A QUANTITATIVE DESCRIPTION OF MESH DEPENDENCE FOR THE DISCRETIZATION OF SINGULARLY PERTURBED NON-CONVEX PROBLEMS

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Abstract. We investigate the limiting description for a finite-difference approximation of a singularly perturbed Allen-Cahn type energy functional. The key issue is to understand the interaction between two small length-scales: the interfacial thickness ε and the mesh size of spatial discretization δ. Depending on their relative sizes, we obtain results in the framework of Γ-convergence for the (i) sub-critical ($\varepsilon \gg \delta$), (ii) critical ($\varepsilon \sim \delta$), and (iii) super-critical ($\varepsilon \ll \delta$) cases. The first case leads to the same area functional just like the spatially continuous case while the third gives the same result as that coming from a ferromagnetic spin energy. The critical case can be regarded as an interpolation between the two.

Key words. spatial discretization, singularly perturbed problems, non-convex functionals, Allen-Cahn functional

AMS subject classifications. 35B25, 49M25, 65K10

1. Introduction.

In this paper we describe the effect of discretization by finite differences on singularly perturbed non-convex variational problems by examining the prototypical case of an Allen-Cahn energy

$$F_\varepsilon(u) = \int_\Omega \left(W(u) + \varepsilon^2|\nabla u|^2\right) dx, \tag{1.1}$$

where $\Omega \subset \mathbb{R}^n$ and W is a double-well energy density with wells in ± 1; e.g., $W(u) = (u^2-1)^2$. Except for the trivial constant functions $u \equiv \pm 1$ (which can be excluded by an integral constraint), a function u_ε that attains very small energy value F_ε (in the sense that $F_\varepsilon(u_\varepsilon) = O(\varepsilon)$) typically partitions the domain Ω into sub-domains on which u_ε takes on the values close to 1 or -1 and make a rapid transition between the sub-domains (see Fig. 1.1).

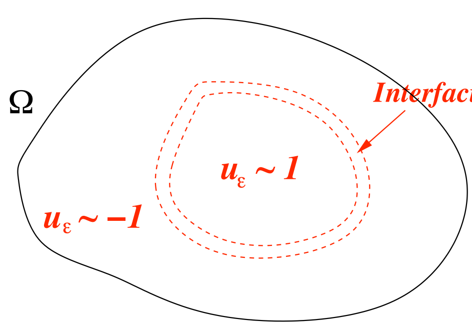

FIG. 1.1. *Partitioning of Ω into sub-regions with $u_\varepsilon \approx 1$ and $u_\varepsilon \approx -1$*

The energy then concentrates on the transition region which is often called the *interfacial region*. Such a description can be made rigorous using the theory of Γ-

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convergence of the functionals F_ε. By now it is well known that as $\varepsilon \to 0$ the functionals F_ε behave as a *sharp-interface phase-transition energy*, finite only on functions taking the values in $\{\pm 1\}$ and which can be written as an interfacial energy (see, e.g., [35, 33, 37]) in the form

$$\varepsilon\, C_W\, \mathcal{H}^{n-1}(\Omega \cap \partial\{u = 1\}), \tag{1.2}$$

where C_W is a constant determined by W and the boundary of $\{u = 1\}$ is suitably defined. In the above $\mathcal{H}^{n-1}$ is the Hausdorff $(n-1)$-dimensional measure which coincides with the $(n-1)$-dimensional surface measure if the surface is a smooth manifold.

Dynamical models associated with energy (1.1) also arise in many applications. A typical equation, derived from the negative L^2-gradient flow with respect to (1.1), is the following Allen-Cahn equation [5]:

$$u_t = \epsilon^2 \triangle u - W'(u). \tag{1.3}$$

The $\varepsilon \to 0$ limit of the above equation is also studied in many works. It is shown that the limiting equation is given by the motion of a sharp interface by its mean curvature. See for example [25, 16, 30, 27].

Due to their wide range of applications, it is thus of practical importance to consider numerical schemes associated with (1.1) and (1.3). In this paper, we only consider stationary problems. Some discussion on dynamical problems will be given. We believe the latter problems are important and yet very challenging.

A formal finite-difference discretization of F_ε can be obtained by introducing another small positive parameter δ which represents the mesh size. The following energy defined on functions $u : \Omega \cap \delta\mathbb{Z}^n \to \mathbb{R}$ is a typical example:

$$E_{\varepsilon,\delta}(u) = \sum_i \delta^n W(u_i) + \frac{\varepsilon^2}{2} \sum_{i,j} \delta^n \left| \frac{u_i - u_j}{\delta} \right|^2, \tag{1.4}$$

where the first sum is taken on $i \in \Omega \cap \delta\mathbb{Z}^n$ and the second sum on all nearest neighbours (n.n. for short) $i, j \in \Omega \cap \delta\mathbb{Z}^n$; i.e., those indices such that $|i - j| = \delta$ (each such pair is thus counted twice, which explains the factor $1/2$). The second term is easily shown to be a discretization of $\varepsilon^2 \int_\Omega |\nabla u|^2\, dx$. Heuristically, if the discretization step is much smaller than ε then the energy $E_{\varepsilon,\delta}$ is an approximation of the sharp-interface energy (1.2). This does not happen in the more realistic case when the two scales may interact. We are interested in describing precisely this interaction.

We will first show that (1.4) is approximated by (1.2) for $\delta \ll \varepsilon$. In the case that $\delta \sim K\varepsilon$ then we will show that the $E_{\varepsilon,\delta}$'s are approximately

$$\varepsilon \int_{\Omega \cap \partial\{u=1\}} \varphi_K(\nu)\, d\mathcal{H}^{n-1} \tag{1.5}$$

where φ_K is some anisotropic convex energy density characterized by a discrete optimal profile problem. In the case $\delta \gg \varepsilon$, we have a different scaling of the energies $E_{\varepsilon,\delta}$, which approximate the crystalline interfacial energy

$$4\frac{\varepsilon^2}{\delta} \int_{\Omega \cap \partial\{u=1\}} \|\nu\|_1\, d\mathcal{H}^{n-1}\,. \tag{1.6}$$

Moreover, in this last scaling $E_{\varepsilon,\delta}$ are also approximated by a ferromagnetic spin energy

$$E^{\rm ferro}_{\varepsilon,\delta}(u) = \frac{\varepsilon^2}{2\delta}\sum_{i,j}\delta^{n-1}|u_i-u_j|^2\,, \tag{1.7}$$

defined for $u:\Omega\cap\delta\mathbb{Z}^n\to\{-1,1\}$. Finally, we will show that the function φ_K acts as an interpolation between the euclidean norm $\|\nu\|_2$ and the crystalline norm $4\|\nu\|_1$.

The asymptotic result described in the present paper has some common features with the analysis in the continuum setting the interaction between phase transitions and microscopic oscillations. Examples include the study of energies of the form (see [7, 14, 21]):

$$F_{\varepsilon,\delta}(u) = \int_\Omega\Big(W(u)+\varepsilon^2\,a\Big(\frac{x}{\delta}\Big)|\nabla u|^2\Big)\,dx,\ \text{ or }\ \int_\Omega\Big(W(u,\frac{x}{\delta})+\varepsilon^2|\nabla u|^2\Big)\,dx. \tag{1.8}$$

(See also [3] where Ising systems with Kac potentials are analyzed.) In the above works, a limiting energy functional, in the form of anisotropic sharp interfacial energy is also obtained. In our case the discrete dimension adds a further constraint on the difference quotients, which implies that $\varphi_K = O(1/K)$ as $K\to+\infty$.

The main difficulty of the type of problems above is due to the combined presence of singular perturbation and the spatial heterogeneity (which can also come from the discreteness of the problem). When the two scales interact, there can be lots of *local minimizers*. This phenomenon manifests itself even more profoundly in dynamical problems (see for example, [38, 26]). Even though there are works which extend the theory of Γ-convergence to evolution equations [36], dynamical version of the problems described here remain largely open. The work [17] proves the convergence of the time dependent problem of the finite difference scheme (1.4) to the motion by mean curvature but only in the sub-critical case ($\delta\ll\varepsilon$). On the other hand, the works [19, 31, 23] consider from a homogenization point of view motion by mean curvature in heterogeneous media. A first-order Hamilton-Jacobi equation is derived in the limit. See also Section 3.5 for further discussion.

2. Setting of the problem. Let $W:\mathbb{R}^n\to[0,+\infty)$ be a locally Lipschitz double-well potential with wells at ±1; i.e., W is a non-negative function and $W(u)=0$ if and only if $u=1$ or $u=-1$. Moreover, we suppose that W is coercive; i.e.,

$$\lim_{u\to\pm\infty}W(u)=+\infty,$$

and that W is convex close to ±1; i.e., there exists $C_0>0$ such that $\{u: W(u)\le C_0\}$ consist of two intervals on each of which W is convex. Standard examples include $W(u)=(1-u^2)^2$ or $W(u)=(1-|u|)^2$ (see Fig. 2.1).

Let Ω be a bounded open subset of $\mathbb{R}^n$ with Lipshitz boundary $\partial\Omega$. We will analyze the asymptotic behaviour of $E_{\varepsilon,\delta}$ defined by (1.4) on functions $u:\Omega\cap\delta\mathbb{Z}^n\to\mathbb{R}$ by computing their Γ-developments ([9, Section 1] and [13]; see also [10, 20] for a general introduction to Γ-convergence). For completeness, we will briefly state the necessary definitions at the end of this section. In this process each u is identified with its piecewise-constant interpolation defined by $u(x)=u_i$ on $i+\frac{\delta}{2}(-1,1)^n$ (and equal to 0 elsewhere), so that Γ-limits can be taken in Lebesgue spaces.

Whatever the dependence of δ on ε, the Γ-limit of $E_{\varepsilon,\delta}$ with respect to the weak L^1-convergence can be easily shown to be simply

$$\int_\Omega W^{**}(u)\,dx,$$

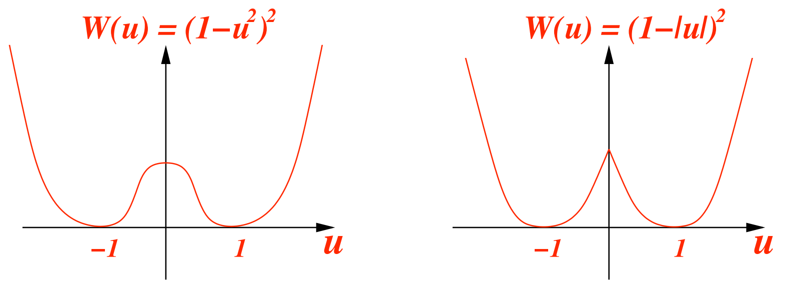

FIG. 2.1. *Examples of double-well potential*

where W^{**} is the convex envelope of W. However, the structure of the interface cannot be described by the above limit. It will only be revealed by the next-order Γ-limit which captures energies at the first relevant scale. This is described by the theorem below. To prepare for its statement and the proof, we denote by Q^ν a fixed n-dimensional cube centered at 0, with side length 1 and one side parallel to ν, $Q^\nu_T = TQ^\nu$ for all $T > 0$, and $Q^\nu_T(x) = x + TQ^\nu$ for all x. The limit energies will be defined on $u \in BV(\Omega; \{\pm 1\})$ (or equivalently on sets of finite perimeter after identifying u with $A = \{u = 1\}$). For such a u, the jump set S_u is defined (corresponding to the reduced boundary of A). Furthermore, on all points of S_u, the measure-theoretical normal ν, pointing inwards to A, is defined (we refer to [8, 29] for precise definitions and details).

THEOREM 2.1. *Let Ω, W and $E_{\varepsilon,\delta}$ be as above, and let $\delta = \delta(\varepsilon)$. We then have the following three regimes for the Γ-limit with respect to the strong L^1-convergence. In all cases the domain of the Γ-limit is $BV(\Omega; \{\pm 1\})$ and is a surface term on the set S_u (which we will called* the interface*).*

(i) (**Subcritical case.**) *If $\delta \ll \varepsilon$ ($\lim_{\varepsilon\to 0} \frac{\delta}{\varepsilon} = 0$), then we have*

$$\Gamma\text{-}\lim_{\varepsilon\to 0} \frac{1}{\varepsilon} E_{\varepsilon,\delta}(u) = C_W\, \mathcal{H}^{n-1}(\Omega \cap S_u), \tag{2.1}$$

where $C_W = 2\int_{-1}^{1} \sqrt{W(s)}\, ds$, as in the continuous case;

(ii) (**Critical case.**) *If $\lim_{\varepsilon\to 0} \frac{\delta}{\varepsilon} = K$ with $0 < K < +\infty$, then*

$$\Gamma\text{-}\lim_{\varepsilon\to 0} \frac{1}{\varepsilon} E_{\varepsilon,\delta}(u) = \int_{\Omega\cap S_u} \varphi_K(\nu)\, d\mathcal{H}^{n-1}, \tag{2.2}$$

where φ_K is given by the asymptotic formula

$$\varphi_K(\nu) = \lim_{N\to+\infty} \frac{1}{N^{n-1}} \inf\Big\{ K \sum_i W(v_i) + \frac{1}{2K} \sum_{i,j} |v_i - v_j|^2 \Big\}, \tag{2.3}$$

where the indices i, j are restricted to the cube Q^ν_N and the infimum is taken on all v that are equal to $u^\nu(x) = \operatorname{sign}\langle x, \nu\rangle$ on a neighbourhood of ∂Q^ν_N. Furthermore, φ_K is continuous in the normal direction ν;

(iii) (**Supercritical case.**) *If $\varepsilon \ll \delta$ $\big(\lim_{\varepsilon\to 0} \frac{\varepsilon}{\delta} = 0\big)$, then we have*

$$\Gamma\text{-}\lim_{\varepsilon\to 0} \frac{\delta}{\varepsilon^2} E_{\varepsilon,\delta}(u) = 4 \int_{\Omega\cap S_u} \|\nu\|_1\, d\mathcal{H}^{n-1}, \tag{2.4}$$

where $\|\nu\|_1 = |\nu_1| + \cdots + |\nu_n|$;

(iv) (**Interpolation**.) *For all* $\nu \in S^{n-1}$ *we have*

$$\lim_{K\to 0}\varphi_K(\nu) = c_W, \qquad \lim_{K\to +\infty} K\varphi_K(\nu) = 4\|\nu\|_1 . \tag{2.5}$$

REMARK 2.2. (1) The existence of the limit in (2.3) and the continuity of φ_K can be proved as in the continuous case (see [7]). Moreover, it is a-posteriori convex (i.e., its one-homogeneous extension is) since it is the integrand of a lower-semicontinuous interfacial energy (see [6]).

(2) In the one-dimensional case formula (2.3) reduces to the computation of an optimal-profile problem

$$C_K = \inf\Big\{K\sum_i W(v_i) + \frac{1}{K}\sum_i |v_i - v_{i-1}|^2 : v(\pm\infty) = \pm 1\Big\} ; \tag{2.6}$$

in particular (taking $v_i \in \pm 1$ as test functions) we have

$$C_K \le \frac{4}{K} . \tag{2.7}$$

(3) It is easily seen that for coordinate directions minimizers for $\varphi_K(e_k)$ are one-dimensional, so that

$$\varphi_K(e_k) = C_K,$$

which gives the estimate

$$\varphi_K(\nu) \le C_K\|\nu\|_1, \tag{2.8}$$

since the right-hand side is the greatest positively one-homogeneous convex function satisfying $\varphi_K(e_k) = C_K$ for all k.

(4) Note that in the super-critical case, the limit interfacial energy is *degenerate, or not uniformly convex*. This is understandable as in this case the nonlinear term $W(u)$ dominates so that the energy concentrates on the spin functions v which takes on only values of 1 or -1. In this case, the energy is equivalent to bond-counting: the number of bonds between 1 and -1. It is likely that φ_K be uniformly convex for $0 < K < \infty$ even though this is not immediately clear from its definition.

(5) For simplicity, in this paper we do not impose any boundary conditions for the function space. Such effects can be considered. However, boundary layer might arise. In addition, the scaling associated with the boundary conditions might be different from that in the bulk. Hence care must be taken. See for example [34, 2] for some works in the continuum case which do consider boundary energy terms.

Further remarks and extensions will be given at the end of this paper. Before the proof, we briefly outline the definition and procedure of proving Γ-convergence. Given a sequence of functionals $f_\varepsilon : X_\varepsilon \longrightarrow \mathbb{R}$. It is said to Γ-converge to $f_0 : X_0 \longrightarrow \mathbb{R}$ if the following two steps are true:

lower bound: for every $x \in X_0$ and sequence $\{x_\varepsilon \in X_\varepsilon\}_{\varepsilon>0}$ such that $x_\varepsilon \longrightarrow x_0$, then

$$\liminf_{\varepsilon\to 0} f_\varepsilon(x_e) \ge f_0(x); \tag{2.9}$$

upper bound: given any $x_0 \in X_0$, one can find a sequence $\bar{x}_\varepsilon \in X_\varepsilon$ such that

$$f_0(x_0) \geq \limsup_{\varepsilon \to 0} f_\varepsilon(\bar{x}_e). \tag{2.10}$$

The fundamental property of Γ-convergence is that if the collection of functionals $\{f_\varepsilon\}$ is *equi-coercive* (every sequence with equibounded energy has a convergent subsequence), then minimizers of f_ε will have a subsequence that converges to a minimizer of f_0.

In the application of this paper, the X_ε's and X_0 will be taken to be subspaces of L^1. We are most interested in the subspace $BV(\Omega; \{\pm 1\})$ of all functions with bounded variations which take values in $\{\pm 1\}$ which can also be identified with *sets of finite perimeter*. We will use in particular the well-known result by Modica and Mortola (see [35]) that

$$\Gamma\text{-}\limsup_{\varepsilon \to 0} \frac{1}{\varepsilon} F_\varepsilon(u) = C_W \mathcal{H}^{n-1}(\Omega \cap S_u) \tag{2.11}$$

with domain $u \in BV(\Omega; \{\pm 1\})$. In this case the sequence of energies is equi-coercive in $L^1(\Omega)$.

Beside the Γ-limit defined above, it is useful to introduce the Γ-lower and upper limits respectively as

$$f'(x) := \Gamma\text{-}\liminf_{\varepsilon \to 0} f_\varepsilon(x) = \inf\{\liminf_{\varepsilon \to 0} f_\varepsilon(x_\varepsilon) : x_\varepsilon \to x\}, \tag{2.12}$$

$$f''(x) := \Gamma\text{-}\limsup_{\varepsilon \to 0} f_\varepsilon(x) = \inf\{\limsup_{\varepsilon \to 0} f_\varepsilon(x_\varepsilon) : x_\varepsilon \to x\}\,, \tag{2.13}$$

which are always defined at all x. The desired lower bound then translates into $f'(x) \geq f_0(x)$ and the upper bound into $f''(x) \leq f_0(x)$.

The Γ-lower and upper limits are lower-semicontinuous function ([9, Proposition 1.28]). This is useful in the computation of the lower inequality, since it allows us to restrict to classes of lower-semicontinuous f_0, which in the present paper will be surface energies with a convex integrand of the normal. Moreover, it allows also to restrict the verification of the upper bound to a dense class of x (see [9, Remark 1.29]), which, in our case will be (functions identified with) polyhedral sets.

3. Proof of the result. In the two extreme cases (i) and (iii) the proof will be achieved by a "separation of scales" argument. First, a lower bound is obtained by comparing the energies with the functionals that are formally obtained by letting, respectively, $\delta \to 0$ with $\varepsilon > 0$ fixed and $\varepsilon \to 0$ with $\delta > 0$ fixed. Second, the bounds will be proved to be sharp by using suitable approximate (or recovering) sequences. In the intermediate case, a new surface energy defined directly by a family of scaled discrete problems has to be constructed.

As is customary, the letter C will denote a strictly positive constant, whose value may vary at each of its appearance.

3.1. Subcritical Case ($\delta \ll \varepsilon$). We will first show that given $\{u_i^\varepsilon\}$ with $\sup_\varepsilon \frac{1}{\varepsilon} E_{\varepsilon,\delta}(u_\varepsilon) \leq C < +\infty$, we can construct continuous functions v_ε such that $\|u_\varepsilon - u_\varepsilon\|_{L^1} = o(1)$ and

$$\liminf_{\varepsilon} \frac{1}{\varepsilon} E_{\varepsilon,\delta}(u_\varepsilon) \geq \liminf_{\varepsilon} \frac{1}{\varepsilon} F_\varepsilon(v_\varepsilon).$$

By the equicoerciveness of $\frac{1}{\varepsilon}F_\varepsilon$, this implies that we may suppose up to subsequences that $v_\varepsilon \to u$ and hence $u_\varepsilon \to u$ in $L^1(\Omega)$.

If $u_\varepsilon \to u$ then from the inequality above and (2.11) we have

$$\liminf_\varepsilon \frac{1}{\varepsilon} E_{\varepsilon,\delta}(u_\varepsilon) \geq \liminf_\varepsilon \frac{1}{\varepsilon} F_\varepsilon(v_\varepsilon) \geq C_W\, \mathcal{H}^{n-1}(\Omega \cap S_u);$$

i.e., the **lower bound** (2.9) for $\frac{1}{\varepsilon}E_{\varepsilon,\delta}$.

To start the proof, upon a truncation argument, we can first suppose that $\|u_\varepsilon\|_\infty \leq 1$. Next we consider the continuous functions v_ε mentioned above to be the piecewise-affine interpolations on a triangularization of u_ε. Then we have,

$$\frac{1}{2}\sum_{i,j} \delta^n \Big|\frac{u_i^\varepsilon - u_j^\varepsilon}{\delta}\Big|^2 = \int_\Omega |\nabla v_\varepsilon|^2\, dx + o(1). \tag{3.1}$$

Next we have to estimate the first sum in $E_{\varepsilon,\delta}(u_\varepsilon)$ in terms of $\int_\Omega W(v_\varepsilon)\, dx$. We will consider the various cases whether u_i^ε together with the values of its nearest neighbours fall into the same convexity region of $W(\cdot)$ or not.

The first and simple scenario is that when for all the neighbours j of i, the values u_i and u_j lie in the same interval of convexity of W as in this case we have by Jensen's inequality,

$$\int_{T^\delta} W(v_\varepsilon)\, dx \leq \frac{1}{n+1}|T^\delta| \sum_{k\in \mathrm{Vertices}(T^\delta)} W(u_k^\varepsilon), \tag{3.2}$$

for each simplex T^δ of the triangulation with vertices on $\delta\mathbb{Z}^n$, where v_ε is a convex combination of the value u_k^ε at the vertices of T^δ and one of the vertices is i as above.

To continue, let C_0 be a fixed number such that $\{z : W(z) < C_0\}$ consists of two intervals. Denote by J_ε^1 the set of indices i such that $W(u_i^\varepsilon) < C_0/2$ and the value u_j^ε of each its nearest neighbour j is in the same interval of $\{z : W(z) < C_0\}$ as u_i^ε, and denote by J_ε^2 the complement of J_ε^1 in $\{i : W(u_i^\varepsilon) < C_0/2\}$. If the simplex T^δ as above is such that one of its vertices is in J_ε^1, then (3.2) holds by the observation above. As for the simplexes with one vertex in J_ε^2, note that

$$C \geq \sum_{i\in J_\varepsilon^2} \delta^n \varepsilon \Big|\frac{u_i^\varepsilon - u_j^\varepsilon}{\delta}\Big|^2 \geq C' \frac{\varepsilon}{\delta}\delta^{n-1}\#(J_\varepsilon^2)$$

so that

$$\#(J_\varepsilon^2) = o\Big(\frac{1}{\delta^{n-1}}\Big).$$

As a consequence, if we sum over all such simplexes and simply take into account that W is bounded on $[-1,1]$ we have

$$\frac{1}{\varepsilon}\sum_{T^\delta\in J_\varepsilon^2} \int_{T^\delta} W(v_\varepsilon)\, dx \leq C\frac{\delta^n}{\varepsilon}\#(J_\varepsilon^2) = o\Big(\frac{\delta}{\varepsilon}\Big). \tag{3.3}$$

In the above and the following, we will make use of the abused notation that $T_\varepsilon \in J_\varepsilon^2$ if any of the vertices of T_e belongs to J_ε^2. It applies to other set of indices also.

We now take into account simplexes for which the functions u_ε may take values outside the convexity domain of W. To this end, with fixed $M>0$, denote by I^1_ε and I^2_ε the sets of indices

$$I^1_\varepsilon=\Big\{i: W(u^\varepsilon_i)>C_0/2, \qquad \Big|\frac{u^\varepsilon_i-u^\varepsilon_j}{\delta}\Big|^2\le\frac{M}{\varepsilon}\text{ for all n.n.}j\Big\}$$
$$I^2_\varepsilon=\Big\{i: W(u^\varepsilon_i)>C_0/2, \qquad \Big|\frac{u^\varepsilon_i-u^\varepsilon_j}{\delta}\Big|^2>\frac{M}{\varepsilon}\text{ for some n.n.}j\Big\}.$$

Since

$$\frac{\delta^n}{\varepsilon}\#(I^1_\varepsilon\cup I^2_\varepsilon)\frac{C_0}{2}\le\frac{1}{\varepsilon}\sum_i\delta^n W(u^\varepsilon_i)\le C$$

and

$$\frac{\delta^n}{\varepsilon}\#(I^2_\varepsilon)\Big(\frac{C_0}{2}+\frac{1}{4}M^2\Big)\le\frac{1}{\varepsilon}\sum_i\delta^n W(u^\varepsilon_i)+\frac{\varepsilon}{4}\sum_{i,j}\delta^n\Big|\frac{u^\varepsilon_i-u^\varepsilon_j}{\delta}\Big|^2\le C$$

then we have

$$\#(I^1_\varepsilon\cup I^2_\varepsilon)\le C\frac{\varepsilon}{\delta^n}, \qquad \#(I^2_\varepsilon)\le\frac{C}{(1+M^2)}\frac{\varepsilon}{\delta^n}\,. \tag{3.4}$$

Let T^δ be a simplex as above, and suppose that one of its vertices i is in I^1_ε; then by the Lipschitz continuity of W for all vertices k of T^δ we have

$$\Big|\int_{T^\delta}W(v_\varepsilon)\,dx-|T^\delta|W(u^\varepsilon_k)\Big|\le\frac{1}{\varepsilon}C\delta^n\sup_{i,j}|u^\varepsilon_j-u^\varepsilon_i|\le C\frac{\delta^{n+1}}{\varepsilon}M,$$

so that

$$\Big|\int_{T^\delta}W(v_\varepsilon)\,dx-\frac{1}{n+1}|T^\delta|\sum_k W(u^\varepsilon_k)\Big|\le C\delta^n\sup_{i,j}|u^\varepsilon_j-u^\varepsilon_i|\le C\frac{\delta^{n+1}}{\varepsilon}M.$$

Summing over such T^δ and taking into account (3.4) we have

$$\Big|\frac{1}{\varepsilon}\sum\int_{T^\delta}W(v_\varepsilon)\,dx-\frac{1}{\varepsilon}\frac{1}{n+1}|T^\delta|\sum\sum_k W(u^\varepsilon_k)\Big|\le\#(I^1_\varepsilon)C\frac{\delta^{n+1}}{\varepsilon^2}M=o(1). \tag{3.5}$$

Next, if we sum over all simplexes with one vertex in I^2_ε, and again simply take into account that W is bounded on $[-1,1]$, by (3.4) we have

$$\frac{1}{\varepsilon}\sum\int_{T^\delta}W(v_\varepsilon)\,dx\le C\frac{\delta^n}{\varepsilon}\#(I^2_\varepsilon)\le\frac{C}{1+M^2}\,. \tag{3.6}$$

Taking into account the estimates in (3.2), (3.3), (3.5) and (3.6) we then obtain

$$\begin{aligned}\frac{1}{\varepsilon}\int_\Omega W(v_\varepsilon)\,dx&\le\frac{1}{\varepsilon}\sum_{T^\delta}\sum_k\frac{|T^\delta|}{n+1}W(u^\varepsilon_k)+o(1)+\frac{C}{1+M^2}\\&=\frac{1}{\varepsilon}\sum_i\delta^n W(u^\varepsilon_i)+o(1)+\frac{C}{1+M^2}.\end{aligned} \tag{3.7}$$

Finally, by (3.1), (3.7) and the arbitrariness of $M > 0$ we have

$$\begin{aligned}\liminf_{\varepsilon\to0}\frac{1}{\varepsilon}E_{\varepsilon,\delta}(u_\varepsilon) &\geq \liminf_{\varepsilon\to0}\int_\Omega\Big(\frac{1}{\varepsilon}W(v_\varepsilon)+\varepsilon|\nabla v_\varepsilon|^2\Big)dx\\ &= \liminf_{\varepsilon\to0}\frac{1}{\varepsilon}F_\varepsilon(v_\varepsilon)\,. \end{aligned}\tag{3.8}$$

As remarked at the beginning of the section, from this inequality we deduce the equicoerciveness of the sequence $\frac{1}{\varepsilon}E_{\varepsilon,\delta}$ with respect to the strong L^1-convergence since the functionals $\frac{1}{\varepsilon}F_\varepsilon$ are equicoercive and the construction above implies that $\|u_\varepsilon - v_\varepsilon\|_1 = o(1)$ as $\varepsilon\to 0$, as well as the desided lower bound.

The **upper bound** (2.10) is obtained by an explicit construction. It is sufficient to show that it holds for S_u a planar interface, since the generalization to a general interface is achieved by the same approximation using polyhedral interfaces as in the continuum case (see for example [1, Section 3.9]). We can also suppose that $\mathcal{H}^{n-1}(S_u\cap\partial\Omega)=0$.

Now consider $u(x) = \mathrm{sign}\langle x,\nu\rangle$. Let v be a minimizer for the optimal profile problem giving C_W; i.e., $v(\pm\infty)=\pm1$ and

$$\int_{-\infty}^{+\infty}\Big(W(v)+|v'|^2\Big)\,dt = C_W\,.$$

The recovery sequence (u_ε) is then defined by

$$u_i^\varepsilon = v\Big(\frac{1}{\varepsilon}\langle i,\nu\rangle\Big)\qquad i\in\delta\mathbb{Z}^n;$$

i.e., it is the discretization of $v(\langle x,\nu\rangle/\varepsilon)$ on the lattice $\delta\mathbb{Z}^n$.

After noting that, if $i-j=\delta e_k$,

$$\frac{u_i^\varepsilon-u_j^\varepsilon}{\delta} = \frac{\nu_k}{\varepsilon}\;v'\Big(\frac{1}{\varepsilon}\langle i,\nu\rangle\Big)(1+o(1))\Big)$$

we have for fixed i

$$\begin{aligned}\frac{\varepsilon}{2}\sum_{k=1}^n\delta^n\Big|\frac{u_i-u_{i\pm\delta e_k}}{\delta}\Big|^2 &= \delta^n\sum_{k=1}^n\nu_k^2\Big|v'\Big(\frac{1}{\varepsilon}\langle i,\nu\rangle\Big)(1+o(1))\Big|^2\\ &= \delta^n\Big|v'\Big(\frac{1}{\varepsilon}\langle i,\nu\rangle\Big)\Big|^2(1+o(1)),\end{aligned}$$

so that

$$\begin{aligned}\frac{1}{\varepsilon}E_{\varepsilon,\delta}(u_\varepsilon) &= \sum_i\delta^n\Big(\frac{1}{\varepsilon}W\Big(v\Big(\frac{1}{\varepsilon}\langle i,\nu\rangle\Big)\Big)+\frac{1}{\varepsilon}\Big|v'\Big(\frac{1}{\varepsilon}\langle i,\nu\rangle\Big)\Big|^2\Big)(1+o(1))\\ &= C_W\mathcal{H}^{n-1}(S_u\cap\Omega)+o(1).\end{aligned}$$

3.2. Critical case ($0<\lim_{\varepsilon\to0}\frac{\delta}{\varepsilon}=K<\infty$). In this case, the proof of the equicoerciveness can be achieved through reduction to the one-dimensional case by a sectional compactness criterion [1, Section 3.7]. In dimension one, the proof is standard and can be obtained following [9, Section 6.2] by replacing integrals with sums. This procedure also shows that the limit is in $BV(\Omega;\{\pm1\})$.

The proof of the lower bound can be achieved by a blow-up procedure as follows. Let $\sup_\varepsilon \frac{1}{\varepsilon} E_{\varepsilon,\delta}(u_\varepsilon) < +\infty$ and $u_\varepsilon \to u$. By equicoercivity (as mentioned above) $u \in BV(\Omega;\{\pm 1\})$. For each $\varepsilon > 0$ we consider the measures

$$\mu_\varepsilon = \sum_i \delta^n \Big(\frac{1}{\varepsilon} W(u_i^\varepsilon) + \frac{\varepsilon}{2}\sum_{k=1}^n \Big|\frac{u_i^\varepsilon - u_{i+\delta e_k}^\varepsilon}{\delta}\Big|^2\Big)\mathbf{1}_{\delta i}$$

(to avoid confusing notation $\mathbf{1}_x$ denotes the Dirac delta in x), where the sum is performed on all $i \in \Omega \cap \delta\mathbb{Z}^n$ such that $i + \delta e_k \in \Omega \cap \delta\mathbb{Z}^n$ for all $k = 1, \dots, n$.

Note that $\frac{1}{\varepsilon} E_{\varepsilon,\delta}(u_\varepsilon) \geq \mu_\varepsilon(\Omega)$ so that the family of measures μ_ε is equibounded. Hence, up to further subsequences we can assume that μ_ε converges weak-$*$ to a finite measure μ. To continue, we will estimate μ on S_u. For this, we will use a covering argument for almost all S_u with cubes as follows:

With fixed $h \in \mathbb{N}$, we consider the collection $\mathcal{Q}_h$ of cubes $Q_\rho^\nu(x)$ such that the following conditions are satisfied:

(a) $x \in S_u$ and $\nu = \nu(x)$ is the normal to S_u at x;

(b) $\Big|(Q_\rho^\nu(x) \cap \{u = 1\}) \,\triangle\, \Pi^\nu(x)\Big| \leq \dfrac{1}{h}\rho^n$, where

$$\Pi^\nu(x) = \{y \in \mathbb{R}^n : \langle y - x, \nu\rangle \geq 0\};$$

(c) $\Big|\dfrac{\mu(Q_\rho^\nu(x))}{\rho^{n-1}} - \dfrac{d\mu}{d\mathcal{H}^{n-1} \llcorner S_u}(x)\Big| \leq \dfrac{1}{h}$;

(d) $\Big|\dfrac{1}{\rho^{n-1}}\displaystyle\int_{Q_\rho^\nu(x)\cap S_u} \varphi_K(\nu(y))d\mathcal{H}^{n-1}(y) - \varphi_K(\nu(x))\Big| \leq \dfrac{1}{h}$

(e) $\mu(Q_\rho^\nu(x)) = \mu(\overline{Q_\rho^\nu(x)})$.

(The notation in (a)–(e) is pictured in Fig. 3.1.)

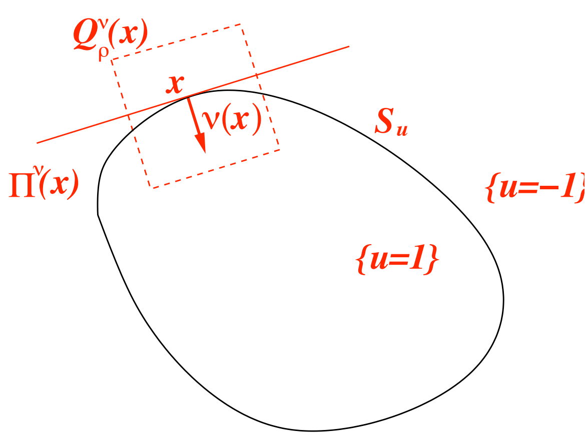

FIG. 3.1. *Description of notations (a)–(e) in the blow-up procedure.*

Note that for fixed $x \in S_u$ and for ρ small enough, (b) is satisfied by the definition of S_u since its blow-up set is a hyperplane. (c) follows from the Besicovitch Derivation Theorem provided that

$$\frac{d\mu}{d\mathcal{H}^{n-1} \llcorner S_u}(x) < +\infty;$$

(d) holds by the same reason, and (e) is satisfied for almost all $\rho > 0$ since μ is a finite measure and hence $\mu(\partial Q^\nu_\rho(x)) = 0$ except for at most countably many ρ's. We deduce that $\mathcal{Q}_h$ is a fine covering of the set

$$S^\mu_u = \Big\{ x \in S_u : \frac{d\mu}{d\mathcal{H}^{n-1} \llcorner S_u}(x) < +\infty \Big\}.$$

By Morse lemma [28, Theorem 1.147], we can extract a countable family of disjoint closed cubes $\{\overline{Q^{\nu_j}_{\rho_j}(x_j)}\}$ still covering S^μ_u. Note that we have

$$\mathcal{H}^{n-1}(S_u \setminus S^\mu_u) = 0$$

since $\mu(S_u) < +\infty$.

We now fix an $x \in S^\mu_u$. For simplicity, it is assumed to be 0. In addition, let $Q^\nu_\rho = Q^\nu_\rho(0)$ the a cube satisfying (b)–(e) above. Then for ε small enough we have

$$\int_{Q^\nu_\rho} |u_\varepsilon - u^\nu| \, dy \le \frac{4}{h} \rho^n \tag{3.9}$$

by (b) above, where $u^\nu(x) = \operatorname{sign}\langle x, \nu\rangle$. Note that in this regime we have

$$\frac{1}{\varepsilon} E_{\varepsilon,\delta}(u^\nu) \le \frac{C}{K} \, \mathcal{H}^{n-1}(\Omega \cap \partial \Pi^\nu) + o(1) \tag{3.10}$$

(with a slight abuse of notation we identify u^ν with its restriction to $\delta\mathbb{Z}^n$) and that the same estimate holds locally. By (3.9) and (3.10), it is not restrictive to suppose that $u_\varepsilon = u^\nu$ near the boundary of Q^ν_ρ. This can be done by using a well-chosen cut-off function close to ∂Q^ν_ρ. This procedure will introduce only an error in the energy functional of order $O(1/h)\rho^{n-1}$. (This is a 'classical' argument in Γ-convergence dating back to De Giorgi (see [24]). For its formalization in a discrete-to-continuous setting we refer e.g. to [12]).

We then have

$$\begin{aligned}
&\liminf_{\varepsilon\to0} \frac{\mu_\varepsilon(Q^\nu_\rho(x))}{\rho^{n-1}} \\
&= \liminf_{\varepsilon\to0} \frac{1}{\rho^{n-1}} \Bigg(\sum_{i \in \delta\mathbb{Z}^n \cap Q^\nu_\rho} \delta^n \Big(\frac{1}{\varepsilon} W(u^\varepsilon_i) + \frac{\varepsilon}{2} \sum_{k=1}^n \delta^n \Big| \frac{u^\varepsilon_i - u^\varepsilon_{i+\delta e_k}}{\delta} \Big|^2 \Big) \Bigg) + O\Big(\frac{1}{h}\Big) \\
&= \liminf_{\varepsilon\to0} \Big(\frac{\delta}{\rho}\Big)^{n-1} \Bigg(\sum_{i \in \delta\mathbb{Z}^n \cap Q^\nu_\rho} \Big(\frac{\delta}{\varepsilon} W(u^\varepsilon_i) + \frac{\varepsilon}{2\delta} \sum_{k=1}^n |u^\varepsilon_i - u^\varepsilon_{i+\delta e_k}|^2 \Big) \Bigg) + O\Big(\frac{1}{h}\Big) \\
&= \liminf_{\varepsilon\to0} \frac{1}{N_\varepsilon^{n-1}} \Bigg(\sum_{i \in \mathbb{Z}^n \cap Q^\nu_{N_\varepsilon}} \Big(K_\varepsilon \, W(w^\varepsilon_i) + \frac{1}{2K_\varepsilon} \sum_{i,j \in \mathbb{Z}^n \cap Q^\nu_{N_\varepsilon}} |w^\varepsilon_i - w^\varepsilon_j|^2 \Big) \Bigg) + O\Big(\frac{1}{h}\Big) \\
&= \liminf_{\varepsilon\to0} \frac{1}{N_\varepsilon^{n-1}} \Bigg(\sum_{i \in \mathbb{Z}^n \cap Q^\nu_{N_\varepsilon}} \Big(K \, W(w^\varepsilon_i) + \frac{1}{2K} \sum_{i,j \in \mathbb{Z}^n \cap Q^\nu_{N_\varepsilon}} |w^\varepsilon_i - w^\varepsilon_j|^2 \Big) \Bigg) + O\Big(\frac{1}{h}\Big),
\end{aligned}$$

where $N_\varepsilon = \rho/\delta$, $K_\varepsilon = \rho/\varepsilon$, and $w^\varepsilon_i = u^\varepsilon_{\delta i}$ for $i \in \mathbb{Z}^n$. Since the functions w_ε are suitable test functions for the problem in (2.3) we obtain

$$\liminf_{\varepsilon\to0} \frac{\mu_\varepsilon(Q^\nu_\rho(x))}{\rho^{n-1}} \ge \varphi_K(\nu(x)) + O\Big(\frac{1}{h}\Big). \tag{3.11}$$

Using condition (d) above, we finally deduce that

$$\begin{aligned}\liminf_{\varepsilon\to 0}\mu_\varepsilon(\Omega) &\geq \sum_j \liminf_{\varepsilon\to 0}\mu_\varepsilon(Q^{\nu_j}_{\rho_j}(x_j)\cap S_u)+O\Big(\frac{1}{h}\Big)\\ &\geq \sum_j \int_{Q^{\nu_j}_{\rho_j}(x_j)\cap S_u}\varphi_K(\nu(y))\,d\mathcal{H}^{n-1}(y)+O\Big(\frac{1}{h}\Big)\\ &= \int_{\Omega\cap S_u}\varphi_K(\nu(y))\,d\mathcal{H}^{n-1}(y)+O\Big(\frac{1}{h}\Big),\end{aligned}$$

which gives the liminf inequality by the arbitrariness of h.

For the upper bound, we again treat explicitly the case $u(x)=\operatorname{sign} x_n$ only. For this it is not restrictive to suppose that $\mathcal{H}^{n-1}(S_u\cap\partial\Omega)=0$. We fix $\eta>0$, $N\in\mathbb{N}$ and v a test function for the problem in (2.3) such that

$$\frac{1}{N^{n-1}}\Big(K\sum_{i\in Q_N}W(v_i)+\frac{1}{2K}\sum_{i,j\in Q_N}|v_i-v_j|^2\Big)\leq\varphi_K(e_n)+\eta\,. \tag{3.12}$$

We may extend u^ε_i periodically in the directions $x_1,\dots,x_{n-1}$ inside the strip $\{|x_n|\leq N/2\}$ and equal to u (i.e., constant ±1) outside this strip. We then set

$$u^\varepsilon_i = v_{i/\delta}\qquad \text{for } i\in\delta\mathbb{Z}^n\,.$$

For such u_ε we have

$$\begin{aligned}\frac{1}{\varepsilon}E_{\varepsilon,\delta}(u_\varepsilon) &\leq \delta^{n-1}\#\Big(\{j\in\mathbb{Z}^{n-1}:(\delta Q_N+\delta j)\cap\Omega\neq\emptyset\}\Big)\times\\ &\qquad\Big(\sum_{i\in\delta Q_N}\frac{\delta}{\varepsilon}W(u^\varepsilon_i)+\sum_{i,j\in Q_N}\frac{\varepsilon}{2\delta}|u^\varepsilon_i-u^\varepsilon_j|^2\Big)\\ &= \Big(\mathcal{H}^{n-1}(S_u\cap\overline{\Omega})+o(1)\Big)\Big(\sum_{i\in Q_N}\frac{\delta}{\varepsilon}W(v_i)+\sum_{i,j\in Q_N}\frac{\varepsilon}{2\delta}|v_i-v_j|^2\Big)\\ &\leq \mathcal{H}^{n-1}(S_u\cap\Omega)\Big(\varphi_K(e_n)+\eta\Big)+o(1)\end{aligned}$$

as $\varepsilon\to0$, which proves the upper inequality by the arbitrariness of $\eta>0$. The case of a general ν is proven likewise, with an almost-periodic extension of v in the directions orthogonal to ν (see e.g. [12]). As remarked above this is sufficient to infer the validity of the upper bound for all u by approximation.

3.3. Supercritical case ($\varepsilon\ll\delta$). In this case, formally letting $\varepsilon\to0$ we obtain the constraint $u_i\in\{\pm1\}$ for all i. This suggests to use as a comparison functional the 'spin energies'

$$G_\delta(u)=\begin{cases}\sum_{i,j}\delta^{n-1}|u_i-u_j|^2 & \text{if } |u_i|=1 \text{ for all } i\\ +\infty & \text{otherwise.}\end{cases} \tag{3.13}$$

These energies have been studied in [4]. They are equicoercive in L^1, their Γ-limit is finite only on $BV(\Omega;\{\pm1\})$, and

$$\Gamma\text{-}\lim_{\delta\to0}G_\delta(u)=4\int_{S_u\cap\Omega}\|\nu\|_1\,d\mathcal{H}^{n-1}. \tag{3.14}$$

Now consider a sequence u_ε with $\sup_\varepsilon(\delta/\varepsilon^2)E_{\varepsilon,\delta}(u_\varepsilon) < +\infty$; i.e.

$$\sum_i \frac{\delta^{n+1}}{\varepsilon^2} W(u_i^\varepsilon) + \sum_{i,j} \delta^{n-1}|u_i^\varepsilon - u_j^\varepsilon|^2 \le C\,. \tag{3.15}$$

From (3.15) in particular, for all $\eta > 0$ we have

$$\#\Big\{i : W(u_i^\varepsilon) > \eta\Big\} \le \frac{C}{\eta}\,\frac{\varepsilon^2}{\delta^{n+1}} = o(1)\frac{1}{\delta^{n-1}} \tag{3.16}$$

for ε small enough.

If we define

$$v_i^\varepsilon = \begin{cases} 1 & \text{if } u_i^\varepsilon > 0 \\ -1 & \text{if } u_i^\varepsilon \le 0 \end{cases}$$

then condition (3.16) ensures that

$$\|u_\varepsilon - v_\varepsilon\|_1 \le C\eta + o(\delta),$$

and in particular $\|u_\varepsilon - v_\varepsilon\|_1 \to 0$ by the arbitrariness of η. We can estimate

$$\frac{\delta}{\varepsilon^2} E_{\varepsilon,\delta}(u_\varepsilon) \ge C_\eta\, G_\delta(v_\varepsilon) \tag{3.17}$$

with $C_\eta \to 1$ as $\eta \to 0$ so that

$$\liminf_\varepsilon \frac{\delta}{\varepsilon^2} E_{\varepsilon,\delta}(u_\varepsilon) \ge \liminf_\varepsilon G_\delta(v_\varepsilon).$$

This implies the coerciveness of the energies $(\delta/\varepsilon^2)E_{\varepsilon,\delta}$ and the desired lower bound.

The proof of the upper bound is trivial since on the domain of G_δ we have

$$\frac{\delta}{\varepsilon^2} E_{\varepsilon,\delta} = G_\delta.$$

It suffices then to take a sequence $u_\varepsilon = v_\delta$, where $v_\delta \to u$ realizes the upper bound for the Γ-limit in (3.14).

3.4. Interpolation. Note that in the proof of the lower inequality, the condition $\delta << \varepsilon$ was used only in the estimate leading to (3.3). So if now $\varepsilon/\delta \to K$, then we get instead

$$\#(J_\varepsilon^2) = \frac{1}{\delta^{n-1}} O(K)\,,$$

which gives a $O(K)$ in (3.3), and as a consequence

$$\liminf_{\varepsilon\to 0} \frac{1}{\varepsilon} E_{\varepsilon,\delta}(u_\varepsilon) \ge \Big(C_W + O(K)\Big)\,\mathcal{H}^{n-1}(\Omega \cap S_u)\,.$$

in (3.8). This proves that

$$\liminf_{K\to 0^+} \varphi_K(\nu) \ge C_W.$$

The opposite inequality with the lim sup is obtained by estimating φ_K taking v_i as in the proof of the upper bound in the case sub-critical case.

Finally, by (2.7) and (2.8) in Remark 2.2 (ii) we obtain

$$\limsup_{K\to+\infty} K\varphi_K(\nu) \le 4\|\nu\|_1.$$

The opposite inequality for the liminf follows from the estimate

$$\frac{K}{\varepsilon}E_{\varepsilon,\delta}(u) \ge (1+o(1))\frac{1}{2}\sum_{i,j}\delta^{n-1}|u_i-u_j|^2\,,$$

and the same argument as after (3.17).

3.5. Remarks and extensions. As mentioned in the Introduction, due to the wide range of applications of singularly perturbed problems, analysis and understanding of their numerical schemes are of practical importance. However, mesh size introduces another small length scale which in essentially all practical settings interacts with the small parameter in the original problem. Such an interaction already gives non-trivial descriptions for the stationary problem, as indicated by our theorem. In this section, we give some further remarks and plausible extensions of our results.

It is natural to perform a similar analysis for dynamical problems, such as (1.3). The situation can be quite intricate due to the presence of a large number of critical points or local minimzers for the discrete functional. This can lead to interesting pinning and de-pinning phenomena. Such have been investigated in both the continuum and discrete cases (see for example [22, 15]). The more recent work [11] is closer in spirit with the current paper, in particular the super-critical case. A time stepping, variational scheme is employed on a lattice model. Depending on the relative magnitude of the mesh and time step sizes, the dynamics demonstrates interesting stick-slip phenomena.

Even though our results do not directly lead to concrete statements for dynamical problems, it does give a quantitative description of the limit interfacial energy functional and more important, the energy scaling in different regimes of ε and δ. They can also provide useful guidelines if other effects are incorporated. Here we provide some examples.

Volume constraints can be imposed:

$$\sum_i \delta^n u_i = C_\delta.$$

If $C_\delta \longrightarrow C$, the same Γ-limit appears as before but with the constraint for the limit u.

$$\int_\Omega u = C.$$

Applied forces can also be considered:

$$E_{\varepsilon,\delta}(u) = \sum_i \delta^n W(u_i) + \frac{\varepsilon^2}{2}\sum_{i,j}\delta^n\Big|\frac{u_i-u_j}{\delta}\Big|^2 + \sum_i \delta^n f_i^{\varepsilon,\delta}u_i.$$

If the forcing terms $f^{\varepsilon,\delta}$ satisfy

$$\frac{1}{\varepsilon}f^{\varepsilon,\delta} \xrightarrow{L^2} f, \text{in (i) and (ii)}$$
$$\frac{\delta}{\varepsilon^2}f^{\varepsilon,\delta} \xrightarrow{L^2} f, \text{(iii)}$$

then the Γ-limit is the same with the addition of the bulk integral term:

$$\int_\Omega fu\,dx.$$

A complete picture of discrete dynamics is not currently available. However, our results can shed light in the realistic critical case (ii) if $K \ll 1$ and $K \gg 1$. For the former case, we believe it is possible to compute asymptotically the limiting dynamics and investigate the underlying anisotropy front propagation. For the latter case, the approach of [11] might still be applicable. This resembles some works in the study of cell-dynamical systems [18, 32]. Stochastic noise can certainly be used to drive the state out of local minima. The incorporation of a non-uniform adaptive mesh is also possible if we have some a priori knowledge about the location of the interface. We will defer quantitative answers to these challenging questions in future works.

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