq \tilde{x}_n$, by minimizing the energy given by

$$\begin{aligned} \mathcal{E} &= \mathcal{E}^{(i)} + \mathcal{E}^{(F)} + \mathcal{E}^{(L)}, \\ \mathcal{E}^{(i)}(\tilde{\mathbf{x}}) &= K \sum_{k=1}^n \sum_{j=0}^{n-k} V \left(\pi \frac{\tilde{x}_{j+k} - \tilde{x}_j}{h} \right), \\ \mathcal{E}^{(F)}(\tilde{\mathbf{x}}) &= \sigma \sum_{i=1}^n \tilde{x}_i, \\ \mathcal{E}^{(L)}(\tilde{\mathbf{x}}) &= \begin{cases} 0, & \text{if } \tilde{x}_n \leq L, \\ \infty, & \text{otherwise.} \end{cases} \end{aligned} \tag{1.1}$$

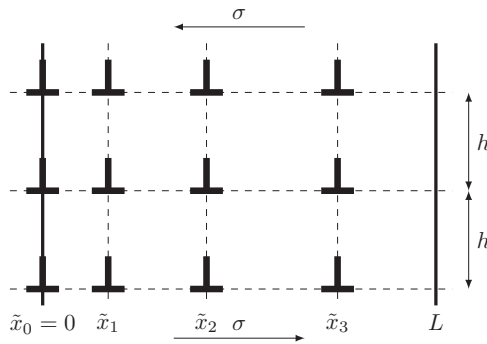


FIGURE 1. Configuration of dislocations in the discrete model.

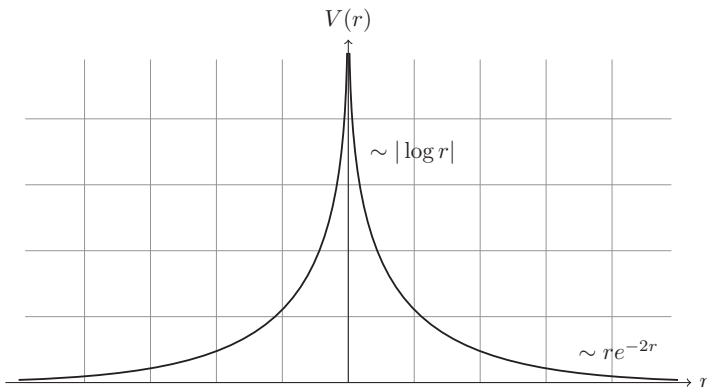


FIGURE 2. The interaction potential V .

Here, V is the interaction potential between walls, which is defined by

$$V(r) := r \coth r - \log |\sinh r| - \log 2, r \in \mathbb{R}. \tag{1.2}$$

The potential V is even, has a logarithmic singularity at the origin, and is strictly convex and monotonic on $(-\infty, 0)$ and $(0, \infty)$ (see Figure 2 for a plot). The energy \mathcal{E} involves five model parameters: n , the number of walls minus 1; h , the distance between two subsequent dislocations in a wall; σ , a constant external load applied to the system; L , the position of the right boundary; K , a material constant.

Let us explain our model in terms of the expression for $\mathcal{E}(\tilde{\mathbf{x}})$. The interaction part $\mathcal{E}^{(i)}$ is minimized by spreading the walls far apart in the interval $(0, \infty)$. The 0 is due to the pinned wall at the impenetrable barrier located at $\tilde{x}_0 = 0$. Due to the logarithmic singularity of V at 0, none of the other walls will be located at \tilde{x}_0 . The parts coming from the external load $\mathcal{E}^{(F)}$ and from the right impenetrable barrier $\mathcal{E}^{(L)}$ are minimized by putting the walls close to 0. The unique minimizer (see Proposition 3.3) of \mathcal{E} balances these effects. A thorough understanding of this balance will explain how the finiteness of the domain changes the results from [16].

1.2 Upscaling

As mentioned in the introduction, the collective behaviour of dislocation walls will be obtained by scaling up the system described above, resulting in an energy functional E which depends only on a dislocation density μ . For this we need to define what it means for μ to be “close to” a vector $\tilde{\mathbf{x}}$ of discrete wall positions. We do this by using the *narrow topology*. Setting

$$\mu_n = \frac{1}{n} \sum_{j=1}^n \delta_{\tilde{x}_j}.$$

we say that μ_n converges in the narrow topology to μ if and only if

$$\int_{[0,\infty)} \varphi d\mu_n \rightarrow \int_{[0,\infty)} \varphi d\mu \quad \text{for all } \varphi \in C_b([0, \infty)). \tag{1.3}$$

As V has a logarithmic singularity at 0, the energy landscape of \mathcal{E} contains $\mathcal{O}(n)$ singularities. Hence \mathcal{E} will never be close to any limiting energy E in any L^∞ -topology. Instead, we aim to prove that \mathcal{E} Γ -converges to E provided that an appropriate scaling is applied. With Γ -convergence, we can show that the minimizer of \mathcal{E} is close to a minimizer of E . Furthermore, Γ -convergence is robust to a perturbation by a continuous functional (which may model another type of external force term, for example).

From now on, all the parameters (L, h, K, σ) depend on n . In order to obtain a meaningful limit we rescale the positions \mathbf{x} and the energy \mathcal{E} in a specific n -dependent manner (see Section 2 for a motivation for the scaling choices made in the following).

There are two natural length scales for the rescaling of $\tilde{\mathbf{x}}$; one given by the size L_n of the domain, and the other provided by an intrinsic scale arising from the balance between the load parameter σ_n and the interaction term $\mathcal{E}^{(i)}$. Inspired by [16] we define this second length scale as

$$\ell_n = \frac{nh_n}{\pi} \hat{\alpha}_n, \tag{1.4}$$

where $\hat{\alpha}_n$ is a parameter which scales like the aspect ratio between the dislocations in Figure 1, i.e. the typical horizontal distance between walls divided by h_n . It depends on the parameters in the following way:

$$\hat{\alpha}_n := f_n \left(\sqrt{\frac{\pi K_n}{n\sigma_n h_n}} \right), \text{ with} \tag{1.5}$$

$$f_n(a) := \begin{cases} na^2, & a < \frac{1}{n}, \\ a, & \frac{1}{n} \leq a \leq 1, \\ \log a + 1, & 1 < a. \end{cases} \tag{1.6}$$

Figure 3 illustrates the typical behaviour of f_n . We define the ratio

$$\gamma_n := \frac{L_n}{\ell_n} \tag{1.7}$$

to characterize the relative size of ℓ_n and L_n .

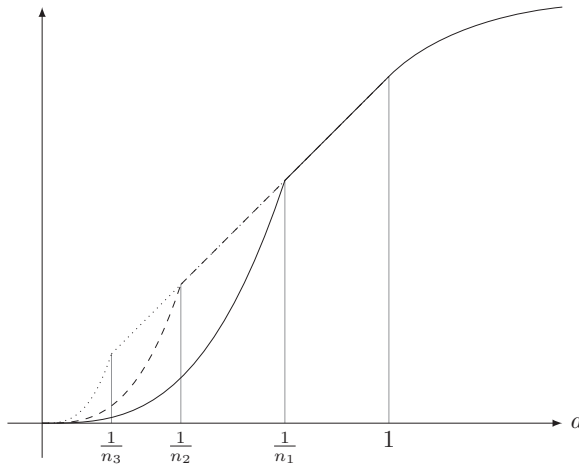


FIGURE 3. Plots of f_n (see (1.6)) for $n_1 < n_2 < n_3$.

Whenever ℓ_n is asymptotically smaller than L_n , i.e. $\gamma_n \gg 1$, it is natural to rescale the positions by ℓ_n . In this case the scaled energy is given by

$$E_n(\mathbf{x}^n) := \begin{cases} \frac{1}{n\sigma_n\ell_n} \mathcal{E}(\ell_n\mathbf{x}^n) - \frac{1}{2} \log \frac{e}{2n\hat{\alpha}_n}, & \text{if } \hat{\alpha}_n \ll 1/n, \\ \frac{1}{n\sigma_n\ell_n} \mathcal{E}(\ell_n\mathbf{x}^n), & \text{otherwise.} \end{cases} \tag{1.8}$$

The Γ -convergence result of E_n to E is stated in [[16], Theorem 1]. There are five expressions for the related limiting energy E , depending on which of five scaling regimes $\hat{\alpha}_n$ belongs to. We come back to this while discussing Table 1.

On the other hand, when $L_n \lesssim \ell_n$, i.e. $\gamma_n \lesssim 1$, the barrier at L_n is likely to determine the typical length scale for $\tilde{\mathbf{x}}$, and we scale $\tilde{\mathbf{x}}$ with L_n . The expression for the aspect ratio then also changes:

$$\alpha_n := \frac{\pi L_n}{nh_n} = \gamma_n \hat{\alpha}_n. \tag{1.9}$$

In this case (i.e. $\gamma_n \ll 1$ or $\gamma_n \sim 1$), we scale the energy as follows:

$$E_n(\mathbf{x}^n) := \begin{cases} \frac{\gamma_n}{n\sigma_n L_n} \mathcal{E}(L_n\mathbf{x}^n) - \frac{1}{2} \log \frac{e}{2n\alpha_n}, & \text{if } \alpha_n \ll 1/n, \\ \frac{\exp(2\alpha_n(1 - 1/\gamma_n))}{n\sigma_n L_n} \mathcal{E}(L_n\mathbf{x}^n), & \text{if } \alpha_n \gg 1, \\ \frac{\gamma_n^2}{n\sigma_n L_n} \mathcal{E}(L_n\mathbf{x}^n), & \text{otherwise.} \end{cases} \tag{1.10}$$

In order to state the main result we extend E_n to apply to measures by setting

$$E_n(\mu) = \begin{cases} E_n(\mathbf{x}^n), & \text{if } \mu = \frac{1}{n} \sum_{j=1}^n \delta_{x_j}, \\ \infty, & \text{otherwise.} \end{cases} \tag{1.11}$$

Table 1. Expressions for $E^{(i)}$, the interaction part of the limit energy. If $\gamma_n \gg 1$, one has to read $\hat{\alpha}_n$ instead of α_n . γ is defined as the limit of γ_n

regime	$E^{(i)}(\mu)$	p
$\alpha_n \ll \frac{1}{n}$	$\frac{1}{2} \int_0^\infty \int_0^\infty \log \frac{1}{ x-y } d\mu(y)d\mu(x)$	1
$n\alpha_n \rightarrow \tilde{c}$	$\frac{\tilde{c}}{2} \int_0^\infty \int_0^\infty V(\tilde{c}(x-y)) d\mu(y)d\mu(x)$	2
$\frac{1}{n} \ll \alpha_n \ll 1$	$\begin{cases} \left(\int_0^\infty V\right) \int_0^\infty \rho^2, & \text{if } d\mu(x) = \rho(x)dx, \\ \infty, & \text{otherwise} \end{cases}$	3
$\alpha_n \rightarrow \tilde{c}$	$\begin{cases} \tilde{c} \int_0^\infty \left(\sum_{k=1}^\infty V\left(k\frac{\tilde{c}}{\rho(x)}\right)\right) \rho(x) dx, & \text{if } d\mu(x) = \rho(x)dx, \\ \infty, & \text{otherwise} \end{cases}$	4
$1 \ll \alpha_n$	$\begin{cases} 2e^{-2} \mathbb{1}_{\{\gamma \leq 1\}}, & \text{if } \frac{d\mu}{d\mathcal{L}} = \rho \leq 1 \text{ } \mathcal{L}\text{-a.e.}, \\ \infty, & \text{otherwise} \end{cases}$	5

Table 2. Expressions for $E^{(F)}$ and $E^{(L)}$, the parts in the limit energy coming from the external force and the second barrier. The constant C is given by (1.12)

regime	$E^{(F)}(\mu)$	$E^{(L)}(\mu)$	q
$\gamma_n \gg 1$	$\int_0^\infty x d\mu(x)$	0	1
$\gamma_n \rightarrow \gamma$	$C(\gamma; (\alpha_n)) \int_0^\infty x d\mu(x)$	$\begin{cases} 0, & \text{if } \text{supp } \mu \subset [0, 1], \\ \infty, & \text{otherwise.} \end{cases}$	2
$\gamma_n \ll 1$	0	$\begin{cases} 0, & \text{if } \text{supp } \mu \subset [0, 1], \\ \infty, & \text{otherwise.} \end{cases}$	3

Theorem 1.1 (Convergence of the energy) *Let α_n and γ_n be such that they satisfy any of the criteria as in the first columns of Tables 1 and 2. Then boundedness of $E_n(\mu_n)$ (as in (1.11)) implies that (μ_n) is compact in the narrow topology. Moreover, E_n Γ -converges with respect to the narrow topology to*

$$E = E^{(i)} + E^{(F)} + E^{(L)},$$

where the components are given in Tables 1 and 2, except for the particular case in which $1 \ll \alpha_n$ and $\exp(2\alpha_n(1 - 1/\gamma_n)) \rightarrow \infty$, which is treated in Theorem 5.1.

The state of the art before this paper is given by Table 1; Table 2 shows our generalization of the results of [16] to finite domains. For a given set of parameters $(n, L_n, h_n, K_n, \sigma_n)$, we can calculate ℓ_n and consecutively γ_n and α_n , and thus we know *a priori* which of the expressions for $E^{(i)}(\mu)$, $E^{(F)}(\mu)$ and $E^{(L)}(\mu)$ we have as limit energy.

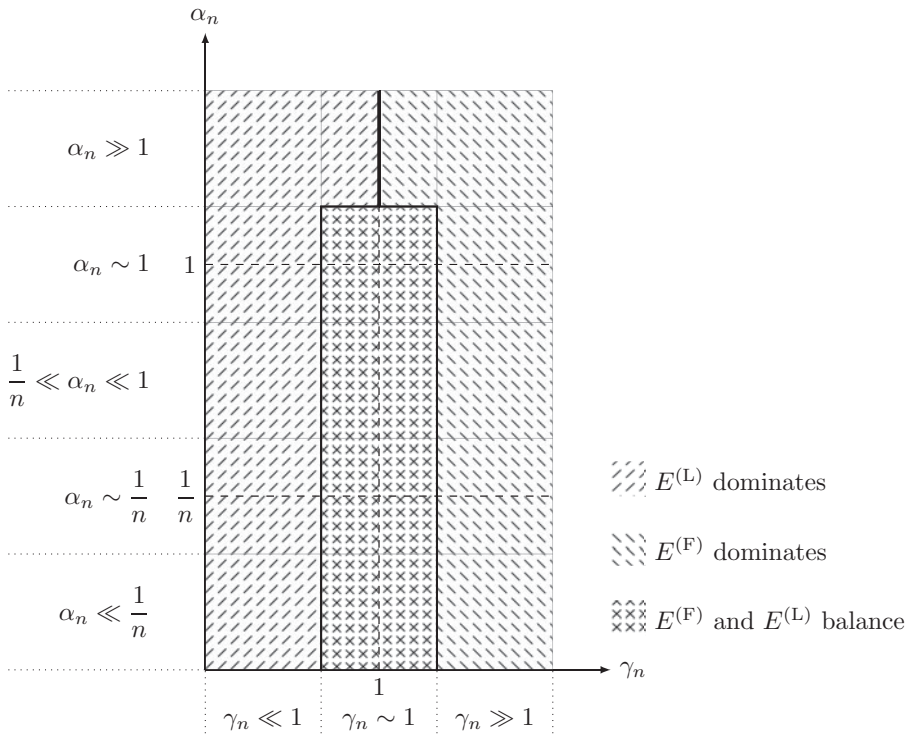


FIGURE 4. Plot of the regions in parameter space in which either $E^{(L)} \ll E^{(F)}$, $E^{(F)} \ll E^{(L)}$, or $E^{(F)} \sim E^{(L)}$. The axes show the asymptotic behaviour of γ_n and α_n . Although the parameter space is divided in a matrix of five by three blocks, their boundaries do not correspond to specific scalings of α_n or γ_n .

In all cases the limit energy gives rise to a well-posed variational problem: minimizers exist and are unique (Theorem 5.2). By the standard results on Γ -convergence, minimizers are the limit of the sequence of the finite- n minimizers (Corollary 5.3).

1.3 Discussion

We started with the question how the finiteness of the domain changes the results from [16]. We now discuss the assertions of Theorem 1.1 from this viewpoint, for which we use a schematic plot of the parameter space (Figure 4).

- First note that if $\gamma_n \gg 1$, i.e. $L_n \gg \ell_n$, then we recover the same limit energy as in [16]. This can be considered a consistency check, showing that the results of this paper generalize [16].
- Moving away from the case of [16], the case $\gamma_n \ll 1$ is the simplest: here the finiteness of the domain completely dominates the external forcing (first column in Figure 4). The scaling is independent of the external forcing, and the limit energy is governed by the balance between the interactions and the finiteness of the domain.

- The critical case $\gamma_n \rightarrow \gamma$ is more subtle (second column in Figure 4), as can be recognized e.g. in the constant that multiplies the force term of the limit energy. This constant is given by

$$C(\gamma; (\alpha_n)) := \begin{cases} \gamma, & \text{if } \alpha_n \ll 1/n, \\ \beta/2, & \text{if } \alpha_n \gg 1, \\ \gamma^2, & \text{otherwise,} \end{cases} \quad (1.12)$$

$$\text{where } \beta := \lim_{n \rightarrow \infty} \exp(2\alpha_n(1 - 1/\gamma_n)). \quad (1.13)$$

It describes the transition between $E^{(L)} \ll E^{(F)}$ (i.e. $C(\gamma; (\alpha_n)) = \infty$), to $E^{(F)} \ll E^{(L)}$ (i.e. $C(\gamma; (\alpha_n)) = 0$). When $C(\gamma; (\alpha_n)) \in (0, \infty)$, both terms of the energy contribute a finite amount. Indeed, for these values of $C(\gamma; (\alpha_n))$ we could have chosen the scaling for $\tilde{\mathbf{x}}$ to be as in (1.8) as well. The Γ -limit would contain just as much information. However, we use the other scaling (1.10) for purely practical reasons.

When $\alpha_n \gg 1$, the transition is very delicate: $C(\gamma; (\alpha_n)) \in (0, \infty)$ if $\beta \in (0, \infty)$, which can only occur if $\gamma = 1$. This is indicated in Figure 4 by the vertical line at $\gamma_n \rightarrow 1$. If $\beta = \infty$, then $E^{(F)}(\mu) = \infty$, and hence the scaling of $\tilde{\mathbf{x}}$ by L_n doesn't give a useful limit energy. That is why the case $\beta = \infty$ is excluded in Theorem 1.1. The scaling as given by (1.8) does work. This is made precise by Theorem 5.1, from which we conclude that $E^{(L)}$ is indeed negligible with respect to $E^{(F)}$ in this case.

- For $\alpha_n \gg 1$ and γ_n bounded such that $\beta \neq \infty$ (i.e. the part of parameter space given by the left half of the first row of Figure 4), the energy E is degenerate in the sense that it is only finite at exactly one point, the measure $\mu = \mathcal{L}|_{(0,1)}$. Hence it only contains information about the minimizer. One way to obtain more information in the limit energy is by using a logarithmic rescaling of E_n . In Theorem 5.4 we state our result that

$$\frac{1}{2\alpha_n} \log E_n \xrightarrow{\Gamma} \left(\mu \mapsto 1 - \left\| \frac{d\mu}{d\mathcal{L}} \right\|_{\infty}^{-1} \right).$$

- It might be instructive to note that the five expressions for $E^{(i)}(\mu)$ only depend on γ_n through the choice of rescaling with $\hat{\alpha}_n$ versus α_n . This observation implies that the presence of the second barrier does not influence the interaction behaviour of the walls. Indeed, if one (numerically) calculates the minimizers of both E_n and E , one observes that the qualitative behaviour of the dislocation walls in the bulk is not affected by the second barrier. Hence, we omit the related plots, and refer to [16] for plots of the minimizers without a second barrier. Regarding the behaviour of the dislocations near the boundaries, we observe the same effect as in [16] (i.e. a boundary layer if and only if α_n scales as in the first two rows of Table 1), but now at both barriers.

This paper is organized as follows. In Section 2 we motivate our choice of scaling for the energy. We prove Theorem 1.1 in Section 4, which requires a detailed description of our setting and its notation (Section 3.1) followed by crucial arguments that support the proof (Section 3.2 up to and including Section 3.4). This leaves us with the small range of parameters which is excluded in Theorem 1.1, with the question whether the limiting energies still have a unique minimizer (and whether the discrete minimizers converge to it),

and with the issue that the limiting energy in the dilute case (i.e. $\alpha_n \gg 1$ and $\gamma \leq 1$) solely contains information about the minimizer. These three issues are all separately solved in Section 5. In Section 6 we reflect on the introduction. In the Appendix we discuss a few technical steps in the proof of Theorem 1.1, and we briefly recall the definition of Γ -convergence together with its basic properties.

2 Scaling of the energy

In this section we give some heuristic arguments for the scaling of (1.8) and (1.10); a more detailed calculation can be found in [32, Sections 4–8].

The crucial step in rescaling the system is the choice of the spatial scale, i.e. the scale of \mathbf{x} . Of the three energy terms, the interaction energy favours spreading, while the other two favour concentration; we determine the resulting spatial scale by comparing the length scale generated by the interaction-forcing pair ($\mathcal{E}^{(i)}$ - $\mathcal{E}^{(F)}$) in (1.1) with the size L of the finite domain. Whichever is smaller determines the resulting spatial scale.

We therefore determine the size of structures that arise from the trade-off between $\mathcal{E}^{(i)}$ and $\mathcal{E}^{(F)}$. As it turns out, the scaling of this size can be found by simply requiring that both terms are of the same order, and it even is enough to test this on the special class of structures that are equispaced, i.e. $x_i^n = i\Delta x/n$, for some Δx . For these structures, one calculates

$$\mathcal{E}^{(i)} = K \sum_{k=1}^n \sum_{j=0}^{n-k} V\left(\pi \frac{k\Delta x}{h}\right) \sim \frac{nhK}{\pi\Delta x} \int_0^{\pi n\Delta x/h} V(s) ds, \quad \mathcal{E}^{(F)} \sim \sigma n^2 \Delta x, \quad (2.1)$$

where we assume $\Delta x/h \lesssim 1$ for the approximation of the sum by the integral.

We can now recognize the different regimes, by assuming some behaviour of the aspect ratio $\Delta x/h$ and deriving the corresponding parameter regime. If $n\Delta x/h \gtrsim 1$, then the integral above is of order 1, and the two terms are of the same order when

$$(\Delta x)^2 \sim \frac{\pi h K}{n\sigma}, \quad \text{or equivalently} \quad \frac{\Delta x}{h} \sim \sqrt{\frac{\pi K}{n\sigma h}}.$$

This suggests that

- $\frac{1}{n} \lesssim \frac{\Delta x}{h} \lesssim 1$ implies $\frac{\Delta x}{h} \sim \sqrt{\frac{\pi K}{n\sigma h}}$.

On the other hand, if $n\Delta x/h \ll 1$, then the integral in (2.1) is of order $(n\Delta x/h) \log(n\Delta x/h)$. It turns out that the logarithm contributes a constant to the energy (see (1.10)₁), but plays no role in the spatial scaling. We therefore find that

- $\frac{\Delta x}{h} \ll \frac{1}{n}$ implies $\frac{\Delta x}{h} \sim \frac{\pi K}{\sigma h} = n \left(\sqrt{\frac{\pi K}{n\sigma h}} \right)^2$.

Finally, when $\Delta x/h \gg 1$, the approximation by the integral in (2.1) breaks down; instead,

$$K \sum_{k=1}^n \sum_{j=0}^{n-k} V\left(\pi \frac{k\Delta x}{h}\right) \sim K n \frac{\Delta x}{h} e^{-2\Delta x/h}.$$

For large $\Delta x/h$ the exponential dominates, leading to

- $\frac{\Delta x}{h} \gg 1$ implies $\frac{\Delta x}{h} \sim \frac{1}{2} \log \frac{K}{n\sigma h} = \log \sqrt{\frac{K}{n\sigma h}}$.

which explains the logarithmic behaviour of f_n in (1.6).

To connect these guesses with the scaling of \mathbf{x} , note that in the equispaced case the total pile-up length ℓ equals $n\Delta x$, so that by (1.4) and (1.6)

$$\frac{\Delta x}{h} = \frac{\ell}{nh} \sim \hat{\alpha} = f_n \left(\sqrt{\frac{\pi K_n}{n\sigma_n h_n}} \right).$$

Up to some constants, the three regimes above can now be recognized in the definition of the function f_n in (1.6).

Having determined the typical length of a pile-up ℓ_n in the case of unconstrained positions, we compare this length with the imposed constraint L_n ; whichever is smaller determines the total length, and therefore also the aspect ratio $\Delta x/h$. This mechanism determines the changeover between $\hat{\alpha}_n$ (L larger than ℓ_n , no effective constraint) and α_n (L_n smaller than ℓ_n , the constraint determines the scale) when $\gamma_n = L_n/\ell_n$ changes from larger to smaller than 1.

3 Preliminaries

3.1 Notation

3.1.1 Basic notation

- We denote a sequence by (a_n) .
- $\chi_{\{A\}} := \begin{cases} 0, & A \text{ is true,} \\ \infty, & A \text{ is false.} \end{cases}$
- $\overline{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\}$.
- We denote the Lebesgue measure by \mathcal{L} .
- For $\zeta \in BV(\mathbb{R})$, we denote the distributional derivative by $D\zeta$. If ζ is at least weakly differentiable, we use the common notation ζ' for the real-valued derivative of ζ .
- $\mathcal{P}([0, \infty)) :=$ space of probability measures.
- Let X be a metric space and $E : X \rightarrow \overline{\mathbb{R}}$. A subset $Y \subset X$ is said to be *energy dense* if

$$\{(y, E(y)) \mid y \in Y\} \subset Y \times \overline{\mathbb{R}} \text{ is dense in } \{(x, E(x)) \mid x \in X\},$$

or equivalently,

$$\forall x \in X \exists (y_n) \subset Y : y_n \rightarrow x \text{ and } \lim_{n \rightarrow \infty} E(y_n) = E(x).$$

The set Y is said to be *lower energy dense* in X with respect to E if

$$\forall x \in X \exists (y_n) \subset Y : y_n \rightarrow x \text{ and } \limsup_{n \rightarrow \infty} E(y_n) \leq E(x).$$

Note that energy density implies lower energy density. We need to prove lower energy density of two sets a number of times, but often it is just as easy to show that they are even energy dense.

- We use the symbols \sim , \ll and \lesssim to precisely denote the different scaling regimes for γ_n and $\hat{\alpha}_n$ or α_n . They are defined as follows. Let $(a_n), (b_n) \in \mathbb{R}$, then

$$a_n \sim b_n \Leftrightarrow \frac{a_n}{b_n} \text{ converges to some } C \in (0, \infty),$$

$$a_n \ll b_n \Leftrightarrow \limsup_{n \rightarrow \infty} \frac{a_n}{b_n} = 0,$$

$$a_n \lesssim b_n \Leftrightarrow a_n \sim b_n \text{ or } a_n \ll b_n.$$

We similarly define \gg and \gtrsim . Two sequences $(a_n), (b_n) \in \mathbb{R}$ do not have to satisfy any of the above criteria. However, these sequences are not important to us, as we shall argue in Remark 3.2.

In the standard asymptotics literature, \sim typically means $a_n/b_n \rightarrow 1$. This is expressed here by writing $a_n = b_n + \mathcal{O}(c_n)$, where a sequence $c_n \ll b_n$ is specified.

3.1.2 Difference in notation compared to [16]

We use a slightly different expression for K and V to simplify formulas. To make the connection clear, we decorate the corresponding quantities in [16] by a sub- or superscript GPPS, in honour of the authors. The connection is given by $K = K_{\text{GPPS}}/\pi^2$ and

$$V(r) := \pi^2 V_{\text{GPPS}}\left(\frac{r}{\pi}\right).$$

Remark 3.1 (Properties of the interaction potential V) V as defined by (1.2) satisfies:

- (i) V is even;
- (ii) $V|_{(0, \infty)}$ is strictly convex;
- (iii) $V(r) = \log \frac{1}{r} + 1 - \log 2 + \mathcal{O}(r^2)$ for $r \ll 1$;
- (iv) $V(r) = 2re^{-2r} + \mathcal{O}(re^{-4r})$ for $r \gg 1$.

3.1.3 Scaling regimes

We use the letter $q \in \{1, 2, 3\}$ to indicate any of the three scaling regimes for γ_n in Table 2. As a result, q labels the columns in Figure 4 in decreasing order. We also use $q = 0$, which corresponds to $\gamma_n = \infty$, to indicate the setting without second barrier (as in [16]). Let us immediately use q to unify the notation for the aspect ratio: let $\alpha_n^{(q)}$ be defined by

$$\alpha_n^{(0)} := \alpha_n^{(1)} := \hat{\alpha}_n, \quad \alpha_n^{(2)} := \alpha_n^{(3)} := \alpha_n. \tag{3.1}$$

Similarly, we introduce $p \in \{1, \dots, 5\}$ to indicate any of the five scaling regimes for $\hat{\alpha}_n$ in Table 1. In decreasing order, p labels the rows in Figure 4. The following list illustrates how we exploit the indices p and q to distinguish scaling regimes:

- (p, q) : we consider any scaling for $\alpha_n^{(q)}$ and γ_n at the same time.

- $(p, 3)$: we consider $\gamma_n \ll 1$, but no restriction on the scaling of $\alpha_n^{(q)}$. We also refer to this by “case $q = 3$ ”.
- $(5, 0)$: $1 \ll \hat{\alpha}_n$ and $\gamma_n \ll 1$.
- $(2, q)$ for $q = 2, 3$: $\alpha_n^{(q)} \sim 1/n$ and $\gamma_n \lesssim 1$.
- $((2 - 4), q)$: short-hand notation for (p, q) for $p = 2, 3, 4$. It means that $1/n \lesssim \alpha_n^{(q)} \lesssim 1$ and no restrictions on the scaling of γ_n .

Not all possible sequences $\alpha_n^{(q)}$ and γ_n can be characterized by a single value for p or q . Fortunately, the following remark shows that these sequences can never yield a unique limit for the related energy functionals.

Remark 3.2 (Explanation for conditions in Theorem 1.1) *Let $\alpha_n^{(q)}$ or γ_n be such that they can not be characterized by a single value for p or q . Then there exist at least two subsequences that belong to a different class (or converge to a different constant \tilde{c} or γ). As can be seen from the expression in Tables 1 and 2, this would give different limit energies, depending along which of these subsequences we take the Γ -limit, and hence the Γ -limit does not exist for such sequences $\alpha_n^{(q)}$ or γ_n .*

3.1.4 Energies for fixed n

From this point on, we denote the energy as stated in (1.8) and (1.10) by

$$E_n^{(p,q)} = E_n^{(p,q;\text{i})} + E_n^{(p,q;\text{F})} + E_n^{(p,q;\text{L})} : \Omega_n \rightarrow \overline{\mathbb{R}},$$

where

$$\Omega_n := \{(x_1, \dots, x_n) \in [0, \infty)^n \mid x_1 \leq x_2 \leq \dots \leq x_n\}.$$

Furthermore, we define $x_0 := 0$ to indicate the pinned dislocation wall at the left barrier.

Now we can explicitly denote all the components of the energies $E_n^{(p,q)}$ in terms of the two parameters $\alpha_n^{(q)}$ and γ_n :

$$\begin{aligned} E_n^{(1,q;\text{i})}(x^n) &= \frac{1}{n^2} \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\alpha_n^{(q)}(x_{j+k}^n - x_j^n)) - \frac{1}{2} \log \frac{e}{2n\alpha_n^{(q)}}, \\ E_n^{((2-4),q;\text{i})}(x^n) &= \frac{\alpha_n^{(q)}}{n} \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\alpha_n^{(q)}(x_{j+k}^n - x_j^n)), \\ E_n^{(5,q;\text{i})}(x^n) &= \frac{\exp(2(\alpha_n^{(q)} - 1))}{n\alpha_n^{(q)}} \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\alpha_n^{(q)}(x_{j+k}^n - x_j^n)), \\ E_n^{(p,(0-1);\text{F})}(x^n) &= \frac{1}{n} \sum_{i=1}^n x_i^n, \end{aligned}$$

$$\begin{aligned}
 E_n^{(1,(2-3);F)}(x^n) &= \gamma_n \frac{1}{n} \sum_{i=1}^n x_i^n, \\
 E_n^{((2-4),(2-3);F)}(x^n) &= \gamma_n^2 \frac{1}{n} \sum_{i=1}^n x_i^n, \\
 E_n^{(5,(2-3);F)}(x^n) &= \exp\left(2\alpha_n \left(1 - \frac{1}{\gamma_n}\right)\right) \frac{1}{n} \sum_{i=1}^n x_i^n, \\
 E_n^{(p,(0-1);L)}(x^n) &= \chi_{\{x_n^n \leq \gamma_n\}}, \\
 E_n^{(p,(2-3);L)}(x^n) &= \chi_{\{x_n^n \leq 1\}}.
 \end{aligned}$$

The constant in $E_n^{(1,q;i)}(x^n)$ is introduced to balance a constant contribution to the energy for each wall-wall interaction, regardless of their intermediate distance. From the expressions above and V being strictly convex on $(0, \infty)$, it is easy to see that the following proposition holds:

Proposition 3.3 $E_n^{(p,q)} : \Omega_n \rightarrow \mathbb{R}$ is strictly convex.

3.1.5 Limit energies

We continue with the notation for the limit energies. Let

$$\begin{aligned}
 E^{(p,q)} &: \mathcal{P}([0, \infty)) \rightarrow \mathbb{R}, \\
 E^{(p,q)}(\mu) &= E^{(p,q;i)}(\mu) + E^{(p,q;F)}(\mu) + E^{(p,q;L)}(\mu),
 \end{aligned}$$

of which the expressions for the components are listed in Tables 1 and 2. To be precise, we need to define $\gamma = \infty$ in case $q = 0, 1$ and $\gamma = 0$ in case $q = 3$, in order to make sense of the expression of $E^{(5,q;i)}(\mu)$. Observe that in case $p = 5$ and $q = 2, 3$, the expression for $E^{(p,q)}(\mu)$ reduces to

$$E^{(5,(2-3))}(\mu) = 2e^{-2} \chi_{\{\mu = \mathcal{L}|_{[0,1]}\}} + \frac{\beta}{2} \mathbb{1}_{\{\gamma=1\}}. \tag{3.2}$$

In some cases, it will be useful to reformulate $E^{(p,q)}$ in terms of elements from

$$X := \{\xi : (0, 1) \rightarrow [0, \infty) \mid \xi \text{ non-decreasing}\}. \tag{3.3}$$

The elements $\xi \in X$ relate to $\mu \in \mathcal{P}([0, \infty))$ by being the inverse of the cumulative distribution of μ . To state this more precisely, we use the following notion of pseudo-invertibility. Let $f : (a, b) \rightarrow (c, d)$ non-decreasing, then we call

$$f^{-1}(y) := \sup\{x \in (a, b) \mid f(x) < y\}$$

the pseudo-inverse of f . By using the pseudo-inverse, we can denote the relation between ξ and μ by

$$\xi = (x \mapsto \mu([0, x]))^{-1}, \quad \mu = D(\xi^{-1}), \tag{3.4}$$

where D stands for the distributional derivative. Later on, in Theorem 3.11, we derive the related metric on X , which allows us to prove Γ -convergence of the energies either on $\mathcal{P}([0, \infty))$ or X .

Before writing out explicitly the components of

$$E^{(p,q)}(\xi) = E^{(p,q;i)}(\xi) + E^{(p,q;F)}(\xi) + E^{(p,q;L)}(\xi),$$

for $\xi \in X$, we note that the following equalities follow from (3.4)

$$\max \operatorname{supp} \mu = \sup \xi, \quad \|\rho\|_\infty = \frac{1}{\inf \xi'},$$

where the second equality only makes sense if $\xi \in W_{\text{incr}}^{1,1}$ and if μ is absolutely continuous with $\rho = d\mu/d\mathcal{L}$. Together with these inequalities, it is easy to see

$$\begin{aligned} E^{(3,(0-3);i)}(\xi) &:= \left(\int_0^\infty V \right) \int_0^1 \frac{1}{\xi'} \\ E^{(4,(0-3);i)}(\xi) &:= \tilde{c} \int_0^1 \left(\sum_{k=1}^\infty V(\tilde{c}k\xi') \right) \\ E^{(5,(0-3);i)}(\xi) &:= \begin{cases} 2e^{-2} \mathbb{1}_{\{\gamma \leq 1\}}, & \text{if } \xi' \geq 1 \text{ a.e.}, \\ \infty, & \text{otherwise,} \end{cases} \\ E^{((1-5),(0-1);F)}(\xi) &:= \int_0^1 \xi, \\ E^{((1-5),2;F)}(\xi) &:= C^{(p)}(\gamma) \int_0^1 \xi, \\ E^{((1-5),3;F)}(\xi) &:= 0, \\ E^{((1-5),(0-1);L)}(\xi) &:= 0, \\ E^{((1-5),(2-3);L)}(\xi) &:= \chi_{\{\sup \xi \leq 1\}}, \end{aligned}$$

where $C^{(p)}(\gamma)$ is the same constant as defined in (1.12) (we have changed the second argument to p for convenience).

In cases $p = 3, 4, 5$, it turns out to be convenient to use both descriptions of $E^{(p,q)}$. Since it will be clear from the context in this paper which of the two descriptions we use, we do not make a distinction notation-wise.

Just as in (1.11) we can regard $E_n^{(p,q)}$ as

$$\begin{aligned} E_n^{(p,q)} &: X \rightarrow \overline{\mathbb{R}}, \\ E_n^{(p,q)}(\xi) &:= \begin{cases} E_n^{(p,q)}(\xi), & \text{if } \exists x \in \Omega_n : \xi = \xi_n \text{ in the sense of Definition 3.9,} \\ \infty, & \text{otherwise.} \end{cases} \end{aligned}$$

Again, we will not make a notational distinction.

3.2 Using density to construct recovery sequences

Lemma 3.4 will serve as the backbone for the proof of Theorem 1.1.

Lemma 3.4 (*lim sup inequality for a dense subset*) Let M be a metric space, $M_1 \subset M$ dense, $F_n, F : M \rightarrow \mathbb{R}$. If

- (i) $\forall v \in M_1 \exists (u_n) \subset M : u_n \rightarrow v$ and $\limsup_{n \rightarrow \infty} F_n(u_n) \leq F(v)$, and
(ii) $\forall u \in M \exists (v_n) \subset M_1 : v_n \rightarrow u$ and $\limsup_{n \rightarrow \infty} F(v_n) \leq F(u)$,
then $\forall u \in M \exists (u_n) \subset M : u_n \rightarrow u$ and $\limsup_{n \rightarrow \infty} F_n(u_n) \leq F(u)$.

Remark 3.5 The proof of Lemma 3.4 is based on a diagonal argument. See e.g. [[9], Proposition 6.2] for the proof of a similar statement. Minor, obvious adjustments to that proof are needed to prove Lemma 3.4.

The following Lemma turns out to be very useful in our application of Lemma 3.4. It gives a sufficient condition for condition (ii), which consists of easier subproblems. In a way, it shows that one can show condition (ii) iteratively. Since the proof can be done by a straight-forward diagonal argument, we do not show it here.

Lemma 3.6 (*Alternative for Lemma 3.4, condition (ii)*) Let M be a metric space, $M_1 \subset M$ dense, $k \in \{2, 3, \dots\}$, $M_1 \subset M_2 \subset \dots \subset M_k := M$, and $F_n, F : M \rightarrow \mathbb{R}$. If

$$\forall j \in \{1, \dots, k-1\} \forall u \in M_{j+1} \exists (v_n) \subset M_j : v_n \rightarrow u \text{ and } \limsup_{n \rightarrow \infty} E(v_n) \leq E(u),$$

then condition (ii) of Lemma 3.4 is satisfied.

3.3 Link between $\mathcal{P}([0, \infty))$ and X

In (3.4) we have shown how elements from $\mathcal{P}([0, \infty))$ relate to those of X . Here, we like to give a topology on X for which Γ -convergence of $E_n^{(p,q)}$ to $E^{(p,q)}$ on X with respect to that topology is equivalent to Γ -convergence of $E_n^{(p,q)}$ to $E^{(p,q)}$ on $\mathcal{P}([0, \infty))$ with respect to narrow convergence. This statement follows easily from Theorem 3.11. Before stating it, we need two definitions:

Definition 3.7 (*Topology on X*) Let $\xi_n, \xi \in X$. We say that $\xi_n \rightarrow \xi$ in $BV_{loc}(0, 1)$ if for all $\delta \in (0, 1)$ we have that $\xi_n \rightarrow \xi$ in $L^1(0, 1 - \delta)$ and $D\xi_n \rightarrow D\xi$ in $\mathcal{P}((0, 1 - \delta))$ with respect to the narrow topology, where D is the distributional derivative.

Remark 3.8 Our motivation for using $\delta \in (0, 1)$ instead of just taking $\delta = 0$, is that $\xi(s)$ may go to ∞ if $s \uparrow 1$. This happens when the related $\mu \in \mathcal{P}([0, \infty))$ has unbounded support.

Definition 3.9 (*Embedding discrete wall density*) For a sequence of $(n+1)$ -tuples denoted by $((x_i^n)_{i=0}^n)_{n \in \mathbb{N}_+}$ that satisfies $x_0^n = 0$ and $x_{i-1}^n \leq x_i^n$ for all $n \in \mathbb{N}_+$ and for all $i \in \{1, \dots, n\}$,

we define $(\mu_n) \subset \mathcal{P}([0, \infty))$ and $(\xi_n) \subset W^{1,\infty}(0, 1)$ by

$$\mu_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i^n}, \tag{3.5a}$$

$$\xi_n(s) := x_{i-1}^n + n(x_i^n - x_{i-1}^n) \left(s - \frac{i-1}{n} \right), \quad \text{for } s \in \left(\frac{i-1}{n}, \frac{i}{n} \right). \tag{3.5b}$$

Remark 3.10 We have made the choice to exclude x_0^n from the definition of μ_n .

A useful interpretation of μ_n and ξ_n is as follows. For a Borel set A of X , the fraction of dislocation walls in A is given by $\mu_n(A)$. ξ_n uses the property that the walls are ordered by their position. $\xi_n(i/n)$ is the position of wall i . All the intermediate values of ξ_n are chosen to be convenient in the Γ -convergence proofs.

Theorem 3.11 (Link between μ and ξ [16]) Let $((x_i^n)_{i=0}^n)_{n \in \mathbb{N}_+}, (\mu_n), (\xi_n)$ as in Definition 3.9. Then the following two statements are equivalent:

- (i) $\xi_n \rightarrow \xi$ in $BV_{loc}(0, 1)$,
- (ii) $\mu_n \rightarrow \mu$.

Moreover, if any of the two statements above hold, and $\xi^{-1} \in W^{1,1}(0, \infty)$, then

$$\rho := \frac{d\mu}{d\mathcal{L}} = (\xi^{-1})'.$$

3.4 Properties of the “F” and “L” part of the energies

The energies $E_n^{(p,q;F)}$ and $E_n^{(p,q;L)}$ have special structure. The related properties are useful in reducing the complexity of the proof of Theorem 1.1. Here, we make these properties precise.

Let

$$C_n^{(p)}(\gamma_n, \alpha_n) := \begin{cases} \gamma_n, & \text{if } p = 1, \\ \gamma_n^2, & \text{if } p \in \{2, 3, 4\}, \\ \exp(2\alpha_n(1 - 1/\gamma_n)), & \text{if } p = 5. \end{cases} \tag{3.6}$$

If $q = 3$, we have $C_n^{(p)}(\gamma_n, \alpha_n) \rightarrow 0$. If $q = 2$, we obtain $C_n^{(p)}(\gamma_n, \alpha_n) \rightarrow C^{(p)}(\gamma)$. We will require $C^{(p)}(\gamma)$ to be finite. This means that for $p = 1$, we have to impose $\beta < \infty$. Note that this is exactly what we require in Theorem 1.1.

Without violating (1.11), we can regard $E_n^{(p,q;F)}, E_n^{(p,q;L)} : \mathcal{P}([0, \infty)) \rightarrow \mathbb{R}$ as

$$E_n^{(p,(0-1);F)}(\mu) := E^{(p,(0-1);F)}(\mu) = \int_0^\infty x d\mu(x), \tag{3.7a}$$

$$E_n^{(p,(2-3);F)}(\mu) := C_n^{(p)}(\gamma_n, \alpha_n) \int_0^\infty x d\mu(x), \tag{3.7b}$$

$$E_n^{(p,(2-3);L)}(\mu) := E^{(p,(2-3);L)}(\mu). \tag{3.7c}$$

The following proposition is now a straightforward consequence of the statements above:

Proposition 3.12 (Continuous convergence of the force term) For any $p \in \{1, \dots, 5\}$ and any $q \in \{0, \dots, 3\}$ (except for the case $p = 5, q = 2$ and $\beta = \infty$ (see (1.13))),

$$E_n^{(p,q;F)} \rightarrow E^{(p,q;F)}, \quad (3.8)$$

where the convergence is as in Definition B.2 (i.e. continuous convergence) on the space $\mathcal{P}([0, 1])$ with respect to the narrow topology.

Remark 3.13 Proposition 3.12 basically allows us to decouple the force term from the energy in the proof of Theorem 1.1 whenever $q = 2, 3$. This is mainly due to Theorem B.3, but we need additional arguments because the energy is defined on $\mathcal{P}([0, \infty))$ instead of $\mathcal{P}([0, 1])$.

Proposition 3.12 does not always apply due to the restriction to $\mathcal{P}([0, 1])$. In that case, we still have lower semicontinuity, which also holds for $E^{(p,(2-3);L)}$:

Proposition 3.14 $E^{(p,(0-1);F)}$ and $E^{(p,(2-3);L)}$ are lower semicontinuous on $\mathcal{P}([0, \infty))$ with respect to the narrow topology.

Proof of Proposition 3.14 Both $E^{(p,(0-1);F)}$ and $E^{(p,(2-3);L)}$ can be written as integrals over lower semicontinuous functions that are bounded from below. Lower semicontinuity of $E^{(p,(0-1);F)}$ and $E^{(p,(2-3);L)}$ follows from the Portmanteau Theorem. □

4 Proof of Theorem 1.1

Theorem 1.1 consists of two statements; a compactness property and Γ -convergence of the energies. The first can be proved in a few lines, which we do next. After that, we continue with the proof of the Γ -convergence.

By the compactness property, we mean that if for some $(\mu_n) \subset \mathcal{P}([0, \infty))$ we have that $E_n^{(p,q)}(\mu_n)$ is bounded, then (μ_n) is compact in the narrow topology. For $q = 0$ this is given by [[16], Theorem 1]. For $q = 1$, we have $E_n^{(p,1)} \geq E_n^{(p,0)}$, so the compactness property follows easily from the case $q = 0$. For $q = 2, 3$, we have $E_n^{(p,(2-3))}(\mu_n) \leq C$ implies $E_n^{(p,(2-3);L)}(\mu_n) = 0$, and hence $\text{supp } \mu_n \subset [0, 1]$. This gives tightness of (μ_n) , and by e.g. Prokhorov's Theorem the compactness property follows.

We prove Γ -convergence of the energies by establishing the two inequalities

$$\text{for all } \mu_n \rightharpoonup \mu, \quad \liminf_{n \rightarrow \infty} E_n^{(p,q)}(\mu_n) \geq E^{(p,q)}(\mu), \quad (4.1a)$$

$$\text{for all } \mu \text{ there exists } \mu_n \rightharpoonup \mu \text{ such that } \limsup_{n \rightarrow \infty} E_n^{(p,q)}(\mu_n) \leq E^{(p,q)}(\mu), \quad (4.1b)$$

for all $p = 1, \dots, 5$ and $q = 0, \dots, 3$ (except for the case $(p, q) = (5, 2)$ and $\beta = \infty$). Here μ_n and μ are probability measures on $[0, \infty)$. Note that it is sufficient to prove (4.1b) for all μ with $E^{(p,q)}(\mu) < \infty$.

In these inequalities, $E_n^{(p,q)}$ and $E^{(p,q)}$ are sums of three terms

$$E_n^{(p,q)} = E_n^{(p,q;i)} + E_n^{(p,q;F)} + E_n^{(p,q;L)}, \quad \text{and} \quad E^{(p,q)} = E^{(p,q;i)} + E^{(p,q;F)} + E^{(p,q;L)},$$

which are given in the list starting on page 760 and in Tables 1 and 2. Since similar results were proved in [16] for similar energies without the final (“L”) term, we will be using many results from [16]. The following lemma lists them. It uses the following (sub)spaces:

$$\begin{aligned} \mathcal{Y} &:= \left\{ \mu \in \mathcal{P}([0, \infty)) \mid \text{supp } \mu \text{ bounded, } \mu \ll \mathcal{L}, \text{ and } \frac{d\mu}{d\mathcal{L}} \in L^\infty(0, \infty) \right\}, \\ X &= \{ \xi : (0, 1) \rightarrow [0, \infty) \mid \xi \text{ non-decreasing} \}, \\ Y^{(4)} &:= W_{\text{incr}}^{1,1}(0, 1), \\ Y^{(3)} &:= \{ \xi \in Y^{(4)} \mid \xi' \geq \varepsilon \text{ for some } \varepsilon > 0 \}, \\ \tilde{Y}^{(5)} &:= \{ \xi \in Y^{(4)} \mid \xi \text{ piece-wise affine} \}. \end{aligned}$$

The tilde on $\tilde{Y}^{(5)}$ is due to us using another definition for $Y^{(5)}$ in the proof of Theorem 1.1.

Lemma 4.1 (Results from [16])

(i) (lim inf inequality). Let $\mu_n, \mu \in \mathcal{P}([0, \infty))$, and $\mu_n \rightarrow \mu$. For all $p \in \{1, \dots, 5\}$ and all $q \in \{0, \dots, 3\}$, we have

$$\liminf_{n \rightarrow \infty} E_n^{(p,q;i)}(\mu_n) \geq E^{(p,q;i)}(\mu). \tag{4.2}$$

In addition, for all $0 \leq I < J \leq n$,

$$\frac{1}{n} \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\alpha_n(x_{j+k} - x_j)) \geq \frac{1}{n}(J - I)V\left(n\alpha_n \frac{x_J - x_I}{J - I}\right). \tag{4.3}$$

(ii) (lim sup inequality). Let $p \in \{1, \dots, 5\}$, $\mu \in \mathcal{P}([0, \infty))$. Then there exists $\mu_n \rightarrow \mu$ such that

$$\limsup_{n \rightarrow \infty} E_n^{(p,0)}(\mu_n) \leq E^{(p,0)}(\mu). \tag{4.4}$$

(iii) (Condition (i) of Lemma 3.4). Fix $p \in \{1, \dots, 5\}$. If $p \leq 2$, let $\mu \in \mathcal{Y}$. If $p = 3, 4$, let $\xi \in Y^{(p)}$; if $p = 5$, let $\xi \in \tilde{Y}^{(5)}$. Let

$$x_i^{(p),n} := \inf \{x \in [0, \infty) \mid \mu([0, x]) \geq i/n\}, \quad \text{for } p = 1, 2, \tag{4.5}$$

$$x_i^{(p),n} := \xi\left(\frac{i}{n}\right), \quad \text{for } p = 3, 4, \tag{4.6}$$

$$x_i^{(p),n} := (1 + \varepsilon_n)\xi\left(\frac{i}{n}\right), \quad \text{for } p = 5, \tag{4.7}$$

for some sequence $\varepsilon_n \downarrow 0$. Let $(\mu_n^{(p)})$ be defined as in (3.5a). Then

$$\limsup_{n \rightarrow \infty} E_n^{(p,0)}(\mu_n^{(p)}) \leq E^{(p,0)}(\mu^{(p)}), \tag{4.8}$$

$$\limsup_{n \rightarrow \infty} E_n^{(p,0;i)}(\mu_n^{(p)}) \leq E^{(p,0;i)}(\mu^{(p)}), \tag{4.9}$$

where $\mu^{(p)} := \mu$ if $p \leq 2$, and $\mu^{(p)} := (\xi^{-1})'$ (as in (3.4)) else.

(iv) (Condition (ii) of Lemma 3.4). Fix $p \in \{1, \dots, 5\}$. If $p \leq 2$, let $M := \mathcal{P}([0, \infty))$ and $M_1 := \mathcal{Y}$, otherwise let $M := X$ and $M_1 := Y^{(p)}$. Then condition (ii) of Lemma 3.4 holds for $F := E^{(p,0)}$.

We now continue with the two inequalities (4.1).

4.1 The liminf inequality (4.1a)

In cases $q = 0, 1$ either the domain is $[0, \infty)$ ($q = 0$) or after rescaling the right-hand bound converges to $+\infty$ ($q = 1$). Therefore the domain restriction enforced by $E_n^{(p,q;L)}$ becomes unimportant in the limit $n \rightarrow \infty$, and for all p we can simply disregard it:

$$\begin{aligned} \liminf_{n \rightarrow \infty} E_n^{(p,q)}(\mu_n) &\stackrel{(4.2),(3.8)}{\geq} E^{(p,q;i)}(\mu) + E^{(p,q;F)}(\mu) + \liminf_{n \rightarrow \infty} E_n^{(p,q;L)}(\mu) \\ &\geq E^{(p,q;i)}(\mu) + E^{(p,q;F)}(\mu) = E^{(p,q)}(\mu), \end{aligned}$$

which proves (4.1a) for all p and for $q = 0, 1$.

In cases $q = 2, 3$, where the rescaled domain is $[0, 1]$, the functional $E_n^{(p,q;L)}$ becomes important. When $q = 2, 3$, $E_n^{(p,q;L)}$ is independent of n (see (3.7c)) and lower semicontinuous with respect to the narrow convergence (see Proposition 3.14). We then calculate for $p \in \{1, \dots, 4\}$ and $q = 2, 3$,

$$\begin{aligned} \liminf_{n \rightarrow \infty} E_n^{(p,q)}(\mu_n) &\stackrel{(4.2),(3.8)}{\geq} E^{(p,q;i)}(\mu) + E^{(p,q;F)}(\mu) + \liminf_{n \rightarrow \infty} E^{(p,q;L)}(\mu_n) \\ &= E^{(p,q;i)}(\mu) + E^{(p,q;F)}(\mu) + E^{(p,q;L)}(\mu) = E^{(p,q)}(\mu). \end{aligned}$$

This proves (4.1a) for these cases.

Finally, we discuss the case $q = 2, 3$ and $p = 5$. Here the boundedness of the domain and the exponential behaviour of the tails of V create a behaviour that is different from that on unbounded domains. We calculate, for any $0 \leq I < J \leq n$,

$$\begin{aligned} E_n^{(5,q;i)}(\mu_n) &= \frac{\exp(2(\alpha_n - 1))}{n\alpha_n} \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\alpha_n(x_{j+k}^n - x_j^n)) \\ &\stackrel{(4.3)}{\geq} \frac{\exp(2(\alpha_n - 1))}{\alpha_n} \frac{1}{n} (J - I) V\left(n\alpha_n \frac{x_J^n - x_I^n}{J - I}\right). \end{aligned} \tag{4.10}$$

Taking $I = 0$ and $J = n$ in this expression, we find that

$$\begin{aligned} E_n^{(5,q;i)}(\mu_n) &\geq \frac{\exp(2(\alpha_n - 1))}{\alpha_n} V(\alpha_n(x_n^n - x_0^n)) \\ &\geq \frac{\exp(2(\alpha_n - 1))}{\alpha_n} V(\alpha_n) && \text{since } x_n^n \leq 1 \\ &= 2e^{-2} + \mathcal{O}(e^{-2\alpha_n}) && \text{by Rem. 3.1(iv)}. \end{aligned} \tag{4.11}$$

Therefore

$$\liminf_{n \rightarrow \infty} E_n^{(5,q)}(\mu_n) \geq 2e^{-2} + \liminf_{n \rightarrow \infty} [E_n^{(5,q;F)}(\mu_n) + E_n^{(5,q;L)}(\mu_n)] \geq 2e^{-2}.$$

In order to show that $\liminf_{n \rightarrow \infty} E_n^{(5,q)}(\mu_n) \geq E^{(5,q)}(\mu)$, we still need to show that $\liminf_{n \rightarrow \infty} E_n^{(5,q)}(\mu_n) = \infty$ whenever $\mu \neq \mathcal{L}|_{[0,1]}$. If $\text{supp } \mu \not\subseteq [0, 1]$, we have that

$E_n^{(5,q;L)}(\mu_n) = \infty$ by (3.7c) and Proposition 3.14. If $\text{supp } \mu \subset [0, 1]$ and $\mu \neq \mathcal{L}|_{[0,1]}$, there exists an interval $(a, b) \subset \mathbb{R}$ such that $\delta := (b - a)^{-1} \mu((a, b)) > 1$. Define I_n and J_n by

$$x_{I_n}^n = \min_i \{x_i^n \mid x_i^n > a\} \quad \text{and} \quad x_{J_n}^n = \max_i \{x_i^n \mid x_i^n < b\}.$$

Using Prokhorov’s characterization of narrow convergence, we calculate

$$\limsup_{n \rightarrow \infty} \delta(x_{J_n}^n - x_{I_n}^n) \leq \delta(b - a) = \mu((a, b)) \leq \liminf_{n \rightarrow \infty} \mu_n((a, b)) = \liminf_{n \rightarrow \infty} \frac{1}{n}(J_n - I_n + 1),$$

and therefore

$$\limsup_{n \rightarrow \infty} n \frac{x_{J_n}^n - x_{I_n}^n}{J_n - I_n} \leq \frac{1}{\delta}.$$

Continuing from (4.10) we then find

$$\begin{aligned} E_n^{(5,q;i)}(\mu_n) &\geq \frac{\exp(2(\alpha_n - 1))}{\alpha_n} \frac{1}{n}(J_n - I_n)V(\alpha_n \delta^{-1}) \\ &\geq 2e^{-2}(b - a) \exp[2\alpha_n(1 - \delta^{-1})] (1 + \mathcal{O}(e^{-2\alpha_n/\delta})). \end{aligned} \tag{4.12}$$

This converges to $+\infty$ since $\delta > 1$.

4.2 The limsup inequality (4.1b)

The case $q = 0$. When $q = 0$, (4.1b) is given by Lemma 4.1.(4.1). However, for the specific case $p = 5$, we present an alternative proof here. The proof is easier and more explicit than the proof as given in [16]. Moreover, the arguments in the following proof are easier to extend to the cases in which $q \neq 0$.

We conclude (4.1b) from Lemma 3.4 after showing that its two conditions are satisfied. We use Lemma 3.4 with the subset

$$Y^{(5)} := \{\xi \in Y^{(4)} \mid \inf \xi' > 1\}.$$

Condition (i). Let $\xi \in Y^{(5)}$. We construct ξ_n by using linear interpolation (see (3.5b)) with $x_i^n := \xi(i/n)$. Observe that for any $i, j \in \{0, \dots, n\}$ with $i > j$, we have the estimate

$$(x_i^n - x_j^n) = |\xi(i/n) - \xi(j/n)| = \int_{j/n}^{i/n} \xi' \geq (\inf \xi') \frac{i - j}{n}. \tag{4.13}$$

Let $m := \inf \xi' > 1$. We calculate

$$\begin{aligned}
 & \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\alpha_n(x_{j+k}^n - x_j^n)) \\
 & \leq \sum_{k=1}^n \sum_{j=0}^{n-k} V\left(n\alpha_n m \frac{k}{n}\right) && \text{by (4.13) and } V \text{ decreasing} \\
 & = \sum_{k=1}^n (n-k+1)2mk\alpha_n e^{-2mk\alpha_n} (1 + \mathcal{O}(e^{-2mk\alpha_n})) && \text{by Rem. 3.1(iv)} \\
 & \leq 2mn\alpha_n (1 + \mathcal{O}(e^{-2m\alpha_n})) \sum_{k=1}^n k e^{-2mk\alpha_n} \\
 & = 2mn\alpha_n (1 + \mathcal{O}(e^{-2m\alpha_n})) e^{-2m\alpha_n} (1 + \mathcal{O}(e^{-2m\alpha_n})), && (4.14)
 \end{aligned}$$

from which it follows that

$$\begin{aligned}
 E_n^{(5,0;i)}(\xi_n) &= \frac{\exp(2(\alpha_n - 1))}{n\alpha_n} \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\alpha_n(x_{j+k}^n - x_j^n)) \\
 &\leq \frac{2m}{e^2} e^{-2\alpha_n(m-1)} (1 + \mathcal{O}(e^{-2m\alpha_n})) \rightarrow 0.
 \end{aligned}$$

It remains to show that the limsup also holds for the force term. As $\xi(1) < \infty$, it is possible to use Proposition 3.12 to conclude that $E_n^{(5,0;F)} \rightarrow E^{(5,0;F)}$ continuously.

Condition (ii). By Lemma 3.6 it is enough to show that the following two inclusions are energy dense:

$$Y^{(5)} \subset Y^{(4)} \subset X \quad \text{with respect to } E^{(5,0)}. \tag{4.15}$$

Energy density of the second inclusion follows from Theorem A.2. The first inequality is easy to prove: take $\xi \in Y^{(4)}$ with $E^{(5,0)}(\xi) < \infty$. This implies $\inf \xi' \geq 1$. Hence $\xi_n := (t \mapsto \xi(t) + t/n) \in Y^{(5)}$, $E^{(5,0;i)}(\xi_n) = 0 = E^{(5,0;i)}(\xi)$, and $E^{(5,0;F)}(\xi_n) \rightarrow E^{(5,0;F)}(\xi)$. This completes the proof for case $(p, q) = (5, 0)$.

Case $q = 1$. Take any μ in any of the dense subsets as listed on page 17. Then $\text{supp } \mu$ is bounded, and by construction the recovery sequence (see Lemma 4.1.iii) satisfies $\text{supp } \mu_n \leq \text{supp } \mu$. Therefore, $E_n^{(p,1)}(\mu_n) = E^{(p,0)}(\mu_n)$ for n large enough, and thus (4.1b) follows from Lemma 4.1.ii.

Cases $q = 2, 3$. Here we separate the proof for $p \leq 4$ and $p = 5$. In the latter case, we have that $E^{(5,q)}(\mu)$ can only be finite if $\mu = \mathcal{L}|_{[0,1]}$, for which the proof requires a different argument.

We start with $p \leq 4$. Note that the energies are much alike for $q = 2, 3$: we have $E_n^{(p,2)} = E_n^{(p,3)}$ and $E^{(p,2)} = E^{(p,3)} + E^{(p,2;F)}$. Hence we take $q \in \{2, 3\}$ arbitrary.

Since we can restrict ourselves to those $\mu \in \mathcal{P}([0, \infty))$ for which $E^{(p,q;L)}(\mu)$ is finite, we can assume that $\text{supp } \mu \subset [0, 1]$ and $E^{(p,q;L)}(\mu) = 0$. We prove (4.1b) by applying Lemma

3.4 to the following spaces:

$$\mathcal{X}_1 := \{\mu \in \mathcal{P}([0, \infty)) \mid \text{supp } \mu \subset [0, 1]\}, \tag{4.16a}$$

$$\mathcal{Y}_1 := \{\mu \in \mathcal{Y} \mid \text{supp } \mu \subset [0, 1]\}, \tag{4.16b}$$

$$X_1 := \{\xi \in X \mid \text{sup } \xi \leq 1\}, \tag{4.16c}$$

$$Y_1^{(p)} := \{\xi \in Y^{(p)} \mid \text{sup } \xi \leq 1\}, \quad \text{for } p = 3, 4. \tag{4.16d}$$

It remains to show that the two conditions of Lemma 3.4 are satisfied:

Condition (i). Let $p = 1, 2$ and $\mu \in \mathcal{Y}_1$. Let μ_n as in Lemma 4.1(iii). Observe that $\text{supp } \mu_n \subset [0, 1]$, so

$$\begin{aligned} & \limsup_{n \rightarrow \infty} E_n^{(p,q)}(\mu_n) \\ & \leq \limsup_{n \rightarrow \infty} E_n^{(p,q;i)}(\mu_n) + \limsup_{n \rightarrow \infty} E_n^{(p,q;F)}(\mu_n) + \limsup_{n \rightarrow \infty} E_n^{(p,q;L)}(\mu_n) \\ & \stackrel{(4.9),(3.8)}{\leq} E^{(p,q;i)}(\mu) + E^{(p,q;F)}(\mu) = E^{(p,q)}(\mu). \end{aligned}$$

For $p = 3, 4$, we can repeat the same argument for $\xi \in Y_1^{(p)}$.

Condition (ii). As $E^{(p,q;F)}$ is continuous on \mathcal{X}_1 , it is sufficient to prove condition (ii) for the interaction part. If $p = 1, 2$, this condition is given by Lemma A.4(ii). For $p = 3, 4$, we use Lemma 3.6 to argue that we can split the proof by showing separately that the following three inclusions are lower energy dense:

$$\begin{aligned} Y_1^{(3)} & \stackrel{(a)}{\subset} Y_1^{(4)} \stackrel{(b)}{\subset} X_1 \quad \text{with respect to } E^{(3,q;i)}, \\ Y_1^{(4)} & \stackrel{(c)}{\subset} X_1 \quad \text{with respect to } E^{(4,q;i)}. \end{aligned}$$

Energy density of inclusions (b) and (c) follows from Theorem A.2. For inclusion (a), let $\xi \in Y_1^{(3)}$ and $\varepsilon_n \downarrow 0$. Take $\xi_n(t) := (1 + \varepsilon_n)^{-1}(\xi(t) + \varepsilon_n t)$. Then

$$\xi_n' = \frac{\xi' + \varepsilon_n}{1 + \varepsilon_n} \geq \frac{\varepsilon_n}{1 + \varepsilon_n} > 0, \quad \text{sup } \xi_n \leq 1,$$

and hence $(\xi_n) \subset Y_1^{(3)}$. Obviously, $\xi_n \rightarrow \xi$ in $BV_{\text{loc}}(0, 1)$, and

$$\begin{aligned} \limsup_{n \rightarrow \infty} E^{(3,q;i)}(\xi_n) & = \|V\|_{L^1(0,\infty)} \limsup_{n \rightarrow \infty} \int_0^1 \frac{1}{\xi_n'} \\ & \leq \|V\|_{L^1(0,\infty)} \limsup_{n \rightarrow \infty} \int_0^1 \frac{1 + \varepsilon_n}{\xi'} = E^{(3,q;i)}(\xi). \end{aligned}$$

Let $p = 5$. As said before, we only have to regard $\mu = \mathcal{L}|_{[0,1]}$, because $E^{(5,q)}(\mu)$ is infinite for any other μ . We take the sequence μ_n related to $x_i^n = i/n$. Clearly $\mu_n \rightarrow \mathcal{L}|_{[0,1]}$. We prove (4.1b) by explicitly calculating the lim sup of all three parts of the energy.

Obviously, $E_n^{(5,q;L)}(\mu_n) = 0$, and

$$E_n^{(5,q;F)}(\mu_n) \xrightarrow{(3.8)} E^{(5,q;F)}(\mathcal{L}|_{[0,1]}) = \frac{\beta}{2},$$

where β is defined in (1.13). It is exactly here that we need the condition $\beta < \infty$ as imposed in Theorem 1.1, because we need $E^{(5,q)}(\mathcal{L}|_{[0,1]})$ to be finite to obtain a non-trivial limit energy.

For the limsup of $E_n^{(5,q;i)}(\mu_n)$, we use estimate (4.14) with $m = 1$ to obtain

$$E_n^{(5,q;i)}(\mu_n) = \frac{\exp(2(\alpha_n - 1))}{n\alpha_n} \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\alpha_n(x_{j+k}^n - x_j^n)) \leq \frac{2}{e^2} (1 + \mathcal{O}(e^{-2\alpha_n})) \rightarrow \frac{2}{e^2}.$$

By gathering the results above, we obtain

$$\begin{aligned} \limsup_{n \rightarrow \infty} E_n^{(5,q)}(\mu_n) &\leq \limsup_{n \rightarrow \infty} E_n^{(5,q;i)}(\mu_n) + \limsup_{n \rightarrow \infty} E_n^{(5,q;F)}(\mu_n) + \limsup_{n \rightarrow \infty} E_n^{(5,q;L)}(\mu_n) \\ &\leq \frac{2}{e^2} + \frac{\beta}{2} = E^{(5,q)}(\mathcal{L}|_{[0,1]}). \end{aligned}$$

5 Further results and applications

Although the proof of Theorem 1.1 is complete, we still need to treat the special case (i.e. $p = 5, q = 2$ and $\beta = \infty$ (see (1.13))) which is not covered by Theorem 1.1. Furthermore, we show that $E^{(p,q)}$ has a unique minimizer, which is, moreover, the limit of the sequence of minimizers of $E_n^{(p,q)}$.

5.1 The particular case $p = 5, q = 2$ and $\beta = \infty$

As mentioned in the introduction, the term coming from the finite domain is negligible with respect to the force term if $p = 5$ and $\beta = \infty$. By considering the scaling of \mathcal{E} as given by $E_n^{(5,2)}$, the only candidate for the Γ -limit would be ∞ (we do not prove this), which means that $E_n^{(5,2)}$ does not contain information in the limit. This is not unexpected, because this scaling of \mathcal{E} is based on balancing the interaction term with the term coming from the finite domain. Here, we consider the scaling coming from balancing the interaction term with the force term (see (1.1)). Let $\hat{E}_n := E_n^{(5,1)}$. Because we only consider the specific case $p = 5$ and $\beta = \infty$ in this section, we do not incorporate it in the notation of \hat{E}_n , nor in its Γ -limit \hat{E} , which is defined by

$$\begin{aligned} \hat{E} &: \mathcal{P}([0, \infty)) \rightarrow \mathbb{R}, \\ \hat{E}(\mu) &:= \hat{E}^{(i)}(\mu) + \hat{E}^{(F)}(\mu) + \hat{E}^{(L)}(\mu), \\ \hat{E}^{(i)}(\mu) &:= E^{(5,0;i)}(\mu), \\ \hat{E}^{(F)}(\mu) &:= E^{(5,1;F)}(\mu), \\ \hat{E}^{(L)}(\mu) &:= \begin{cases} 0, & \text{if } \text{supp } \mu \subset [0, \gamma], \\ \infty, & \text{otherwise.} \end{cases} \end{aligned} \tag{5.1}$$

We emphasize that $\hat{E}^{(i)}(\mathcal{L}|_{(0,1)}) = 0$, even when $\gamma = 1$. Just as before, we regard \hat{E} as a mapping from X to \mathbb{R} whenever that is more convenient.

Theorem 5.1 (Convergence of the energy; particular case) *Let $p = 5, q = 2$ and $\beta = \infty$, and consider $\mathcal{P}([0, \infty))$ equipped with the narrow topology. If $(\mu_n) \subset \mathcal{P}([0, \infty))$ is such that $\hat{E}_n(\mu_n)$ is bounded, then (μ_n) is compact. Moreover, \hat{E}_n Γ -converges to \hat{E} .*

Proof of Theorem 5.1 The proof is similar to the proof of Theorem 1.1. In fact, the proof for the compactness statement is the same, so we do not repeat it here. The proof for the Γ -convergence again consists of proving the following two inequalities:

$$\text{for all } \mu_n \rightharpoonup \mu, \quad \liminf_{n \rightarrow \infty} \hat{E}_n(\mu_n) \geq \hat{E}(\mu), \tag{5.2a}$$

$$\text{for all } \mu \text{ there exists } \mu_n \rightharpoonup \mu \text{ such that } \limsup_{n \rightarrow \infty} \hat{E}_n(\mu_n) \leq \hat{E}(\mu), \tag{5.2b}$$

For (5.2a), note that by (4.2) we have $\liminf_{n \rightarrow \infty} \hat{E}_n^{(i)}(\mu_n) \geq \hat{E}^{(i)}(\mu)$, and by (3.7) and Proposition 3.14, we have

$$\liminf_{n \rightarrow \infty} \hat{E}_n^{(F)}(\mu_n) \geq \hat{E}^{(F)}(\mu), \quad \liminf_{n \rightarrow \infty} \hat{E}_n^{(L)}(\mu_n) \geq \hat{E}^{(L)}(\mu).$$

Together these prove (5.2a).

We prove (5.2b) separately for $\gamma > 1$ and $\gamma = 1$. In the first case, we use Theorem 3.11 to prove (5.2b) for non-decreasing functions ξ . We can restrict ourselves to proving (5.2b) only for $\xi \in X_\gamma$; for these $\xi, \hat{E}^{(L)}(\xi) = 0$. The subscript in the notation for X refers to the upper bound for $\sup \xi$, just as it did in the spaces defined by (4.16). By Proposition 3.12, this upper bound on ξ implies that the force term is a continuous perturbation to \hat{E}_n , so by Theorem B.3 it is enough to prove

$$\begin{aligned} &\text{for all } \xi \in X_\gamma \text{ there exists } \xi_n \rightharpoonup \xi \text{ in } BV_{\text{loc}}(0, 1) \text{ such that} \\ &\limsup_{n \rightarrow \infty} \hat{E}_n^{(i)}(\xi_n) + \hat{E}_n^{(L)}(\xi_n) \leq \hat{E}^{(i)}(\xi), \end{aligned} \tag{5.3}$$

We prove (5.3) by applying Lemma 3.4 with the subset

$$Z_\gamma^{(5)} := \{\xi \in Y_\gamma^{(5)} \mid \xi(1) < \gamma\}.$$

This requires its two conditions to be satisfied:

Condition (i). Let $\xi \in Z_\gamma^{(5)}$ and take $(\xi_n) \subset X_\gamma$ as defined by (4.7). Note that $\sup \xi_n \rightarrow \sup \xi < \gamma$, which together with $\gamma_n \rightarrow \gamma$ implies that indeed $(\xi_n) \subset X_\gamma$ for all n large enough. Furthermore, we have $\sup \xi_n \leq \gamma_n$ for all n large enough, which implies $\hat{E}_n^{(L)}(\xi_n) = 0$. Hence

$$\limsup_{n \rightarrow \infty} \hat{E}_n^{(i)}(\xi_n) + \hat{E}_n^{(L)}(\xi_n) = \limsup_{n \rightarrow \infty} E_n^{(5,0;i)}(\xi_n) \stackrel{(4.9)}{\leq} E^{(5,0;i)}(\xi).$$

Condition (ii). By Lemma 3.6 it is enough to show that the following three inclusions are energy dense:

$$Z_\gamma^{(5)} \subset Y_\gamma^{(4)} \subset X_\gamma \quad \text{with respect to } \hat{E}^{(i)}. \tag{5.4}$$

Energy density of the second inclusion follows from Theorem A.2. To show the first inclusion, we take $\xi \in Y_\gamma^{(4)}$. This implies that $\xi \in W_{\text{incr}}^{1,1}$, $\xi(1) \leq \gamma$ and $\inf \xi' \geq 1$. It is enough to construct $\xi_n \rightharpoonup \xi$ in BV_{loc} such that $\xi_n \in W_{\text{incr}}^{1,1}$, $\xi_n(1) < \gamma$ and $\inf \xi_n' > 1$,

because then $(\zeta_n) \subset Z_\gamma^{(5)}$ and $\hat{E}_n^{(i)}(\zeta_n) + \hat{E}_n^{(L)}(\zeta_n) = 0$. It is easy to see that $\check{\zeta}_n$ as defined by

$$\check{\zeta}_n(t) := \frac{1 - \varepsilon_n}{1 + \varepsilon_n}(\zeta(t) + \varepsilon_n \gamma t) + \varepsilon_n t$$

for some $\varepsilon_n \downarrow 0$, satisfies all these requirements. Note that the strict inequalities in the requirements for $\check{\zeta}_n$ are obtained solely by using $\gamma > 1$. This completes the proof for (5.2b) under the assumption that $\gamma > 1$.

We now turn to the case $\gamma = 1$. As the following proof is similar to the proof of Theorem 1.1 in case $p = 5$ and $q = 2, 3$ (see page 20), we do this in terms of measures instead of using non-decreasing functions. Again, we have that $\hat{E}(\mu)$ can only be finite when $\mu = \mathcal{L}|_{(0,1)}$, but now we take μ_n as defined by $x_i^n := \gamma_n i/n$. This is to ensure that $\hat{E}_n^{(L)}(\mu_n) = 0$. Clearly $\hat{E}_n^{(F)}(\mu_n) \rightarrow 1/2 = \hat{E}^{(F)}(\mathcal{L}|_{(0,1)})$, so it is only left to prove that $\hat{E}_n^{(i)}(\mu_n) \rightarrow 0$. Due to $x_i^n = \gamma_n i/n$, we get

$$\sum_{k=1}^n \sum_{j=0}^{n-k} V(n\hat{\alpha}_n(x_{j+k}^n - x_j^n)) \stackrel{(4.14)}{\leq} 2n\hat{\alpha}_n\gamma_n e^{-2\gamma_n\hat{\alpha}_n} + \mathcal{O}(e^{-4\gamma_n\hat{\alpha}_n}),$$

and hence

$$\begin{aligned} \hat{E}_n^{(i)}(\mu_n) &= \frac{\exp(2(\hat{\alpha}_n - 1))}{n\hat{\alpha}_n} \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\hat{\alpha}_n(x_{j+k}^n - x_j^n)) \\ &\leq \frac{2}{e^2}\gamma_n(e^{2\hat{\alpha}_n(1-\gamma_n)} + \mathcal{O}(e^{-2\hat{\alpha}_n})) \\ &\stackrel{(1.9)}{\leq} \frac{2}{e^2}\gamma_n(e^{2\alpha_n(1/\gamma_n-1)} + \mathcal{O}(e^{-2\hat{\alpha}_n})) \rightarrow 0, \end{aligned}$$

in which the convergence to 0 follows from $\beta = \infty$. □

5.2 Existence, uniqueness and convergence of minimizers

The following Theorem is an extension of [[16], Thm. 2]. It is easy to extend its proof due to $E^{(p,q;L)}$ having narrowly compact level sets and being l.s.c. and convex.

Theorem 5.2 (Existence and uniqueness of minimizers) *Let $p \in \{1, \dots, 5\}, q \in \{0, \dots, 3\}$. The minimization problem*

$$\min_{\mu \in \mathcal{D}([0, \infty))} E^{(p,q)}(\mu)$$

has a unique minimizer. The energy \hat{E} (as defined in (5.1)) has a unique minimizer as well.

Corollary 5.3 (Convergence of minimizers) *For each $n \in \mathbb{N}_+$, let μ_n^* and μ^* be the minimizers of respectively $E_n^{(p,q)}$ and $E^{(p,q)}$ (or \hat{E}_n and \hat{E} whenever $p = 5$ and $\beta = \infty$). Then $\mu_n^* \rightharpoonup \mu^*$.*

Proof of Corollary 5.3 The proof is the same for $p = 5$ and $\beta = \infty$ as for the other cases. Hence we restrict ourselves to the other cases, and so we use the energies $E_n^{(p,q)}$ and $E^{(p,q)}$.

By Theorem 1.1, the sequence (μ_n^*) is narrowly compact, and converges along a subsequence to a limit μ . By standard properties of Γ -convergence, μ is a minimizer of $E^{(p,q)}$. Since minimizers of $E^{(p,q)}$ are unique by Theorem 5.2, the whole sequence converges. \square

5.3 Rescaling $E_n^{(5,(2-3))}$

As mentioned in Section 1.3, the Γ -limit of $E_n^{(5,(2-3))}$ is unsatisfactory, because it only contains information about the unique minimizer. One way to keep more information in the limit, is to consider a logarithmic scaling. More precisely, we define

$$\mathfrak{E}_n(\mu_n) := \frac{1}{2\alpha_n} \log E_n^{(5,(2-3))}(\mu_n)$$

and show that it Γ -converges to \mathfrak{E} , which is given by

$$\mathfrak{E}(\mu) = \begin{cases} 1 - \frac{1}{M}, & \text{if } \text{supp } \mu \subset [0, 1], \\ \infty, & \text{otherwise,} \end{cases}$$

where

$$M := \sup_{a < b} \frac{\mu((a, b))}{b - a}.$$

We can also express \mathfrak{E} in terms of non-decreasing functions as

$$\mathfrak{E}(\xi) = \begin{cases} 1 - m_\xi, & \text{if } \text{sup } \xi \leq 1, \\ \infty, & \text{otherwise,} \end{cases}$$

where

$$m_\xi := \inf_{a < b} \frac{D\xi((a, b))}{b - a},$$

and $D\xi$ is the distributional derivative of ξ .

Before proving Γ -convergence, we argue why this rescaling of the energy is useful. First, it implicitly shows that any rescaling of $E_n^{(5,(2-3))}$ by a constant gives the same degenerate Γ -limit as in Theorem 1.1. Second, it shows exactly how this problem can be solved by a specific non-linear scaling, in our case a logarithmic one. As a result, we can compare different dislocation wall densities μ by computing $\mathfrak{E}(\mu)$, which gives a finite value for a large class of densities (as opposed to $E^{(5,(2-3))}$). Third, it provides a setting in which upscaling of dislocation wall dynamics may be possible. As pointed out at the end of the introduction, these dynamics are usually modelled by a linear drag law, i.e.

$$\frac{d\mathbf{x}^n}{dt} = -\nabla E_n^{(5,(2-3))}(\mathbf{x}^n), \tag{5.5}$$

where we have used the characterization of μ_n in terms of $\mathbf{x}^n \in \mathbb{R}^n$ as in (1.11). Upscaling this gradient flow is not expected to lead to a sensible limit evolution equation due to

$E^{(5,(2-3))}$ being degenerate. However, one sees from

$$-\nabla \mathfrak{E}_n(\mathbf{x}^n) = -\frac{\nabla E_n^{(5,(2-3))}(\mathbf{x}^n)}{2\alpha_n E_n^{(5,(2-3))}(\mathbf{x}^n)} = \frac{1}{2\alpha_n E_n^{(5,(2-3))}(\mathbf{x}^n)} \frac{d\mathbf{x}^n}{dt},$$

how to rescale time in order to make the discrete gradient flow with respect to \mathfrak{E}_n consistent with (5.5). Moreover, its limit is expected to be a gradient flow with respect to \mathfrak{E} , which would be a non-trivial evolution equation. This is a very tentative discussion, and it is beyond the scope of this paper to prove convergence of gradient flows. Nonetheless, the first step would be to show Γ -convergence, which is exactly the topic of this section.

Theorem 5.4 (*Γ -Convergence of the logarithm of the energy*) *Let $p = 5$, $q \in \{2, 3\}$ and $\gamma < 1$, and consider $\mathcal{P}([0, \infty))$ equipped with the narrow topology. If $(\mu_n) \subset \mathcal{P}([0, \infty))$ is such that $\mathfrak{E}_n(\mu_n)$ is bounded, then (μ_n) is precompact. Moreover, \mathfrak{E}_n Γ -converges to \mathfrak{E} .*

Proof of Theorem 5.4

The structure of the proof is similar to the Γ -convergence proof of $E_n^{(5,(2-3))}$. Compactness follows from the same argument as used for showing compactness for $E_n^{(5,(2-3))}$, because we still require for any fixed n that $E_n^{(5,(2-3);L)}(\mu_n) < \infty$ in order for $\mathfrak{E}_n(\mu_n)$ to be finite.

To show the liminf inequality, we separate three cases: $\mu = \mathcal{L}|_{(0,1)}$, $\text{supp } \mu \not\subset [0, 1]$, and all other $\mu \in \mathcal{P}([0, \infty))$.

If $\mu = \mathcal{L}|_{(0,1)}$, we see from (4.11) for any $\mu_n \rightarrow \mu$ that

$$\liminf_{n \rightarrow \infty} \mathfrak{E}_n(\mu_n) \geq \liminf_{n \rightarrow \infty} \frac{1}{2\alpha_n} \log(2e^{-2} + \mathcal{O}(e^{-2\alpha_n})) = 0.$$

If $\text{supp } \mu \not\subset [0, 1]$, it follows from lower semi-continuity (see (3.7c) and Proposition 3.14) that $E_n^{(5,(2-3);L)}(\mu_n) = \infty$ for n large enough for any $\mu_n \rightarrow \mu$, so that $\mathfrak{E}_n(\mu_n) = \infty$ as well.

If $\text{supp } \mu \subset [0, 1]$ and $\mu \neq \mathcal{L}|_{(0,1)}$, we have that $1 < M$. As we like to have explicit values for a, b in the calculation below (rather than the supremum over them as in the definition of M), we fix $0 < \varepsilon < M - 1$, and take $a_\varepsilon < b_\varepsilon$ such that $(b_\varepsilon - a_\varepsilon)^{-1} \mu((a_\varepsilon, b_\varepsilon)) > M - \varepsilon =: M_\varepsilon$. We follow the same reasoning as for (4.12) to find

$$\begin{aligned} \liminf_{n \rightarrow \infty} \mathfrak{E}_n(\mu_n) &\geq \liminf_{n \rightarrow \infty} \frac{1}{2\alpha_n} \log\left(2e^{-2}(b_\varepsilon - a_\varepsilon) \exp(2\alpha_n(1 - M_\varepsilon^{-1})) (1 + \mathcal{O}(e^{-2\alpha_n/M_\varepsilon}))\right) \\ &= \liminf_{n \rightarrow \infty} (1 - (M - \varepsilon)^{-1} + \mathcal{O}(\alpha_n^{-1})) = 1 - (M - \varepsilon)^{-1}. \end{aligned}$$

Since ε was chosen arbitrarily, we obtain

$$\liminf_{n \rightarrow \infty} \mathfrak{E}_n(\mu_n) \geq 1 - \frac{1}{M}.$$

We continue with the proof of the limsup inequality. We can restrict to $\xi \in X_1$, because otherwise \mathfrak{E} is infinite. We conclude the limsup inequality from Lemma 3.4 after showing that its two conditions are satisfied. We use Lemma 3.4 with the subset $X_1^{(5)} := \{\xi \in X_1 \mid m_\xi > 0\}$.

Condition (i). Let $\xi \in X_1^{(5)}$. We construct ξ_n by using linear interpolation (see (3.5b)) with $x_i^n := \sup_{t < i/n} \xi(t)$ (because ξ need not be in $W^{1,1}$, ξ can not be evaluated at specific values). From Proposition 3.12 we conclude that for n large enough

$$E_n^{(5,(2-3);F)}(\xi_n) < E^{(5,(2-3);F)}(\xi) + 1 \leq \frac{\beta}{2} + 1.$$

Observe that for any $i, j \in \{0, \dots, n\}$ with $i > j$, we have the estimate

$$(x_i^n - x_j^n) = D\xi([j/n, i/n]) \geq m_\xi \frac{i - j}{n}.$$

This is a similar estimate to (4.13). This allows us to use (4.14) to derive the following upper bound

$$\begin{aligned} E_n^{(5,(2-3);i)}(\xi_n) &= \frac{\exp(2(\alpha_n - 1))}{n\alpha_n} \sum_{k=1}^n \sum_{j=0}^{n-k} V(n\alpha_n(x_{j+k}^n - x_j^n)) \\ &\leq \frac{2m_\xi}{e^2} e^{2\alpha_n(1-m_\xi)} (1 + \mathcal{O}(e^{-2m_\xi\alpha_n})) \rightarrow 0. \end{aligned}$$

By combining the estimates on $E_n^{(5,(2-3);i)}(\xi_n)$ and $E_n^{(5,(2-3);F)}(\xi_n)$ we obtain

$$\begin{aligned} \limsup_{n \rightarrow \infty} \mathfrak{E}_n(\xi_n) &= \limsup_{n \rightarrow \infty} \frac{1}{2\alpha_n} \log (E_n^{(5,(2-3);i)}(\xi_n) + E_n^{(5,(2-3);F)}(\xi_n)) \\ &\leq \limsup_{n \rightarrow \infty} \frac{1}{2\alpha_n} \log \left(\frac{2m_\xi}{e^2} e^{2\alpha_n(1-m_\xi)} (1 + \mathcal{O}(e^{-2m_\xi\alpha_n})) + \frac{\beta}{2} + 1 \right) \\ &= 1 - m_\xi = \mathfrak{E}(\xi). \end{aligned}$$

Condition (ii). Let $\xi \in X_1$, and define

$$\xi_n(t) := \frac{\xi(t) + t\varepsilon_n}{1 + \varepsilon_n}$$

for some $\varepsilon_n \downarrow 0$. By construction, $\xi_n \in X_1^{(5)}$, which follows from

$$\begin{aligned} \sup \xi_n &= \frac{\sup \xi + \varepsilon_n}{1 + \varepsilon_n} \leq 1, \quad \text{and} \\ m_{\xi_n} &= \inf_{b > a} \frac{D\xi((a, b)) + \varepsilon_n \mathcal{L}((a, b))}{b - a} = m_\xi + \varepsilon_n > 0. \end{aligned}$$

Clearly $\xi_n \rightarrow \xi$ in $BV_{\text{loc}}(0, 1)$, and

$$\mathfrak{E}(\xi_n) = 1 - m_{\xi_n} = 1 - (m_\xi + \varepsilon_n) \rightarrow \mathfrak{E}(\xi).$$

□

6 Conclusion

The finiteness of the domain induces a second length scale—the length of the domain L_n —in addition to the length scale ℓ_n generated by the external forcing. We specified three qualitatively different limiting behaviours for the energy, which correspond to the cases L_n being asymptotically bigger, smaller, or equal to ℓ_n . This result enables us to test the mutually contradicting dislocation-density models (as mentioned in the introduction) with more freedom in the discrete setting. As a special case, we are able to test these models when no loading is applied (i.e. $\sigma_n = 0$).

On the other hand, for the parameter regime in which the forcing term is negligible with respect to the effect of the finite domain, it seems unphysical to ignore the effect of negative edge dislocations. One of the reasons that we do not consider a model with negative edge dislocations, is that the effect of nucleation and annihilation of dislocations with opposite sign results in an energy that is not bounded from below. Various methods have been used to circumvent this issue [3,8], but they each have their drawbacks. We plan to explore the extension of the present results to the case of multiple signs in the future.

A significant step towards applicability would be to replace the assumption of equispaced slip planes by a stochastic spacing, as also suggested by other authors [21,36]). If one maintains the wall assumption, then stochastic spacing leads to a different interaction potential V , for which no explicit expressions exist, and for which the large-distance behaviour is not yet completely understood [21]. However, in the case of stochastically spaced slip planes, dislocations do not form exact walls [30] so that one requires a fully two-dimensional description. A rigorous upscaling in the two-dimensional framework would be the ultimate goal, but that is still far away.

Besides extending the discrete model to have more freedom in space, one can also consider dislocation dynamics, which is paramount for understanding plasticity. In the case of a linear drag law [23, Ch. 7], these dynamics are described by a gradient flow of the energy. Upscaling the dynamics of the discrete dislocation walls to dislocation densities requires more than just Γ -convergence of the energies (see e.g. [33]); one also needs lower bounds on the slopes. We plan to return to this question in a future publication.

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Appendix A Technical steps

Lemma A.1 (*A support property of narrow convergence*) *Let $\mu_n, \mu \in \mathcal{P}([0, \infty))$ and $a_n, a \in \mathbb{R}$ such that $\mu_n \rightarrow \mu$ and $a_n \rightarrow a$. If $\text{supp } \mu \not\subseteq [0, a]$, then $\text{supp } \mu_n \not\subseteq [0, a_n]$ for all n large enough.*

Proof of Lemma A.1 The proof goes by contradiction. Suppose there exists a subsequence (μ_n) such that $\text{supp } \mu_n \subset [0, a_n]$. $\text{supp } \mu \not\subset [0, a]$ and inner regularity imply that there is a closed interval K in (a, ∞) such that $\mu(K) > 0$. It is straightforward to choose a test function $\varphi \in C_b([0, \infty))$ such that

$$\int_0^\infty \varphi \, d\mu_n = 0$$

for n large enough, and

$$\int_0^\infty \varphi \, d\mu > 0,$$

which contradicts $\mu_n \rightarrow \mu$. □

The following theorem is a generalization of [[16], Theorem 4], in the sense that it applies to the sets X_γ and $Y_\gamma^{(4)}$ (see (4.16)) not only for $\gamma = \infty$, but also for any $\gamma \in (0, \infty)$. The proof in [16] holds for finite γ as well.

Theorem A.2 (A sufficient condition for energy density) *Let $f : (0, \infty) \rightarrow \bar{\mathbb{R}}$ be convex and decreasing, such that $\lim_{t \rightarrow \infty} f(t) = 0$. Let $E : X_\gamma \rightarrow \bar{\mathbb{R}}$,*

$$E(u) := \int_0^1 f(u'(t)) \, dt.$$

Then $Y_\gamma^{(4)}$ is energy dense in X_γ with respect to E .

Remark A.3 *Just as in [16], we use Theorem A.2 for $E^{(p,q)}$ for $p = 3, 4, 5$ and $q = 0, \dots, 3$. In these cases, we take for $f(t)$ respectively*

$$\frac{1}{t}, \quad \sum_{k=1}^\infty V(kt), \quad \chi_{\{t \geq 1\}}.$$

Lemma A.4 (Energy density results) *Let $p \in \{1, 2\}$, and \mathcal{X}_1 and \mathcal{Y}_1 as defined by (4.16). Then*

- (i) \mathcal{Y} is energy dense in $\mathcal{P}([0, \infty))$ with respect to $E^{(p,q)}$ for $q = 0, 1$.
- (ii) \mathcal{Y}_1 is energy dense in \mathcal{X}_1 with respect to $E^{(p,q)}$ for $q = 2, 3$.

Proof of Lemma A.4 Lemma A.4.(i) is proved by using Lemma 3.6. It involves the intermediate space

$$\tilde{\mathcal{Y}} := \left\{ \mu \in \mathcal{P}([0, \infty)) \mid \mu \ll \mathcal{L}, \frac{d\mu}{d\mathcal{L}} \in L^\infty(0, \infty) \right\}.$$

The proof of $\tilde{\mathcal{Y}}$ being energy dense in $\mathcal{P}([0, \infty))$ is stated in [[16], proof of limsup inequality Theorem 5]. The related sequence of the limsup inequality is given by the measures corresponding to the densities given by

$$\rho_n(x) := n\mu([x, x + 1/n)). \tag{A 1}$$

It is still to be shown that for all $\mu \in \tilde{\mathcal{Y}}$ there exists $(\mu_n) \subset \mathcal{Y}$ such that $\mu_n \rightarrow \mu$ and $\limsup_{n \rightarrow \infty} E^{(p,0)}(\mu_n) \leq E^{(p,0)}(\mu)$. Let $\rho := \frac{d\mu}{d\mathcal{L}}$, and take $\rho_n = \frac{1}{\mu([0,n])} \rho \mathbb{1}_{[0,n]}$. For the related μ_n , it is easy to see that $\mu_n \rightarrow \mu$ and that $E^{(p,0;F)}(\mu_n) \leq E^{(p,0;F)}(\mu)$. By using the Dominated Convergence Theorem, one can prove $E^{(p,0;i)}(\mu_n) \rightarrow E^{(p,0;i)}(\mu)$.

The proof above works just as well for proving Lemma A.4.(ii), because we can identify $E^{(p,(2-3);i)}|_{\mathcal{X}_1}$ by $E^{(p,0;i)}|_{\mathcal{X}_1}$, since $\hat{\alpha}_n$ and α_n play the same role. \square

Appendix B Γ -convergence

Here, we state the basic properties of Γ -convergence, which can be found, for example, in [28]. Throughout this section, (X, d) denotes a metric space and $E_n, E : X \rightarrow \overline{\mathbb{R}}$.

Definition B.1 (Γ -convergence) *The sequence E_n Γ -converges to E with respect to d iff the following two conditions are satisfied:*

- (i) $\forall x \in X \forall x_n \xrightarrow{d} x : \liminf_{n \rightarrow \infty} E_n(x_n) \geq E(x)$,
- (ii) $\forall x \in X \exists y_n \xrightarrow{d} x : \limsup_{n \rightarrow \infty} E_n(y_n) \leq E(x)$.

The sequence (y_n) , if it exists, is called the *recovery sequence*. Γ -convergence between functionals is often denoted by $\xrightarrow{\Gamma}$.

The next Theorem [[28], Proposition 6.20] states one of the most important properties of Γ -convergence. We need the following definition first:

Definition B.2 (*Continuous convergence*) *Let $F_n, F : X \rightarrow \mathbb{R}$. Then $F_n \rightarrow F$ continuously iff*

$$\forall x \in X : \lim_{\varepsilon \rightarrow 0} \limsup_{n \rightarrow \infty} \sup_{y \in B(x, \varepsilon)} |F_n(y) - F(x)| = 0.$$

Theorem B.3 (*Stability of Γ -convergence under continuously converging perturbations*)

Let $F_n, F : X \rightarrow \mathbb{R}$. If $E_n \xrightarrow{\Gamma} E$ and $F_n \rightarrow F$ continuously, then

$$E_n + F_n \xrightarrow{\Gamma} E + F.$$

Remark B.4 *Note that $R(F) \subset \mathbb{R} \subseteq \overline{\mathbb{R}}$ is required in Definition B.2.*

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