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by

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BOUNDARY-LAYER ANALYSIS OF A PILE-UP OF WALLS OF EDGE DISLOCATIONS AT A LOCK

ADRIANA GARRONI, PATRICK VAN MEURS, MARK PELETIER, AND LUCIA SCARDIA

Abstract. In this paper we analyse the behaviour of a pile-up of vertically periodic walls of edge dislocations at an obstacle, represented by a locked dislocation wall. Starting from a continuum non-local energy $E_c$ modelling the interactions—at a typical length scale of $1/c$—of the walls subjected to a constant shear stress, we derive a first-order approximation of the energy by $\Gamma$-convergence in the limit $c \to \infty$. While the first term in the expansion, the $\Gamma$-limit of $E_c$, captures the ‘bulk’ profile of the density of dislocation walls in the pile-up domain, the next-order term in the expansion is a ‘boundary-layer’ energy that captures the profile of the density in the proximity of the lock.

This study is a first step towards a rigorous understanding of the behaviour of dislocations at obstacles, defects, and grain boundaries.

1. Introduction and motivation

Dislocations are defects in the arrangement of the atoms in a metal lattice, and their distribution and motion greatly affect the macroscopic behaviour of the material. Dislocations not only interact with other dislocations, but also with impurities, other defects, and interfaces. Understanding the behaviour of dislocations at grain boundaries and phase boundaries, in particular, has been the object of intensive research in academia and industry, but is still far from being achieved.

The analysis of idealised pile-ups of two-dimensional point dislocations, representing the intersections of a system of straight and parallel dislocations with a cross-sectional plane, is a first attempt to shed a light on this complex subject. The simplest case is that of a one-dimensional array of points, corresponding to dislocations in a single glide plane, forced against an obstacle by an external load. For this setup Eshelby, Frank and Nabarro [EFN51] pioneered a method for finding the equilibrium density of the dislocations, based on a polynomial representation, which is enabled by the specific structure of the interaction potential. This method has since been extended in various ways [VCMO09, VCOA07, VCO07]. Other approaches to the upscaling of dislocations are obtained via $\Gamma$-convergence for phase-field energies [GM05, FG07, CGM11], for core-radius regularized models [GLP10, ADLGP14], and via homogenization for evolution equations [EHIM09, FIM12, MP12].

In this paper we study a model that lies half-way between one and two dimensions. At the microscopic level, the system contains a large number of periodic walls of edge dislocations with the same Burgers vector (see Figure 1 and [RPGK08, GPPS13, SPPG14, vMMP14, Hal11]). The coordinate system is chosen so that the $n+1$ walls are vertical, and represented by their horizontal positions $x^n = (x^n_i)_{i=0}^n \in [0, \infty)^{n+1}$, with $x^n_0 = 0$. The energy of this system is given by

$$E_n(x^n) := \frac{c_n}{n^2} \sum_{k=1}^{n} \sum_{j=0}^{n-k} V(c_n(x^n_{j+k} - x^n_j)) + \frac{1}{n} \sum_{i=1}^{n} x^n_i,$$  \hspace{1cm} (1.1)

where $c_n > 0$ is a single dimensionless parameter, and the interaction energy potential $V$ (see Figure 1(b)) is

$$V(s) := s \coth s - \log(2 \sinh s) = \frac{2|s|}{(e^{2|s|} - 1)} - \log(1 - e^{-2|s|}).$$  \hspace{1cm} (1.2)

The potential $V$ arises from summing up the interaction potentials generated by all the individual dislocations in a wall [HL82, (19–75)].
The second term in (1.1) is a confinement potential, and corresponds to a constant shear stress acting on the system, forcing the walls against the obstacle at \( x = 0 \), represented as a fixed dislocation wall. The first term models the purely repulsive interaction between pairs of walls.

Note that the energy \( E_n \) is non-dimensional; its dimensional equivalent has a number of parameters, which can be reduced by scaling to the two parameters \( n \) and \( c_n \).

In [GPPS13] upscaled continuum models were derived from \( E_n \), by \( \Gamma \)-convergence, in the “many-walls” limit \( n \to \infty \), for different asymptotic behaviours of the parameter \( c_n \).\(^1\) In particular, for the scaling regime \( 1 \ll c_n \ll n \) (corresponding to an arrangement where dislocations are closer horizontally than vertically, and the length of the pile-up region is larger than the in-wall spacing), the \( \Gamma \)-limit of \( E_n \) was proved to be the continuum energy \( E \) given by

\[
E(\mu) = \frac{1}{2} \left( \int_{\mathbb{R}} V \right) \int_{-\infty}^{\infty} \rho(x)^2 \, dx + \int_{0}^{\infty} \rho(x) \, dx, \quad \text{if} \quad \mu(dx) = \rho(x) \, dx, \quad \text{supp} \rho \subset [0, \infty), \tag{1.3}
\]

where \( \mu_n := \frac{1}{n} \sum_i \delta_{x_n,i} \to \mu \) as \( n \to \infty \).

Figure 2 shows a comparison between the minimiser of the discrete energy \( E_n \), for \( c_n = \sqrt{n} \) and for large \( n \), and the minimiser \( \rho_* \) of the continuum energy \( E \). Note that the continuous minimiser \( \rho_* \) is an affine function with slope \( -(\int_{\mathbb{R}} V)^{-1} \) (see Remark 2.2). In this figure we compare the two minimisers by plotting densities; the discrete density \( \rho_n \) is defined in terms of the minimiser \( x_n^{\ast} \) of \( E_n \) as

\[
\rho_n(x_n^{\ast,i}) := \frac{2/n}{x_n^{\ast,i+1} - x_n^{\ast,i-1}}, \quad i = 1, \ldots, n - 1. \tag{1.4}
\]

The figure illustrates well the starting point of this paper. The upscaled continuum model \( E \) fits very well with the discrete model \( E_n \) in the bulk of the pile-up region; however, it fails to capture the distribution of dislocations at the two ends of the domain, where boundary layers appear.

Inspired by this observation, the goal of this paper is to analyse the boundary layer at the lock at \( x = 0 \), in the scaling regime \( 1 \ll c_n \ll n \). We do this by studying a \( \Gamma \)-expansion [AB93, BC07, BT08] in terms of the small parameter \( 1/c_n \). The zero-order term of the expansion is the \( \Gamma \)-limit of the energy (namely \( E \) in (1.3)), which describes correctly the bulk behaviour of the minimiser; the term of order \( 1/c_n \) in the expansion, instead, is a first-order correction that captures boundary layer effects.

\(^1\)In [GPPS13] the dimensionless parameter is called \( \beta_n \), where \( \beta_n = c_n/n \).
In order to capture the main features of the asymptotic expansion by $\Gamma$-convergence, and isolate them from the more technical issues related with the passage from discrete to continuum, we study the $\Gamma$-expansion of a continuum version of $E_n$. To motivate this continuum version, note that the discrete energies $E_n$ can formally be written in terms of discrete integrals with respect to the measures $\mu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_n^i}$, as

$$E_n(x^n) = \frac{1}{2} c_n \int_{0}^{\infty} \int_{0}^{\infty} V(c_n(x-y)) \mu_n(dx) \mu_n(dy) + \int_{0}^{\infty} x \mu_n(dx).$$

(1.5)

Inspired by this we define the continuum energy

$$E_c(\mu) := \frac{1}{2} c \int_{0}^{\infty} \int_{0}^{\infty} V(c(x-y)) \mu(dx) \mu(dy) + \int_{0}^{\infty} x \mu(dx),$$

(1.6)

which now is considered to be defined for all $\mu \in P(0,\infty)$ – not only for sums of Diracs. This is the functional that we will study in this paper, in the limit $c \to \infty$.

1.1. Approximation of $E_c$ by $\Gamma$-expansion. The discrete energies $E_n$ in (1.1) and their continuous counterpart $E_c$ in (1.6) both have as $\Gamma$-limit the energy $E$ in (1.3), as we show in Theorem 2.1. The limit energy $E$ is therefore the first term of the approximation of $E_c$ by $\Gamma$-convergence, in the limit $c \to \infty$. Following [AB93], the next term of the expansion would be the $\Gamma$-limit of the rescaled energies

$$c(E_c(\mu) - E_c(\rho^*)).$$

(1.7)

as $c \to \infty$. This energy, however, does not seem appropriate for isolating the boundary layer contribution at the lock $x = 0$. Indeed, it is possible to show that there are two order-one contributions in (1.7): one is due to the presence of the boundary layer (namely to the difference between $\rho^*$ and the minimiser of $E_c$), and the other one to the approximation of $E_c$ with $E$. The latter is actually a constant with respect to the variable $\mu$ (namely $c(E_c(\rho^*) - E(\rho^*))$) and does not affect the behaviour of the minimisers.

To focus on the boundary-layer energy contribution only, we analyse the asymptotic behaviour of the following closely related functional

$$c(E_c(\mu) - E_c(\rho^*)).$$

(1.8)

The energy in (1.8) has the advantage of measuring the difference between the minimiser of $E_c$, which exhibits boundary layers, and its approximate bulk behaviour $\rho^*$, in terms of the same energy $E_c$ (rather than two different energies, as in (1.7)). For this reason it is genuinely a

\[2\]This expression is formal since $V(0) = +\infty$; to make it rigorous we should remove the diagonal $i = j$ from the product measure $\mu_n \otimes \mu_n = n^{-2} \sum_{i,j} \delta_{(x_n^i,x_n^j)}$.\]
‘boundary layer energy’, since the only contribution of order one in (1.8) is due to the behaviour at \( x = 0 \).

In order to capture the boundary-layer behaviour, we need to blow up the region next to \( x = 0 \). The scaling factor for the blow up arises naturally from (1.6), since the typical length scale of \( cV(c \cdot) \) is \( 1/c \). As \( c \to \infty \), we have \( cV(c \cdot) \to (\int_0^x V)\delta_0 \), which connects to the limiting energy \( E \) (1.3). This implies that fluctuations on the length scale \( 1/c \) contribute to the energy difference (1.8), which suggests that the boundary layer is likely to have the same length scale.

The boundary layer having length scale \( 1/c \) agrees with the formal analysis of Hall’s [Hal11] for the discrete problem with \( c_n = \sqrt{n} \). Figure 3 illustrates this scaling, by showing how spatially-rescaled densities constructed from the discrete minimisers are similar close to the lock.

\[ F_c(\nu) := \frac{1}{2} \int_0^\infty \int_0^\infty V(x - y)\nu(dx)\nu(dy) - \frac{1}{\sqrt{a}} \int_0^\infty \left( \int_x^\infty V(y)dy \right) \nu(dx) \]

\[ + \frac{1}{2ac} \int_0^\infty \int_0^\infty [V(y + (2c\sqrt{a} - x)) - V(y + x)]dy \nu(dx), \]

where \( a = \int_0^\infty V \), and all integrals (here and everywhere in the paper) denote integration over closed intervals.

The main result (see Theorem 3.5) is that the first two terms of \( F_c \) equal its Γ-limit as \( c \to \infty \):

Theorem 1.1. The functionals \( F_c \) Γ-converge as \( c \to \infty \), with respect to the vague topology, to the energy \( F \) defined as

\[ F(\nu) := \frac{1}{2} \int_0^\infty \int_0^\infty V(x - y)\nu(dx)\nu(dy) - \frac{1}{\sqrt{a}} \int_0^\infty \left( \int_x^\infty V(y)dy \right) \nu(dx), \]

Figure 3. Rescaled discrete densities \( \tilde{\rho}_n \) (see (4.2)), for \( c_n = \sqrt{n} \) and for different values of \( n \). At the left-hand end, close to the lock, the data points seem to lie on a single curve, confirming Hall’s result that the length scale of the boundary layer is \( O(1/\sqrt{n}) = O(1/c_n) \). To capture effects on the length scale \( 1/c \) we zoom in to \( x = 0 \) by a factor \( c \). Since this rescaling operation will be used many times we introduce a corresponding notation: given a measure \( \mu \), the rescaled measure \( c \to \mu \) is the measure \( c \to \mu : = c (x \mapsto cx)\#\mu \), or, in terms of Lebesgue densities, \( (c \to \mu)(x) := \mu(x/c) \). (1.9)

This transformation zooms in to the origin at rate \( c \), but preserves the amplitude of the (Lebesgue density of) the measure. The inverse transformation is written as \( c \leftarrow \mu \). Given a measure \( \mu \), the appropriate zoomed-in version of \( \mu \) is the measure obtained by blowing up the difference \( \mu - \rho_\ast \),

\[ \nu := c \to [\mu - \rho_\ast]. \]

(1.10)

We then rewrite (see Section 3.1) the energy (1.8) in terms of \( \nu \) as

\[ F_c(\nu) := \frac{1}{2} \int_0^\infty \int_0^\infty V(x - y)\nu(dx)\nu(dy) - \frac{1}{\sqrt{a}} \int_0^\infty \left( \int_x^\infty V(y)dy \right) \nu(dx) \]

\[ + \frac{1}{2ac} \int_0^\infty \int_0^\infty [V(y + (2c\sqrt{a} - x)) - V(y + x)]dy \nu(dx), \]

(1.11)
provided \( \nu \) belongs to the admissible class of measures \( \mathcal{A} \) defined in (3.14). In addition, a sequence \( \nu_c \) with \( \sup_c F_c(\nu_c) < \infty \) is compact in the vague topology.

Recall that convergence in the vague topology is defined as convergence against continuous functions with compact support. We discuss in more detail below why the vague topology is the natural choice for our problem.

As a consequence of this theorem the functional \( F \) achieves its minimum in \( \mathcal{A} \); since \( \mathcal{A} \) is convex and \( F \) is strictly convex, this minimum is also unique.

1.2. Approximation of the minimiser of \( E_c \) by ‘matching’. The \( \Gamma \)-convergence result in Theorem 1.1 suggests an improved approximation of the minimiser of the energy \( E_c \) at the left boundary of the pile-up domain, where the bulk density \( \rho_* \) failed to describe the profile of the discrete density (see Figure 2).

Defining \( \nu_* \) as the minimiser of \( F \), \( \rho_*(0) + \nu_* \) is the blown-up boundary layer profile, which corresponds to the behaviour of the minimiser of \( E_c \) close to the lock. In view of the \( \Gamma \)-convergence result, we can therefore define a ‘matched’ continuous density in terms of the original, unscaled variables, as

\[
\rho_c^* := \rho_* + c \nu_*,
\]

or, in terms of Lebesgue densities,

\[
\rho_c^*(x) = \rho(x) + \nu_*(cx),
\]

as the improved approximation of the minimiser of \( E_c \) in (1.6). In fact, this expression appears also to be a good approximation of the discrete optimal density \( \rho_n \), as shown in Figure 4. The agreement between \( \rho_c^* \) and the discrete density is striking, even for a small number of dislocation walls, except for the free end of the pile-up region, where a second boundary layer appears, whose analysis is beyond the scope of this paper.

![Figure 4](image-url)

**Figure 4.** Comparison between the discrete pile-up profile \( \rho_n \) in (1.4), the ‘bulk’ density \( \rho_* \) and the ‘matched’ density \( \rho_c^* = \rho_* + c \nu_* \), for \( n = 27 \) and \( c = \sqrt{n} \). The length of the \( x \)-axis in the left plot equals \( \sqrt{a/c} \).

1.3. Conclusion and comments. Theorem 1.1 gives a clear description of the boundary-layer behaviour of the pile-up at the lock through the minimiser of the limit energy. This theorem however only describes the boundary layer of the continuous energy \( E_c \), while the ‘real’ problem is discrete and described by \( E_n \). Still, the predictions we obtain from Theorem 1.1 are remarkably accurate (see Figure 4). We now comment on some of the aspects of the result and the proof.

*The functional-analytic setting and the vague topology.* The admissible measures \( \nu_c \in \mathcal{A}_c \) are obtained by blowing up probability measures, and consequently we cannot expect their total variation to stay bounded in the limit \( c \to \infty \). Indeed, Corollary 3.4 and (3.22) guarantee only local boundedness for sequences \( \nu_c \) with bounded energy \( F_c(\nu_c) \), and therefore the vague convergence is the natural choice for compactness.
Conditions on $V$. The $\Gamma$-convergence of $E_n$ to $E$ is proved in [GPPS13] under the following assumptions on $V$: $V$ is even, integrable on $\mathbb{R}$, and decreasing and convex on the positive real line. As a consequence of these properties, $V$ is non-negative. In this paper we do not use that $V$ is convex. Instead, we only require the Fourier transform of $V$ to be positive, which is a weaker requirement. On the other hand, we do require that $V$ has finite first moment, in addition to the properties mentioned above. This is necessary to control the contribution to the energy difference in (1.8) which is related to the bulk of the full pile-up.

Boundary layers in the discrete system. The ultimate goal of this work is to state and prove an analogue of Theorem 1.1 for the discrete energy $E_n$ in the limit $n \to \infty$. The current results can be seen as a first step towards such a convergence result, in which we tackle the scaling and compactness issues, but side-step the discreteness. Extending the results to a first-order $\Gamma$-convergence result in the discrete setting is work in progress by C. L. Hall, T. Hudson and PvM.

Unexpected ‘dip’ in the minimiser $\nu_*$. Figure 5 gives another view on the comparison between the discrete and continuous densities, showing the boundary layers at both ends of the pile-up region in the same figure. Note that $\nu_*$ attains negative values in the region where the boundary layer matches with the bulk density $\rho_*$. This ‘dip’ indicates that in this region the dislocation walls tend to separate slightly farther than predicted by the bulk density. It is unclear to us why such a ‘dip’ occurs.

Figure 5. Comparison between the discrete density $\nu_n$ and $\nu_*$ for $c_n = \sqrt{n}$ and for different values of $n$. Many points are omitted to enhance readability. See Section 4.3 for a detailed description of these graphs.

After briefly proving the zero-order limit $E_c \Gamma \rightarrow E$ in Section 2, we prove the main result Theorem 1.1 in Section 3. We conclude in Section 4 with numerical illustrations.

1.4. Assumptions and notation. Although the expression (1.2) is the inspiration for this paper, and although we use (1.2) in the numerical calculations, the convergence results hold for a broader class of functions $V$. In Sections 2 and 3 we make the following assumptions on $V$:

- (V1) $V : \mathbb{R} \rightarrow \mathbb{R}$ is even, and, on $(0, \infty)$, $V$ is decreasing;
- (V2) $V \in L^1(\mathbb{R})$ has finite first moment, i.e., $\int_\mathbb{R} |V(x)| \, dx, \int_\mathbb{R} |x|V(x) \, dx < \infty$;
- (V3) $V$ has a non-negative and bounded Fourier transform.

Note that by (V1) and (V2), $V$ is non-negative.

Here we list some symbols and abbreviations that we use throughout the paper.

3To see that convexity of $V$ implies positivity of $\hat{V}$, note that $V(\xi) = 2 \int_0^\infty V(x) \cos 2\pi \xi x \, dx = -\left(\pi \xi^2\right)^{-1} \int_0^\infty V'(x) \sin 2\pi \xi x \, dx; this expression can be seen to be positive by considering each period of the sine, and using the monotonicity of $V'$.
Proof. Compactness, i.e., tightness, is a simple consequence of the inequality $E = \rho h$ hence the rescaled version of $a$ in (2.1).

Theorem 2.1. The $\Gamma$-limit of $E_c$ as $c \to \infty$ with respect to the narrow topology is given by

$$E(\mu) = a \int_0^\infty \rho(x)^2 \, dx + \int_0^\infty x \rho(x) \, dx,$$

where $a := \int_0^\infty V$. In addition, sequences with bounded $E_c$ are compact in the narrow topology.

Proof. Compactness, i.e., tightness, is a simple consequence of the inequality $E_c(\mu) \geq \int_0^\infty x \mu(dx)$. The proof of the liminf inequality follows from a simple modification of the proof of the discrete-to-continuum convergence in [GPPS13, Theorem 7].

As for the limsup inequality, we first reduce by density arguments to bounded upper semicontinuous functions $\rho \in L^2(0, \infty)$ with bounded support. Then we take as recovery sequence the constant sequence $\rho_c := \rho$. Note that $V_c(x, y) := cV(c(x - y))$ converges vaguely to $2aH^1(D)$, where $D$ is the diagonal of the first quadrant,

$$D := \{(x, y) \in (0, \infty)^2 \mid x = y\}.$$

Then we conclude the limsup inequality from

$$\limsup_{c \to \infty} \int_0^\infty \int_0^\infty V_c(x, y) \rho(x) \rho(y) \, dx \, dy \leq 2a \int_0^\infty \int_0^\infty \rho(x) \rho(y) H^1(D) \, dx \, dy = 2a \int_0^\infty \rho^2.$$

Remark 2.2. We recall that the minimiser of $E$ is given by

$$\rho_*(x) := \left(\frac{1}{\sqrt{a}} - \frac{x}{2a}\right)^+, \quad E(\rho_*) = \frac{4}{3} \sqrt{a},$$

hence the rescaled version of $\rho_*$ is, according to the definition (1.9),

$$\tilde{\rho}_*(x) := c \rho_*(x) = \left(\frac{1}{\sqrt{a}} - \frac{x}{2ca}\right)^+. \quad (2.2)$$
3. First-order Gamma-convergence

In this section we prove Theorem 1.1 (see Theorem 3.5), which states the \( \Gamma \)-convergence of \( F_c \) in (1.11) to \( F \) in (1.12).

3.1. Preliminary results. Rewriting the energy. In the introduction we mentioned that under the blow-up transformation (1.10), which transforms \( \mu \) into \( \nu \), the energy \( E_c \) converts into the expression for \( F_c \) in (1.11). Here we do that calculation explicitly.

Setting \( \tilde{\mu}^c := c \rightarrow \mu \), we write

\[
\frac{1}{2} \int_0^\infty \int_0^\infty V(x - y)\tilde{\mu}^c(dx)\tilde{\mu}^c(dy) + \frac{1}{c} \int_0^\infty x\tilde{\mu}^c(dx) =: \bar{E}_c(\tilde{\mu}^c).
\]

Note that \( \int_0^\infty \tilde{\mu}^c = c \). By defining as in (1.10) \( \nu^c := \tilde{\mu}^c - c \rightarrow \rho_* \) we write, by using Fubini’s theorem,

\[
F_c(\nu^c) := c (E_c(\mu) - E_c(\rho_*)) = \bar{E}_c(\tilde{\mu}^c) - \bar{E}_c(\tilde{\rho}_*)
\]

\[
= \frac{1}{2} \int_0^\infty \int_0^\infty V(x - y)\nu^c(dx)\nu^c(dy) + \int_0^{\infty} \int_0^{\infty} V(x - y)\rho_*(y/c)dy + \frac{1}{c} \int_0^\infty \nu^c(dx).
\]

(3.1)

For the sake of notation, we omit the superscript \( c \). The measures \( \nu \) obtained via the rescaling (1.10) belong to the admissible class \( \mathcal{A}_c \) defined as

\[
\mathcal{A}_c := \left\{ \nu \in \mathcal{M}([0,\infty)) : \int_0^\infty |\nu| \leq 2c, \quad \int_0^\infty \nu = 0, \quad \nu \geq -\tilde{\rho}_* \right\}.
\]

(3.2)

Note that by (3.2) and (2.2),

\[
\text{supp} \nu^c \subset \text{supp} \tilde{\rho}_* = [0, 2c\sqrt{a}] \quad \text{for each } \nu \in \mathcal{A}_c.
\]

(3.3)

Next we rewrite \( F_c(\nu) \). By using the explicit expression of \( \rho_* \) (see Remark 2.2) and the fact that \( V \) is even, the integrand of the second term in (3.1) can be cast into

\[
\int_0^\infty V(x - y)\rho_*(y/c)dy + \frac{1}{c} \int_0^\infty \nu^c(dx)
\]

\[
= \frac{1}{\sqrt{a}} \int_0^{2c\sqrt{a}} V(x - y)dy + \frac{1}{2ac} \int_0^{2c\sqrt{a}} V(x - y)dy + \frac{1}{2ac} \int_0^\infty \nu(x)dx
\]

\[
= \frac{1}{\sqrt{a}} \int_0^{2c\sqrt{a}} V(x - y)dy + \frac{1}{2ac} \int_0^\infty \nu(x)dx
\]

\[
= 2\sqrt{a} - \frac{1}{\sqrt{a}} \int_x^\infty V(y)dy + h_c(x),
\]

(3.4)

where we have set

\[
h_c(x) := \frac{1}{2ac} \int_0^\infty \nu(y)dy
\]

\[
= \frac{1}{2ac} \left[ \int_0^\infty (V * \nu)(y)dy + h_c(x) \right].
\]

(3.5)

Substituting (3.4) in (3.1) and using the fact that \( \int \nu = 0 \) results into

\[
F_c(\nu) = \frac{1}{2} \int_0^\infty (V * \nu)(x)\nu(x)dx - \int_0^\infty g(x)\nu(dx) + \int_0^\infty h_c(x)\nu(dx),
\]

(3.6)

where \( g(x) := \frac{1}{\sqrt{a}} \int_x^\infty V(y)dy \).

(3.7)

Note that, due to assumption (V2), the positive function \( g \) is integrable on \( (0,\infty) \). Moreover, \( g \) is decreasing in \( (0,\infty) \) and \( g(0) = \sqrt{a} \); hence it is bounded in \( (0,\infty) \).

Properties of the auxiliary function \( h_c \). In the following lemma we derive some useful estimates on the behaviour of \( h_c \). The qualitative behaviour of \( h_c \) is illustrated in Figure 6.
Lemma 3.1. The function $h_c$ defined in (3.5) is non-decreasing and satisfies the bounds
\begin{align}
|h_c| &\leq C\frac{1}{c} \text{ in } [0, 2c\sqrt{a}], \\
|h_c| &\leq \frac{\sigma(c)}{c} \text{ in } [\sqrt{c}, 2c\sqrt{a} - \sqrt{c}],
\end{align}
for some $\sigma(c) \to 0$ as $c \to \infty$.

**Proof.** The function $h_c$ is non-decreasing, since it is defined as the convolution of a non-negative function with a non-decreasing function.

To prove (3.8) we note that by the monotonicity of $h_c$, for all $x \in [0, 2c\sqrt{a}]$,
\begin{align}
-C\frac{1}{c} \leq h_c(0) \leq h_c(x) \leq h_c(2c\sqrt{a}) \leq C\frac{1}{c},
\end{align}
with $C = \frac{1}{2a} \int_0^\infty V(y)ydy$. (3.10)

As for (3.9), we estimate
\begin{align}
h_c(2c\sqrt{a} - \sqrt{c}) = -h_c(\sqrt{c}) \leq \frac{1}{2ac} \int_0^{\infty} V(y + \sqrt{c})ydy \leq \frac{1}{2ac} \int_{\sqrt{c}}^{\infty} V(z)zdz,
\end{align}
which implies (3.9) by assumption (V2). \hfill \Box

**Writing $V = W*W$.** We formally write the interaction potential $V$ as a convolution $V = W*W$. In [GPPS13, Appendix] it was shown that, for the special case of (1.2),
\begin{align}
\hat{V}(\xi) = \frac{1}{2\xi \sinh(\pi^2\xi)} \left( \cosh(\pi^2\xi) - \frac{\pi^2\xi}{\sinh(\pi^2\xi)} \right).
\end{align}
This function is even, bounded, and strictly positive on $\mathbb{R}$, and decays to zero at infinity at rate $1/|\xi|$. Since the function $p(\xi) := \sqrt{\hat{V}(\xi)}$ decays at rate $|\xi|^{-1/2}$, it fails to be in $L^2(\mathbb{R})$; therefore the inverse Fourier transform of $p$ may not be a function $W$, and it is not clear whether there exists any function $W : \mathbb{R} \to \mathbb{R}$ such that $V = W*W$.

In this paper we also want to generalize to different functions $V$. We therefore work around these difficulties by defining ‘convolution with $W$’ as an operator on the space of tempered distributions [SW71, Chapter 1], as follows. For a general function $V$ satisfying conditions (V1 – 3), set again $p(\xi) := \sqrt{\hat{V}(\xi)}$; by (V3), the function $p$ is well-defined and bounded. We first define the operator $T$ on the Schwarz space of rapidly decreasing smooth functions $\mathcal{S}(\mathbb{R})$, by
\begin{align}
T : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R}), \quad \varphi \mapsto T\varphi := (p\hat{\varphi}).
\end{align}
The operator $T$ is trivially extended to the space $\mathcal{S}'(\mathbb{R})$ of tempered distributions by
\begin{align}
\text{for } \xi \in \mathcal{S}'(\mathbb{R}), \varphi \in \mathcal{S}(\mathbb{R}), \quad \mathcal{S}'(\mathbb{R})(T\xi, \varphi)_{\mathcal{S}(\mathbb{R})} := \mathcal{S}'(\mathbb{R})(\xi, T\varphi)_{\mathcal{S}(\mathbb{R})}.
\end{align}
Formally, one should think of $T\varphi$ as $W * \varphi$, where $V = W * W$. The following lemma summarises some properties of $T$.

**Lemma 3.2.** The operator $T$ defined in (3.11)-(3.12) enjoys the following properties:

1. $T$ is weakly-continuous on $S'(\mathbb{R})$;
2. $T$ is a bounded mapping from $L^2(\mathbb{R})$ to $L^2(\mathbb{R})$, with operator norm $\|T\| = \left( \int_{\mathbb{R}} V \right)^{\frac{1}{2}} = \sqrt{2}a$;
3. $T(T(\varphi)) = V * \varphi$ for all $\varphi \in S'(\mathbb{R})$.

**Proof.** The weak-$*$ continuity follows directly from the definition: if $\xi_n \rightharpoonup \xi$, then for any $\varphi \in S(\mathbb{R})$, 

$$\langle T\xi_n, \varphi \rangle = \langle \xi_n, T\varphi \rangle \to \langle \xi, T\varphi \rangle = \langle T\xi, \varphi \rangle.$$  

The fact that $T$ maps $L^2(\mathbb{R})$ into itself follows from the boundedness of the function $p$ and Parseval's identity; the norm of the operator $T$ on $L^2$ is the $L^\infty$-norm of $p$, which is achieved at $\xi = 0$ with value $\left( \int_{\mathbb{R}} V \right)^{\frac{1}{2}}$. The fact that $T^2\varphi = V * \varphi$ follows from the property that $p^2 = \tilde{V}$. \hfill $\square$

**Definition of the limit energy.** We slightly rewrite the limiting functional $F$ from the introduction as

$$F(\nu) = \begin{cases} \frac{1}{2} \int_0^\infty \int_0^\infty V(x-y)\nu(dx)\nu(dy) - \int_0^\infty g(x)\nu(dx), & \text{if } \nu \in \mathcal{A}, \\ \infty, & \text{otherwise}, \end{cases}$$

(3.13)

where $g$ is defined in (3.7) and $\nu \in \mathcal{A}$, with

$$\mathcal{A} := \left\{ \nu \in \mathcal{M}([0,\infty)) : \nu \geq -\rho_*(0), \sup_{x \geq 0} \nu^+([x,x+1]) < \infty \right\},$$

(3.14)

where $\nu^+$ is the positive part of $\nu$.

While for finite $c$ the set $\mathcal{A}_c$ consists of measures with uniformly bounded total variation, in the limiting set $\mathcal{A}$ this bound has vanished, and a priori it is unclear why a sequence in $\mathcal{A}$ could not acquire infinite total variation in the limit. Corollary 3.4 below will show that finiteness of $F(\nu)$ implies a local bound on $|\nu|$, but no global bound. Maybe minimising sequences have bounded total variation, but we have not investigated this. The requirement of $\nu^+$ in (3.14) about being uniformly bounded on compacta ensures $\nu \in S'(\mathbb{R})$, which implies that $T\nu$ is well-defined.

3.2. **Key estimates.** The following estimates are central in much of what follows.

**Lemma 3.3.** Let $\eta > 0$. For any bounded interval $[\alpha, \beta] \subset [0,\infty)$ with $\beta - \alpha \geq \eta$ there exist constants $C > 0$ and $C_\eta > 0$ (decreasing in $\eta$) such that for all $\nu \in \mathcal{M}([0,\infty)) \cap S'(\mathbb{R})$ with $\nu \geq -\rho_*(0)$, the following estimates involving $\lambda := T\nu$ hold

$$\nu^+([\alpha, \beta]) \leq C_\eta (\sqrt{\beta - \alpha} \|\lambda\|_{L^2(\mathbb{R})} + \beta - \alpha),$$

(3.15)

$$\int_{-\infty}^0 T\lambda = \int_{-\infty}^\infty V * \nu \leq C(\|\lambda\|_{L^2(\mathbb{R})} + 1).$$

(3.16)

**Proof.** It is not restrictive to prove the claim only for $\nu$ with $T\nu \in L^2(\mathbb{R})$, the bounds (3.15) and (3.16) being trivial otherwise.

Since $V$ is positive, we obtain

$$\int_{\alpha}^{\beta} V * \nu^+ = \int_{\alpha}^{\beta} \int_0^\infty V(x-y)\nu^+(dy)dx \geq \int_{\alpha}^{\beta} \left( \int_{\alpha}^{\beta} V(x-y)dx \right) \nu^+(dy) \geq \tilde{C}_\eta \nu^+([\alpha, \beta]),$$

where $\tilde{C}_\eta$ is a strictly positive constant increasing in $\eta$ and converging to 0 as $\eta \searrow 0$. Note that since we assumed that $T\nu \in L^2(\mathbb{R})$, $T^2\nu \in L^2(\mathbb{R})$, and $\|T^2\nu\|_2 \leq C\|T\nu\|_2$. We then get the desired
Moreover, if $F$ there is finiteness of upper bound (3.15) from $\nu$ of $\lambda$. This proves (3.19).

Theorem 3.5. (First-order $\Gamma$–convergence) Any sequence $(\nu_c) \subset \mathcal{A}_c$ with bounded energies $F_c(\nu_c)$ is pre-compact in the vague topology. Furthermore, $F_c \Gamma$–converges to $F$ as $c \to \infty$ with
with respect to the vague topology, i.e.

for all \( \nu_c \rightharpoonup \nu \) vaguely,

\[
\liminf_{c \to \infty} F_c(\nu_c) \geq F(\nu),
\]

(3.20a)

for all \( \nu \in \mathcal{A} \) there exists \( \nu_c \rightharpoonup \nu \) vaguely such that

\[
\limsup_{c \to \infty} F_c(\nu_c) \leq F(\nu).
\]

(3.20b)

**Proof.** Compactness. Let \( \nu_c \in \mathcal{A}_c \subset \mathcal{A} \); combining (3.6) and (3.13) we write

\[
F_c(\nu_c) - F(\nu) = \int_0^\infty h_c \nu_c.
\]

(3.21)

We split the proof into several steps.

**Step 1. Lower bound for \( \int_0^\infty h_c \nu_c \).** Since \( h_c \) is non-decreasing (Lemma 3.1) and by (3.3) \( \text{supp} \nu_c^- \subseteq [0, 2c\sqrt{\lambda}] \), we deduce the bound

\[
\int_0^\infty h_c \nu_c = \int_0^\infty h_c \nu_c^+ - \int_0^{2c\sqrt{\lambda}} h_c \nu_c^- \geq h_c(0) \int_0^\infty \nu_c^+ - h_c(2c\sqrt{\lambda}) \int_0^\infty \nu_c^- \geq -C,
\]

(3.22)

where the last inequality follows from (3.2) and (3.10). From this estimate we conclude in particular that finiteness of \( F_c(\nu_c) \) implies finiteness of \( F(\nu_c) \).

**Step 2. Convergence of \( \nu_c \) and \( T \nu_c \).** Let \( \nu_c \in \mathcal{A}_c \) be a sequence with bounded energy \( F_c(\nu_c) \leq C \). Then, by Step 1 we deduce that \( F(\nu_c) \leq C \), and by Lemma 3.3 and (3.19) we have

\[
C \geq F(\nu_c) = \frac{1}{2} \| \lambda_c \|_2^2 - \frac{1}{\sqrt{2}} \int_0^\lambda T \lambda_c \geq \frac{1}{2} \| \lambda_c \|_2^2 - C(\| \lambda_c \|_2 + 1),
\]

(3.23)

where \( \lambda_c := T \nu_c \); hence \( \lambda_c \) is bounded in \( L^2(\mathbb{R}) \).

In addition, \( \nu_c([\alpha, \beta]) \) is uniformly bounded in \( c \) for any bounded interval \( [\alpha, \beta] \subset [0, \infty) \), with a bound that only depends on \( \beta - \alpha \) and \( \| \lambda_c \|_2 \). This follows from Lemma 3.3, since \( -(\beta - \alpha) \rho_c(0) \leq \nu_c([\alpha, \beta]) \leq \nu_c^+([\alpha, \beta]) \). Therefore, along a subsequence,

\[
\nu_c \rightharpoonup \nu \text{ vaguely, and } \lambda_c = T \nu_c \rightharpoonup \lambda \text{ in } L^2.
\]

(3.24)

**Step 3. Characterisation of the limits \( \nu \) and \( \lambda \).** We claim that \( \nu_c \) converges weakly-* as tempered distribution to \( \nu \in \mathcal{S}'(\mathbb{R}) \). If so, the weak continuity of \( T \) (Lemma 3.2) and (3.24) imply that \( \lambda = T \nu \in L^2(\mathbb{R}) \). Consequently, by Lemma 3.3, \( \nu \in \mathcal{A} \).

To prove this claim, we take \( \varphi \in \mathcal{S}(\mathbb{R}) \) and a large \( M > 0 \) fixed and write

\[
\int_0^\infty \varphi \nu_c = \int_0^M \varphi \nu_c + \int_M^\infty \varphi \nu_c.
\]

The first term in the right-hand side converges to \( \int_0^M \varphi \nu \) as \( c \to \infty \) because of the vague convergence of \( \nu_c \) to \( \nu \). We now show that the second term is small for large \( M \), uniformly in \( c \). To see this, we first notice that there exists \( C > 0 \) such that \( |\varphi(x)| < C x^{-2} \) for \( x > M \). Then by Lemma 3.3 we obtain

\[
\left| \int_M^{\infty} \varphi \nu_c \right| \leq \sum_{k=0}^{\infty} \int_{M+k}^{M+k+1} C x^{-2} |\nu_c|(dx) \leq \frac{\tilde{C}}{M},
\]

with \( \tilde{C} \) independent of \( c \).

**Lower bound.** To prove (3.20a), we see from (3.21) that it is sufficient to show that

\[
\liminf_{c \to \infty} \int_0^\infty h_c \nu_c \geq 0, \quad \text{and} \quad \liminf_{c \to \infty} F(\nu_c) \geq F(\nu).
\]

(3.25)

We start with the first inequality in (3.25). First of all, if we write \( h_c = h_c^+ - h_c^- \) and \( \nu_c = \nu_c^+ - \nu_c^- \), we have

\[
\int_0^\infty h_c \nu_c \geq - \int_0^\infty h_c^+ \nu_c^- - \int_0^\infty h_c^- \nu_c^+.
\]
the other terms being non-negative. Therefore the first inequality in (3.25) follows if we prove that
\[ \limsup_{c \to \infty} \int_0^{\infty} h_c^+ - \nu_c^- = 0, \quad \text{and} \quad \limsup_{c \to \infty} \int_0^{\infty} h_c^- + \nu_c^+ = 0. \] (3.26)

We note that, since supp \( \nu_c^- \) \( \subseteq [0, 2c \sqrt{a}] \) and \( \nu_c^- \) \( \leq \rho_*(0) \),
\[ \int_0^{\infty} h_c^+ \nu_c^- = \int_0^{2c \sqrt{a}} h_c^+ \nu_c^- \leq \rho_*(0) \int_0^{2c \sqrt{a}} h_c^+. \]
The bounds (3.8) and (3.9) on \( h_c \) entail
\[ \int_0^{2c \sqrt{a}} h_c^+ = \int_0^{\sqrt{a}} h_c^+ + \int_{\sqrt{a}}^{2c \sqrt{a} - \sqrt{a}} h_c^+ + \int_{2c \sqrt{a} - \sqrt{a}}^{2c \sqrt{a}} h_c^+ \leq \frac{C}{\sqrt{a}} + C \sigma(c), \] (3.27)
which converges to zero as \( c \to \infty \). Analogously, since \( \text{supp} \ h_c^- \cap [0, \infty) \subseteq [0, 2c \sqrt{a}] \), by (3.8)-(3.9) and Lemma 3.3 we have
\[ \int_0^{\infty} h_c^- \nu_c^+ = \int_0^{\sqrt{a}} h_c^- \nu_c^+ + \int_{\sqrt{a}}^{2c \sqrt{a} - \sqrt{a}} h_c^- \nu_c^+ + \int_{2c \sqrt{a} - \sqrt{a}}^{2c \sqrt{a}} h_c^- \nu_c^+ \leq \frac{C}{\sqrt{a}} + C \sigma(c), \]
\[ \int_0^{\infty} h_c^- \nu_c^+ \leq \frac{C}{\sqrt{a}} + C \sigma(c) \to 0 \quad \text{as} \quad c \to \infty. \] (3.28)
The bounds (3.27) and (3.28) above imply (3.26), and hence the first inequality in (3.25).

We now prove the second inequality in (3.25). We proceed from the expression of \( F \) in (3.19). From (3.24) we immediately obtain
\[ \liminf_{c \to \infty} \mu_c \geq \| \lambda \|_2^2. \]
To conclude the proof of the liminf inequality it remains to show that
\[ \limsup_{c \to \infty} \int_{-\infty}^{0} T(\lambda_c - \lambda) = 0. \] (3.29)
Let \( M > 0 \) and \( C_F > 0 \) be fixed and large constants. We write, using Fubini and the fact that \( V \)
\[ \int_{-\infty}^{0} T(\lambda_c - \lambda) = \int_{-\infty}^{0} V * (\nu_c - \nu) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} V(x-y)(\nu_c(dy) - \nu(dy)) \]
\[ = \int_0^M (\nu_c(dy) - \nu(dy)) \int_0^\infty V(x+y)dx + \int_0^M (\nu_c(dy) - \nu(dy)) \int_0^\infty V(x+y)dx. \] (3.30)
Since the function
\[ y \mapsto \int_0^\infty V(x+y)dx \]
is continuous and bounded for \( y \geq 0 \), and \( \nu_c \to \nu \) vaguely, it follows that
\[ \lim_{c \to \infty} \int_0^M (\nu_c(dy) - \nu(dy)) \int_0^\infty V(x+y)dx = 0. \] (3.31)
We now prove that, for every \( \nu \in A \) with \( F(\nu) \leq C_F \),
\[ \int_M^\infty \nu^+(dy) \int_0^\infty V(x+y)dx \leq C(M, C_F), \quad C(M, C_F) \to 0 \quad \text{as} \quad M \to \infty. \] (3.32)
Note that (3.32), together with (3.31) and (3.30), imply the claim (3.29), by letting \( M \to \infty \), since
\[ \int_M^\infty (\nu_c(dy) - \nu(dy)) \int_0^\infty V(x+y)dx \leq \int_M^\infty (\nu^+_c(dy) + \nu^-_c(dy)) \int_0^\infty V(x+y)dx. \]
Using the fact that \( \nu^\pm(\alpha, \beta) \) is bounded for any bounded interval \( [\alpha, \beta] \subset [0, \infty) \) and that \( V \) is decreasing on the positive real axis, we immediately have

\[
\int_M^n \nu^\pm(dy) \int_0^\infty V(x + y)dx \leq \sum_{k = |M|}^{\infty} \int_k^{k+1} \nu^\pm(dy) \int_0^\infty V(x + k)dx
\]

\[
\leq C \sum_{k = |M|}^{\infty} \int_0^\infty V(x + k)dx
\]

\[
= C \sum_{k = |M|}^{\infty} \int_k^{\infty} V,
\]

which implies (3.32) since the last term in (3.33) tends to zero as \( M \to \infty \) by assumption (V2).

This concludes the proof of the liminf inequality.

\textbf{Upper bound.} Let \( \nu \in A \) with \( F(\nu) < \infty \). We first prove some density results for the limit energy that will allow us to prove (3.20b) for a smaller class of measures.

\textbf{Step 1. Approximation of \( \nu \) by smooth truncation.} Given \( \nu \in A \), we first show that we can approximate \( \nu \) both in the vague topology and in energy by a modified measure \( \nu_\alpha \) which decays at infinity. For this, define for any \( \alpha > 0 \) the Gaussian \( G_\alpha(x) := \exp(-\pi \alpha x^2) \), and note that \( \hat{G}_\alpha = \alpha^{-1/2} G_{\alpha^{-1}} \) is an approximation of the identity (it converges distributionally to a delta function at zero as \( \alpha \to 0 \)).

We now define \( \nu_\alpha(dx) := G_\alpha(x)\nu(dx) \); note that \( \nu_\alpha \) converges to \( \nu \) in the vague topology. We claim that also \( \lim_{\alpha \downarrow 0} F(\nu_\alpha) = F(\nu) \). Considering the two terms in (3.13), the second term converges because \( G_\alpha \) converges to \( \nu \) as \( \alpha \to 0 \), since \( g \) is continuous and bounded in \( [0, \infty) \) and \( \nu \) fixed. The first term in (3.13) we rewrite as

\[
\frac{1}{2} \int_0^\infty \int_0^\infty V(x - y)\nu_\alpha(dx)\nu_\alpha(dy) = \frac{1}{2} \int_\mathbb{R} |T(G_\alpha \nu)|^2 = \frac{1}{2} \int_\mathbb{R} |\hat{G}_\alpha \ast \hat{\nu}|^2(\xi)p^2(\xi) d\xi,
\]

and since \( \hat{\nu} \in L^2(p^2(\xi) d\xi) \), where \( p^2 = \hat{V} \) as above, this converges as \( \alpha \downarrow 0 \) to

\[
\frac{1}{2} \int_\mathbb{R} |\hat{\nu}|^2(\xi)p^2(\xi) d\xi \leq \frac{1}{2} \int_0^\infty \int_0^\infty V(x - y)\nu(dx)\nu(dy).
\]

Therefore the set \( \cup_{\alpha > 0} G_\alpha A \) is energy-dense in \( A \). Note that for all \( \alpha > 0 \) and \( \nu \in A \), Lemma 3.3 gives exponential decay of \( \nu_\alpha^+([x, x + 1]) \) and \( \nu_\alpha^+([x, x + 1]) \) as \( x \to \infty \).

\textbf{Step 2. Hard truncation.} We now choose \( \nu \in G_\alpha A \), for some \( \alpha > 0 \). Let \( \nu_n := \nu_n[0, n] \). We claim that \( F(\nu_n) \to F(\nu) \) as \( n \to \infty \), where

\[
F(\nu_n) = \frac{1}{2} \int_0^n \int_0^n V(x - y)\nu(dx)\nu(dy) - \frac{1}{\sqrt{n}} \int_{-\infty}^0 V \ast \nu_n.
\]

We rewrite the first term in the right-hand side of (3.34) as follows, by using  \( \nu = \nu^+ - \nu^- \):

\[
\frac{1}{2} \int_0^n \int_0^n V(x - y)\nu(dx)\nu(dy) = \frac{1}{2} \int_0^n \int_0^n V(x - y)\nu^+(dx)\nu^+(dy)
\]

\[
+ \frac{1}{2} \int_0^n \int_0^n V(x - y)\nu^-(dx)\nu^-(dy) - \int_0^n \int_0^n V(x - y)\nu^+(dx)\nu^-(dy).
\]

Now we observe that each of the integrals in the right-hand side of (3.35) is of the form

\[
\int_0^n \int_0^n V(x - y)\chi_{[0,n]}(x,y)\nu^+(dx)\nu^+(dy),
\]

and that

\[
0 \leq V(x - y)\chi_{[0,n]}(x,y) \leq V(x - y)
\]
pointwise, as \( n \to \infty \). By the monotone convergence theorem each of these integrals converges; since \( \nu^\pm ([x, x + 1]) \) decays exponentially as \( x \to \infty \), each of the limiting integrals is finite. We conclude that

\[
\lim_{n \to \infty} \frac{1}{2} \int_0^n \int_0^n V(x - y) \nu(dx) \nu(dy) = \frac{1}{2} \int_0^\infty \int_0^\infty V(x - y) \nu(dx) \nu(dy),
\]

namely the convergence of the first term in the right-hand side of (3.34) to the corresponding term of \( F(\nu) \).

For the second term of (3.34) we observe that

\[
\left| \int_{-\infty}^0 V \ast (\nu_n - \nu) \right| \leq \int_{-\infty}^0 dx \int_n^\infty V(x - y)(\nu^+ + \nu^-)(dy) = \int_n^\infty (\nu^+ + \nu^-)(dy) \int_0^\infty V(x + y)dx,
\]

and this converges to zero as \( n \to \infty \) by (3.32). Therefore

\[
\lim_{n \to \infty} \frac{1}{\sqrt{a}} \int_{-\infty}^0 V \ast \nu_n = \frac{1}{\sqrt{a}} \int_{-\infty}^0 V \ast \nu,
\]

which concludes the proof of Step 2.

**Step 3. Approximation of \( \nu \) with measures with bounded density.** By the previous step we can assume that supp\( \nu \) is bounded. Let now \( \nu_n \) be defined as \( \nu_n(A) := \nu^+_n(A) - \nu^-(A) \), and \( \nu^+_n(A) := \nu^+(A) \wedge n|A| \) for any set \( A \subseteq [0, \infty) \), where \( |A| \) is the Lebesgue measure of \( A \); since \( \nu \) has bounded support, now \( \nu_n \) also has finite mass. Note that \( \nu^+_n = \nu^- \). We are going to prove that

\[
\lim_{n \to \infty} \sup \int_0^\infty (V \ast \nu_n) \nu \leq \int_0^\infty (V \ast \nu) \nu \quad \text{and} \quad \lim_{n \to \infty} \int_{-\infty}^0 V \ast \nu_n = \int_{-\infty}^0 V \ast \nu.
\]

(3.36)

From (3.36) follows immediately the claim

\[
\lim_{n \to \infty} \sup F(\nu_n) \leq F(\nu),
\]

by the definition of the functional \( F \).

To prove the first result in (3.36) we proceed as follows. Writing \( \nu_n = \nu^+_n - \nu^- \) and using the fact that \( V \) is even, we have

\[
\int_0^\infty (V \ast \nu_n) \nu = \int_0^\infty (V \ast \nu^+_n) \nu^+ + \int_0^\infty (V \ast \nu^-) \nu^- - 2 \int_0^\infty (V \ast \nu^-) \nu^+_n \\
\leq \int_0^\infty (V \ast \nu^+) \nu^+ + \int_0^\infty (V \ast \nu^-) \nu^- - 2 \int_0^\infty (V \ast \nu^-) \nu^+_n,
\]

(3.37)

since \( \nu^+_n \leq \nu^+ \), and \( V \ast \nu^+_n \leq V \ast \nu^+ \). It remains to prove that

\[
\lim_{n \to \infty} \int_0^\infty (V \ast \nu^-) \nu^+_n = \int_0^\infty (V \ast \nu^-) \nu^+.
\]

(3.38)

First of all, as \( (V \ast \nu^-) \) is non-negative and bounded, and \( \nu^+_n \leq \nu^+ \), we have

\[
0 \leq \int_0^\infty (V \ast \nu^-)(\nu^+ - \nu^+_n) \leq C \int_0^\infty (\nu^+ - \nu^+_n) = C(\nu^+ - \nu^+_n)(\text{supp} \nu),
\]

and the last term converges to zero as \( n \to \infty \) by the definition of \( \nu_n \). This concludes the proof of the first claim in (3.36). The second result in (3.36) follows by monotone convergence, since \( 0 \leq V \ast \nu^+_n \uparrow V \ast \nu^+ \) pointwise.

In conclusion, by Steps 1-3, we can restrict our attention to \( \nu \in \mathcal{A} \) with bounded support and bounded Lebesgue density. Without loss of generality we can assume in addition that \( \nu > -\rho_\ast(0) \), by slightly retracting \( \nu \) if necessary. For such a \( \nu \), we take as recovery sequence

\[
\nu_c := \nu - \sigma_c \tilde{p}_c, \quad \sigma_c := \frac{1}{c} \int_0^\infty \nu.
\]

(3.39)
Note that $\int_0^\infty \nu_c = 0$ and that $\nu_c \geq -\bar{\rho}_*$ for $c$ sufficiently large. Hence $\nu_c \in \mathcal{A}_c$, and it is an admissible sequence for $F_c$.

Next we prove that $F_c(\nu_c) \to F(\nu)$ as $c \to \infty$. We first write explicitly

$$F_c(\nu_c) = \frac{1}{2} \int_0^\infty \int_0^\infty V(x-y)\nu(dx)\nu(dy)$$

$$+ \frac{2}{\nu} \int_0^\infty \int_0^\infty V(x-y)\bar{\rho}_*(x)\nu(dy)$$

$$+ \sigma_c \int_0^\infty g\bar{\rho}_* + \int_0^\infty h_c\nu - \sigma_c \int_0^{\infty} h_c\bar{\rho}_*.$$

(3.40)

For the second term in the right-hand side of (3.40) we have, since $\bar{\rho}_* \leq \rho_*(0) = 1/\sqrt{a}$,

$$\left| \int_0^\infty \int_0^\infty V(x-y)\nu(x)\nu(dy) \right| \leq 2\sqrt{a}\sigma_c \int_0^{\infty} (\nu^+ + \nu^-)(dy) \leq C \sigma_c \to 0$$

as $c \to \infty$, since, in view of the density arguments in Steps 1-3, we have assumed that the mass of $(\nu^+ + \nu^-)$ is finite.

The third term also converges to zero as $c \to \infty$, since, by the definition of $\rho_*$,

$$\frac{\sigma_c^2}{2} \int_0^\infty \int_0^\infty V(x-y)\bar{\rho}_*(x)\bar{\rho}_*(y) = \frac{\sigma_c^2}{2} \int_0^{2\sqrt{a}} \int_0^{2\sqrt{a}} V(x-y)\bar{\rho}_*(x)\bar{\rho}_*(y)$$

$$\leq 2\sqrt{a}\sigma_c^2 \to 0.$$

To show that the fifth term is small, we use that $g$ has finite integral on the positive real line, which is a consequence of assumption (V2). As $g > 0$, we obtain, by the definition of $\rho_*$,

$$\left| \sigma_c \int_0^\infty g\bar{\rho}_* \right| \leq \frac{\sigma_c}{\sqrt{a}} \int_0^{\infty} g \to 0.$$

The sixth and seventh term tend to zero thanks to the fact that $\nu$ has compact support together with the bound on $h_c$ given in (3.8).

By combining the results above, we can pass to the limit in (3.40) as $c \to \infty$, yielding $F_c(\nu_c) \to F(\nu)$. This concludes the proof of the limsup inequality and of the theorem.

\[ \square \]

4. NUMERICS

In this section we present some numerical results which illustrate the scaling properties of the boundary layer and the degree of fit or misfit between the predictions of the continuum limit energies $E$ and $F$, and the minimisers of the discrete energy $E_n$. The numerical simulations presented in this section are all obtained for the specific choice of the potential given in (1.2).

4.1. Rescaling of the density. The density $\nu$ appearing in the boundary layer energy $E_c$ in (3.6) is defined by blowing up the pile-up domain by a factor $c$. This behaviour is confirmed by the $\Gamma$-convergence result.

We now illustrate some formal calculations and numerical results that suggest a similar scaling for the discrete densities.

In [Hal11] Hall performs some formal asymptotics to obtain a first quantitative estimate on the size of the boundary layer region at the lock in the case $c_n = \sqrt{n}$. These asymptotics suggest that the minimiser $x_n^*$ of the discrete energy $E_n$ (1.1) exhibits a boundary layer of order $1/\sqrt{n}$. In Figure 7 we illustrate his result for different values of $n$, using Newton’s method to solve $\nabla E_n(x) = 0$ to obtain the optimal positions $x_n^*$ of the walls. Since we prefer to plot density rather than position, we define the corresponding optimal discrete density in original variables as

$$\rho_n(x_n^*) := \frac{2/n}{x_n^*+1 - x_n^*-1}, \quad i = 1, \ldots, n-1.$$  \hspace{2cm} (4.1)

We then define the new density $\bar{\rho}_n$ by imposing the following rescaling of the spatial coordinates,

$$\bar{\rho}_n(x) := \rho_n(x/c_n), \quad x \in \{c_n x_n^*: i = 1, \ldots, n-1\}.$$  \hspace{2cm} (4.2)
Figure 7 shows the profiles of $\tilde{\rho}_n$ for $c_n = \sqrt{n}$, and different values of $n$.

![Figure 7](image1)

**Figure 7.** Rescaled densities $\tilde{\rho}_n$ (4.2) close to the lock, for $c_n = \sqrt{n}$ and for different values of $n$.

The rescaled densities agree well at the left-end of the domain, even for a relatively small number of particles. This suggests that there is a fixed curve (independent of the choice of $n$) describing the boundary layer profile at the lock, and that $1/\sqrt{n}$ is indeed the right spatial scaling.

Note however that the slopes of the densities at the right-end of the domain seem to be different. This is due to the fact that, although the unscaled densities $\rho_n$ are close to the same bulk profile $\rho_*$ away from the boundary layer region, the rescaled densities are close to the rescaled (and now $n$- and $c_n$-dependent) profile $\tilde{\rho}_n(x) = \rho_*(x/c_n)$.

For this reason it is more instructive to compare the densities $\nu_n := \tilde{\rho}_n - \rho_*$, which we do in Figure 8. The good agreement between the profiles of $\nu_n$ for different values of $n$ and different scaling of $c_n$ (conform $1 \ll c_n \ll n$) suggest that also in the discrete case the density must be rescaled as in (4.2).

4.2. **Rescaling of the energy.** From the analysis in this paper one could try to infer that also for the discrete energies $E_n$ in (1.1) the right scaling to analyse the boundary layer at the lock is
1/c_n, namely that |E_n(x^n) - E_n(p_n^*)| \propto 1/c_n. Here, p_n^* are the discrete dislocation wall positions generated by \rho_n, i.e.

\[ \rho_n^* = \frac{1}{n} \sum_{i=1}^{n} \delta y_i^n, \quad \text{where} \quad y_i^n := 2\sqrt{a} \left(1 - \sqrt{1 - \frac{i}{n}}\right) \text{ solves } \int_0^{y_i^n} \rho_\star = \frac{i}{n}. \]

We investigate this question by means of numerical computations, for c_n being a power of n. Setting \( \alpha_n := \frac{|E_n(x^n) - E_n(p_n^*)|}{c_n^n} \), and assuming a power-law relation also for \( \alpha_n \), namely \( \alpha_n \propto n^{-p} \), we try to determine \( p \) by computing

\[ p_n := \frac{\log \alpha_n - \log \alpha_{2n}}{\log 2}, \quad \text{for } n = 2^3, 2^4, \ldots, 2^{11}, \quad (4.3) \]

for different expressions of \( c_n \). The results are shown in Table 1. The data in the first two columns support our conjecture that \( p_n \approx \log n c_n \) for sufficiently large \( n \), although the third column seems to contradict it. This disagreement could be due to a much slower convergence to the correct value, or to the presence of a second boundary layer at the free end of the pile-up (see Figure 5), whose energy contribution interferes with the contribution of the boundary layer at the lock. At this stage we can only guess as to the reasons for this discrepancy, and we will return to this issue in a future publication.

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Table 1. Exponents \( p \) in (4.3) for a power law fit of \( |E_n(x^n) - E_n(p_n^*)| \propto n^{-p} \), for different values of \( n \) and \( c_n = n^{1/4}, n^{1/2}, n^{3/4} \). The lower-right value is missing because of memory limitations in Matlab.

4.3. Minimiser of the continuum energy \( F \). In this section we analyse the minimiser of \( F \), namely we consider the minimisation problem:

\[ \min_{\nu \in \mathcal{A}} F(\nu), \]

where \( F \) and \( \mathcal{A} \) are defined in (3.13) and (3.14). We assume in addition that the minimiser \( \nu_\star \) satisfies the strict inequality\(^4\) \( \inf \nu_\star > -\rho_\star(0) \), and derive a first-order necessary condition for minimality for \( \nu_\star \). We consider variations \( \nu_\star + t\mu \in \mathcal{A} \) for \( \mu \in \mathcal{M}(0,\infty) \) with bounded support and bounded Lebesgue density, and \( |t| \) sufficiently small. Then

\[ 0 = \frac{d}{dt} F(\nu_\star + t\mu)|_{t=0} = \int_0^\infty (V \ast \nu_\star)\mu - \int_0^\infty g\mu, \]

and since \( \mu \) is arbitrary, this implies that

\[ V \ast \nu_\star = g = \frac{1}{\sqrt{a}} V \ast \chi_{(-\infty,0]} \quad \text{a.e. on } (0,\infty). \quad (4.4) \]

\(^4\)Note that the numerically calculated minimisers (Figure 5) are consistent with this assumption.
To approximate the solution $\nu_*$ to (4.4) numerically, we follow the method in Section 10.5 of [Hea01]. We approximate $\nu_*$ by a step function of the form

$$\nu_* \approx \sum_{i=1}^{N} \lambda_i \chi_{I_i},$$

(4.5)

where $\lambda_i$ are the unknowns, while $N$ and the sets $I_i$ are chosen beforehand. Figure 8 suggests to take small intervals $I_i = (a_i, a_i + 1)$ close to 0, and larger intervals in the region $x > 1$. We choose the intervals $I_i$ so that $|I_i| = Cb^i$, and then tune $C$, $b$ and $N$ such that $a_1 = 3 \cdot 10^{-5}$, $200 \in I_N$, and the interval $I_j$ containing the element 1 has length $|I_j| = 0.1$. This results in $C = 2.727 \cdot 10^{-5}$, $b = 1.1$, and $N = 141$.

After having fixed $a_i$ and $N$, we substitute the approximation (4.5) in the Euler-Lagrange equation (4.4), and we solve for $\lambda_i$ the linear system

$$\sum_{i=1}^{N} \lambda_i (V * \chi_{I_i})(y_j) = \frac{1}{\sqrt{a}} (V * \chi_{(-\infty,0)})(y_j) \quad \text{for } y_j = \frac{a_j - a_j - 1}{2}, \quad j = 1, \ldots, N.$$  

(4.6)

This amounts to an asymmetric Galerkin (collocation) approximation, in which the solution space is approximated by piecewise constant functions, and the test space by sums of delta functions supported on the midpoint of each interval.

Note that we can identify $(V * \chi_{I_i})(y_j) = \int_{x_j-a_i}^{x_j-a_i+1} V$, and that we have explicitly

$$\int_{y}^{\infty} V = \text{Li}_2(e^{-2y}) - y \ln(1-e^{-2y}),$$

where $\text{Li}_2$ is the polylogarithm,

$$\text{Li}_2(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^2}.$$  

The solution to the linear system (4.6) results in the profile of $\nu_*$ (4.5) as depicted in Figure 9.

![Figure 9](image_url)

**Figure 9.** Numerical approximation of $\nu_*$ (4.5). The intervals $I_i$ are depicted on the $x$-axis. The circles indicate the coordinates $(y_i, \nu_*(y_i))$.

In Figure 10 we compare $\nu_*$ to the discrete density $\nu_n = \bar{\rho}_n - \hat{\rho}_n$ constructed from the minimiser $\rho_n$ of $E_n$. In order to make the figure cleaner, instead of plotting the (mathematically correct) piecewise-constant version of Figure 9, we plot the affine interpolation of the coordinates $(y_i, \nu_*(y_i))$. The figure shows a very good agreement between $\nu_n$ and $\nu_*$ in the boundary-layer region. As we have seen from Figure 8, the profile of $\nu_n$ depends neither on $n$ nor on the scaling of $c_n$. Therefore, together with Figure 10, we conclude that $\nu_*$ is the boundary layer profile of the dislocation density at the lock $x = 0$. 
Figure 10. Comparison between the discrete density $\nu_n$ for $n = 2^{12}$ and $c_n = \sqrt{n}$ and the minimiser $\nu_*$ of $F$. Only the interval $(0, 1)$ is shown, which corresponds to the region $(0, 1/c_n)$ for the unscaled densities.

On the other hand, the agreement between $\nu_n$ and $\nu_*$ is not very good outside of the boundary layer region, as shown in Figure 5, where we plot the densities on $(1, 2c_n\sqrt{a})$ on a logarithmic scale (remember that $(0, 2c_n\sqrt{a})$ is the whole of the pile-up domain, after blowing up the variables by $c_n$). In Section 3 we proved that $F_c$ $\Gamma$-converges to $F$ with respect to vague convergence, hence minimisers of the energies $F_c$ converge to $\nu_*$, minimiser of the limit energy $F$, only on bounded domains. It is therefore not surprising that the densities $\nu_n$, the discrete analogue of the minimiser of $F_c$, do not agree with $\nu_*$ on the whole pile-up domain, which is of order $c_n$ in the blown-up variables, and hence growing in size with $n$.

From Figure 5 we can actually infer that there is another ‘continuous’ boundary layer at the right-end of the pile-up domain, since there is a large number of particles deviating from the bulk distribution $\tilde{\rho}_*$ (i.e. with density $\nu_n$ deviating from 0). We expect the profile of this boundary layer to resemble the bulk behaviour of the optimal discrete density of the energy (1.1) for $c_n = n$.

We refer to [GPPS13, Theorem 8] and to Figure 6 in the same paper for the analysis of that case. The analysis of the boundary layer at the free end of the pile-up region is however beyond the scope of this paper.

Finally, as noted in the introduction, $\nu_n$ (or $\nu_*$) curiously attains small negative values before matching the line $y = 0$. As this ‘dip’ is present in the numerical approximations of both $\nu_n$ and $\nu_*$, it does not appear to be a numerical artefact. We remain with questions regarding how this ‘dip’ relates to the choice of $V$. Does every convex decreasing $V$ with finite first moment have such a ‘dip’? Are there choices of $V$ for which $\nu_*$ is decreasing? Does $V$ have more than one ‘dip’ (the numerical solutions for $\nu_n$ and $\nu_*$ are too coarse to give a speculative answer), and how does the answer depend on the choice of $V$? The answers to these questions are beyond the scope of this paper.

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References


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