Upper bounds on the coarsening rate for an epitaxial growth model

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Abstract

We study a specific example of energy-driven coarsening in two space dimensions. The energy is $\int |\nabla\nabla u|^2 + (1-|\nabla u|^2)^2$; the evolution is the fourth order PDE representing steepest descent. This equation has been proposed as a model of epitaxial growth for systems with slope selection. Numerical simulations and heuristic arguments indicate that the standard deviation of u grows like $t^{1/3}$, and the energy per unit area decays like $t^{-1/3}$. We prove a weak, one-sided version of the latter statement: the time-averaged energy per unit area decays no slower than $t^{-1/3}$. Our argument follows a strategy introduced by Kohn and Otto in the context of phase separation, combining (i) a dissipation relation, (ii) an isoperimetric inequality, and (iii) an ODE lemma. The interpolation inequality is new and rather subtle; our proof is by contradiction, relies on recent compactness results for the Aviles-Giga energy.

1 Introduction

We analyze the coarsening of solutions of the fourth-order PDE

$$u_t + \Delta^2 u + \nabla\cdot(2(1-|\nabla u|^2)\nabla u) = 0 \tag{1}$$

in two space dimensions. This is steepest descent for the functional

$$\frac{1}{2}\int |\nabla\nabla u|^2 + (1-|\nabla u|^2)^2.$$

With suitable boundary conditions it has the property that

$$\frac{d}{dt}\int u = 0,$$

so we shall always assume that u has mean value 0. Equation (1) has been proposed as a model of epitaxial growth, for systems with slope selection [MG, ORS, RK, SP]. In this setting u represents the deviation between the surface height and its mean.

Numerical simulations and heuristic arguments indicate that the standard deviation of u grows as $t^{1/3}$, and the energy per unit area decays like $t^{-1/3}$. Our main accomplishment is a one-sided, time-averaged version of the latter assertion.

In studying coarsening, we are interested in bulk behavior, not finite-size effects. But we need a convenient scheme for averaging. Therefore we shall use periodic boundary conditions, with a square $Q \subset \mathbb{R}^2$ as period cell. Our interest is mainly in the case when Q is large; in particular, our estimates are independent of the size of Q.

The energy per unit area is

$$E = \frac{1}{2}\fint_Q |\nabla\nabla u|^2 + (1-|\nabla u|^2)^2, \tag{2}$$

where we write $\fint_Q f$ for the average of a Q-periodic function f. Notice that if Q has sidelength $1/\varepsilon$ then

$$\fint_Q |\nabla\nabla u|^2 + (1-|\nabla u|^2)^2 = \varepsilon\int_{Q_1} \varepsilon|\nabla\nabla v|^2 + \varepsilon^{-1}(1-|\nabla v|^2)^2 \tag{3}$$

with $v(x) = \varepsilon u(x/\varepsilon)$. Thus in the large-system-size limit, we are effectively considering steepest descent for the singularly perturbed variational problem

$$\int_{Q_1} \varepsilon |\nabla \nabla u|^2 + \varepsilon^{-1}(1 - |\nabla u|^2)^2$$

in the limit $\varepsilon \to 0$. This limit has recently been the object of much attention, see e.g. [ADM, AG, DKMO, JK, JP, JOP]. We shall make essential use of this recent analytical progress.

The phenomenology of coarsening for (1) is explained quite clearly in [MG] and [ORS]. The initial data is taken to be a random perturbation of the unstable constant value $u = 0$. For large system sizes (after an initial transient) the solution develops ridges and valleys where ∇u changes rapidly. Away from these defects $|\nabla u| \approx 1$. As time evolves, the defects move and gradually get eliminated. This reduces the energy, and increases the standard deviation

$$L = \left(\fint_Q u^2 \right)^{1/2}. \tag{4}$$

The observed scaling laws

$$L(t) \sim t^{1/3}, \quad E(t) \sim t^{-1/3}$$

can be motivated as follows (see e.g. [BR, MG, ORS]). The energy is carried mostly in the defects, so we expect that

$$E \sim \text{defect length per unit area.}$$

The solution has slope 1 away from the defects so we expect that

$$L \sim \text{typical distance between defects.}$$

For a reasonably regular arrangement of one-dimensional defects in a two-dimensional domain, we have

$$\text{defect length per unit area} \sim \frac{1}{\text{typical distance between defects}},$$

so we expect that

$$EL \sim 1. \tag{5}$$

But from the steepest descent character of the PDE we have

$$\frac{dE}{dt} = -\fint_Q u_t^2 \tag{6}$$

and

$$\frac{dL^2}{dt} = \partial_t \fint_Q u^2 = 2 \fint_Q u u_t \le 2 \left(\fint_Q u^2 \right)^{\frac{1}{2}} \left(\fint_Q u_t^2 \right)^{\frac{1}{2}}, \tag{7}$$

which together give

$$\dot{L} \le (-\dot{E})^{1/2} \tag{8}$$

using the notation $\dot{L} = dL/dt$. To capture the essential impact of (5) and (8), consider what happens if the former is replaced by $EL = 1$ and the latter by $\dot{L} \sim (-\dot{E})^{1/2}$. Then differentiation of $E = 1/L$ gives

$$\dot{E} = -\frac{1}{L^2}\dot{L}$$

and substitution into the modified (8) gives

$$\frac{dL^3}{dt} \sim 1.$$

Integration gives $L^3(t) - L^3(0) \sim t$. Thus $E^{-1} \sim L \sim t^{1/3}$ for $t \gg L(0)^3$, as expected.

The coarsening rate is physically relevant, because it is the most readily observed consequence of the model. There is, at present, no convincing argument linking continuum growth models like (1) to atomic-scale models of growth. Therefore the main technique for connecting atomic-scale and continuum-scale models is comparison of their solutions. The robust observables are the statistical properties of solutions such as the coarsening rate.

The PDE under consideration is well-posed: given reasonable initial data, it has a unique smooth solution, which exists for all time [KSW]. However there has been, up to now, no rigorous analysis of its coarsening behavior. The main accomplishment of the present paper is a (weak, one-sided) result of this type. Our analysis is parallel to the recent work of Kohn and Otto on phase separation [KO]. Here is the basic strategy:

1. *Seek only upper bounds on the coarsening rate.* A lower bound can be true at best generically, or with probability one, if the energy has critical points. But an upper bound should be true universally, for all initial data. Therefore it should be accessible via deterministic PDE methods. Use of periodic boundary conditions is convenient, and quite natural: it matches the numerical simulations, facilitates averaging, and avoids pollution by finite-size effects so long as the microstructural length scale is much smaller than the period. As the solution coarsens, finite-size effects eventually kick in, slowing and ultimately stopping the coarsening. This does not falsify our results, because we prove only upper bounds (not lower bounds) on the coarsening rate.

2. *Identify two distinct measures of the local length scale, one based on energy per unit area, the other involving a negative norm of the order parameter.* In the present context these are E and L, defined by (2) and (4). We say L is a negative norm of the order parameter ∇u because $\|u\|_{L^2} = \|\nabla u\|_{H^{-1}}$. It is obvious that L has dimensions of length, since ∇u, being a slope, is dimensionless. It is less obvious that E has dimensions of 1/length. This is most easily seen by considering the large-system-size limit, i.e. the behavior of RHS of (3) as $\varepsilon \to 0$. Since that formula was obtained by scaling from a period cell of size $1/\varepsilon$, the prefactor ε has dimension 1/length. The integral itself is dimensionless, with asymptotic behavior (at least formally) a constant times

$$\int_{\text{defects in } Q_1} |[\frac{\partial v}{\partial n}]|^3,$$

see e.g. [AG, JK]. Here v is a continuous function satisfying $|\nabla v| = 1$ almost everywhere; the integration is over its defect set, where the graph of v has a sharp ridge or valley; and $[\frac{\partial v}{\partial n}]$ is the jump of the normal derivative of v across the defect.

3. *Find a dissipation inequality relating $\dot{L}$ and $\dot{E}$.* This step is easy – a direct consequence of the steepest-descent structure of the PDE. In the present context it is simply Eqn. (8). The proof sketched above is entirely rigorous.

4. *Find a pointwise inequality relating L and E.* We shall show that if E is sufficiently small then $EL \geq C$ for some constant $C > 0$. This amounts to a rigorous, one-sided version of (5). Its proof is the main technical achievement of this paper. We call it an isoperimetric inequality, because it relates the defect energy E (analogous to perimeter) and the standard deviation L (analogous to volume). To understand the essence of the matter, consider the large system-size limit as in (3). Asymptotically as $\varepsilon \to 0$ we are considering continuous functions $v : \mathbb{R}^2 \to \mathbb{R}$ with period 1 in each variable such that $|\nabla v| = 1$; our assertion is that

$$\left(\int_{\text{defects in } Q_1} |[\frac{\partial v}{\partial n}]|^3 \right) \left(\int_{Q_1} v^2 \right)^{1/2} \geq C$$

for some absolute constant C, independent of v.

5. *Deduce the desired upper bound by an ODE argument.* This step is unconventional but entirely elementary. The relevant ODE result is proved in [KO]. Focusing on a special case for simplicity, it asserts that if $E(t)$ and $L(t)$ are functions satisfying (a) $EL \gtrsim 1$, and (b) $\dot{L}^2 \lesssim -\dot{E}$, then we have the following lower bound on the time-averaged value of E:

$$\fint_0^T E^2 dt \gtrsim \fint_0^T (t^{-\frac{1}{3}})^2 dt \qquad \text{for } T \gg L_0^3 \gg 1 \gg E_0. \tag{9}$$

Here $L_0 = L(0)$, $E_0 = E(0)$, and our notation $\gtrsim$, $\gg$, etc. is best explained by repeating assertion (9) in more standard notation: there exists a (possibly large) constant C such that

$$\frac{1}{T}\int_0^T E^2 dt \geq \frac{1}{C}T^{-\frac{2}{3}} \qquad \text{provided } T \geq C L_0^3 \text{ and } E_0 \leq \frac{1}{C}.$$

Assertion (9) is a special case of our main result, Theorem 6. It is a time-averaged, one-sided confirmation of the expected result $E \sim t^{-1/3}$. Unfortunately our methods are not sufficient to prove $E \gtrsim t^{-1/3}$ pointwise, and they do not give even a time-averaged version of $L \lesssim t^{1/3}$; see Section 4.4 of [KO] for discussion of this point.

In its outline this program is identical to that of [KO]. However our functionals E and L are quite different from those in [KO], and proving the inequality $EL \geq C$ requires an entirely different approach. We shall argue by contradiction, making essential use of recent results from [ADM, DKMO, JP] on the large-system-size limit. Our analysis is restricted to space dimension two, because the results in [ADM, DKMO, JP] are two-dimensional. Fortunately, space dimension two is the case of primary interest for epitaxial growth.

Anisotropic analogues of (1) have also been considered as models of epitaxial growth [MG, S1, S2]. These models prefer a few symmetry-related values of ∇u rather than the entire circle $|\nabla u| = 1$. The energy is therefore of the form

$$E = \frac{1}{2}\fint_Q |\nabla \nabla u|^2 + W(\nabla u)$$

where $W \geq 0$ vanishes at the vertices of a regular N-sided polygon. Our analysis extends easily to this case, giving a time-averaged version of $E \gtrsim t^{-1/3}$ for any N (see Theorem 7). This matches the numerically-observed coarsening rate if N is large enough, e.g. for $N = 6$ [MG]. When $N = 4$, however, the phenomenology is different: simulation suggests that $L \sim t^{1/4}$ and $E \sim t^{-1/4}$. This does not contradict our upper bound, but it suggests that the bound may not be sharp for $N = 4$. A heuristic explanation of the observed $t^{1/4}$ scaling is given in [MG].

The rest of this introduction provides some remarks on equation (1) as a model for epitaxial growth. A central feature of this approach is its emphasis on slope selection. Indeed, when the system size is large the energy strongly favors $|\nabla u| = 1$ (see (3)). The solution of the PDE therefore develops a pattern of ridges and valleys ("defects"), where $|\nabla u|$ changes rapidly, delimiting regions ("grains") where $|\nabla u|$ is of order 1 and relatively smooth. The energy is concentrated on these ridges and valleys; since the PDE is steepest descent for this energy, its basic hypothesis is that the system's evolution is driven by this "defect energy."

Slope selection is indeed observed experimentally; see e.g. [MG] for references. At least one atomic-scale mechanism for slope selection has been suggested, see e.g. [AF1, AF2, AF3]. However there is no systematic derivation of (1) from an atomic-scale model.

In fact, (1) is but one of many continuum models for epitaxial growth; see e.g. [K, PV, V]. A major deficiency is its up-down symmetry: if u solves this equation then so does $-u$. The underlying physics does not share this symmetry: nucleation occurs mainly at peaks, not valleys. Therefore physical peaks are typically one-dimensional while valleys are typically two-dimensional. Alternative models sharing this asymmetry include variants of the KPZ equation (see e.g. [K]), a model which includes desorption effects via a forcing term [SRK], and a coupled system for the surface height and adatom density [LK]. The up-down symmetry of (1) can also be broken by the initial data [ORS, St].

In focusing on (1), our goal is not to promote this model over its competitors. Rather, our goal is to advance the understanding of energy-driven coarsening. The analysis of (1) is a natural target, because of its similarities to – and differences from – the recent work of Kohn and Otto.

2 The isoperimetric inequality

This section proves the essential inequality

$$EL \gtrsim 1 \text{ when } E \ll 1. \tag{10}$$

Here

$$E = \frac{1}{2} \fint_Q |\nabla\nabla u|^2 + (1 - |\nabla u|^2)^2, \quad \text{and} \quad L = \left(\fint_Q u^2 \right)^{\frac{1}{2}}$$

and u is any Q-periodic function. The period cell Q is a square in $\mathbb{R}^2$, and the constants implicit in (10) are independent of the size of Q.

It is convenient to rescale, so all the serious work can be done on the unit square Q_1. We may suppose without loss of generality that Q is centered at 0, with side length $1/\varepsilon$. Expressed in terms of $v(x) = \varepsilon u(x/\varepsilon)$, (10) asserts that

$$\left(\int_{Q_1} \varepsilon |\nabla\nabla v|^2 + \varepsilon^{-1}(1 - |\nabla v|^2)^2 \right) \cdot \left(\int_{Q_1} v^2 \right)^{\frac{1}{2}} \gtrsim 1$$

whenever

$$\int_{Q_1} \varepsilon^2 |\nabla\nabla v|^2 + (1 - |\nabla v|^2)^2 \ll 1.$$

This is an easy consequence of the following result.

Theorem 1 *There is a constant c_* with the following property: for any Q_1-periodic function v and any $\varepsilon > 0$,*

$$\left(\int_{Q_1} \varepsilon |\nabla\nabla v|^2 + \varepsilon^{-1}(1 - |\nabla v|^2)^2 \right) \left(\int_{Q_1} v^2 \right)^{\frac{1}{2}} + \int_{Q_1} \varepsilon^2 |\nabla\nabla v|^2 + (1 - |\nabla v|^2)^2 \geq c_*.$$

Our proof of Theorem 1 is by contradiction. The argument makes essential use of results from compactness results for the Aviles-Giga energy [ADM, DKMO, JP], through the following two lemmas.

Lemma 2 *Define*

$$E_\varepsilon(v) = \int_{Q_1} \varepsilon |\nabla\nabla v|^2 + \varepsilon^{-1}(1 - |\nabla v|^2)^2$$

where Q_1 is the unit square in $\mathbb{R}^2$. There exists constant $a_0 > 0$ such that for any $\varepsilon \leq 1$, v Q_1-periodic, we have

$$E_\varepsilon(v) \geq a_0. \tag{11}$$

Proof of Lemma 2: If the conclusion of (11) is false then there is a sequence such that

$$E_{\varepsilon_j}(v_j) \leq \frac{1}{j}, \qquad j = 1, 2, 3 \cdots .$$

Let $\tilde{v}_j(x) = \frac{1}{j} v_j(jx)$. Evidently $\tilde{v}_j$ is Q_1-periodic and

$$\begin{aligned} &\int_{Q_1} \frac{\varepsilon_j}{j} |\nabla\nabla \tilde{v}_j|^2 + \frac{j}{\varepsilon_j}(1 - |\nabla \tilde{v}_j|^2)^2 = \int_{Q_1} \frac{\varepsilon_j}{j} j^2 |\nabla\nabla v_j|^2 + \frac{j}{\varepsilon_j}(1 - |\nabla v_j|^2)^2 \\ &= j \int_{Q_1} \varepsilon_j |\nabla\nabla v_j|^2 + \frac{1}{\varepsilon_j}(1 - |\nabla v_j|^2)^2 \leq 1. \end{aligned} \tag{12}$$

We also have

$$\int_{Q_1} \tilde{v}_j^2 = \frac{1}{j^2} \int_{Q_1} v_j^2 \to 0, \tag{13}$$

since $\int_{Q_1} v_j = 0$ and $\int_{Q_1} (1 - |\nabla v_j|^2)^2 \leq 1$ implies a uniform bound on $\int_{Q_1} v_j^2$.

We now conclude from (12) (using the compactness theorem from [ADM, DKMO, JP]) that $\{\nabla \tilde{v}_j\}$ stays compact in L^2 with $\nabla \tilde{v}_j \to \nabla \tilde{v}_\infty$, $|\nabla \tilde{v}_\infty| = 1$. But (13) gives $\int_{Q_1} \tilde{v}_\infty^2 = 0$. This contradiction shows that (11) must be true for some $a_0 > 0$.

Remark 3 We remark that Lemma 2 is also an easy consequence of Theorem 1 in [JOP].

Lemma 4 *Let $E_\varepsilon(v)$ be as in Lemma 2. For any $c \le \frac{1}{2}$, there exists $\gamma > 0$ such that for all $\varepsilon \le 1$, if $\int_{Q_1} v^2 \le \gamma$, then $E_\varepsilon(v) \ge c$.*

Proof of Lemma 4: If the lemma is false, then for some $c \le \frac{1}{2}$, there exist v_j, ε_j such that

$$\int_{Q_1} v_j^2 \le \frac{1}{j} \text{ but } E_{\varepsilon_j}(v_j) < c. \tag{14}$$

Consider the limit as $j \to \infty$. If $\liminf_j \varepsilon_j > 0$, one can restrict attention to $\varepsilon_j \ge$const> 0, so $\{\int_{Q_1} |\nabla\nabla v_j|^2\}$ stay bounded. From this, one concludes easily that ∇v_j is compact in L^2. If $\liminf_j \varepsilon_j = 0$, compactness theorem of [ADM, DKMO, JP] implies compactness of ∇v_j (passing to a subsequence if necessary) in L^2. Either way one gets a limit v_∞ such that $\nabla v_j \to \nabla v_\infty$ strongly in $L^2(Q_1)$.

On the other hand, (14) implies $v_\infty = 0$. Therefore $\nabla v_\infty = 0$, while by (14), compactness of ∇v_j in L^2 and Fatou's Lemma, we have

$$1 = \int_{Q_1} (|\nabla v_\infty|^2 - 1)^2 \le \liminf_{j\to\infty} \int_{Q_1} (|\nabla v_j|^2 - 1)^2 \le c\varepsilon_j \le \frac{1}{2}.$$

This contradiction shows that the lemma is true.

We continue laying necessary groundwork for the proof of Theorem 1. The most difficult (and interesting) case is when $\varepsilon \to 0$. As explained in the Introduction, in this limit the formal content of the theorem is that

$$(\text{defect energy of } v) \cdot (\text{standard deviation of } v) \gtrsim 1$$

for Q_1-periodic functions v with $|\nabla v| = 1$. The heart of the proof uses the following idea: suppose the standard deviation of v is small; then v is close to 0 on average. So if we subdivide Q_1 into a grid of squares, v is relatively small on most blocks in the grid. But if the restriction of v is small on a block, yet $|\nabla v| = 1$ a.e., then v must surely have a lot of defect energy in the block. This is a consequence of Lemma 4 after rescaling. The following Proposition provides a rigorous basis for this argument.

Proposition 5 *For any $c_0 \le \frac{1}{2}$, there exist constant $c_1 > 0$ with the following property. Consider any square $Q \subset \mathbb{R}^2$, and any $v : Q \to \mathbb{R}$ (not necessarily periodic) satisfying*

$$\int_Q v^2 dx \le c_1 |Q|^2.$$

Then we have

Case a

$$\int_Q \varepsilon|\nabla\nabla v|^2 + \varepsilon^{-1}(1 - |\nabla v|^2)^2 \ge c_0 |Q|^{\frac{1}{2}} \qquad \text{if } |Q|^{\frac{1}{2}} \ge \varepsilon; \tag{15}$$

Case b

$$\int_Q \varepsilon|\nabla\nabla v|^2 + \varepsilon^{-1}(1 - |\nabla v|^2)^2 \ge c_0 \varepsilon^{-1} |Q| \qquad \text{if } \varepsilon \ge |Q|^{\frac{1}{2}}. \tag{16}$$

Proof of Proposition 5: We address Case A first. Define $u(x) = \frac{1}{\lambda} v(\lambda x + x_0)$, where $\lambda = |Q|^{\frac{1}{2}}$ and x_0 is the center of Q. Then (15) is equivalent to proving for any $c_0 \le \frac{1}{2}$, the existence of c_1 such that if

$$\frac{\varepsilon}{\lambda} \le 1, \qquad \int_{Q_1} u^2 \le c_1,$$

then

$$\int_{Q_1} \left(\frac{\varepsilon}{\lambda}\right)|\nabla\nabla u|^2 + \left(\frac{\lambda}{\varepsilon}\right)(1-|\nabla u|^2)^2 \geq c_0.$$

This is exactly the conclusion of Lemma 4.
We turn now to Case B. Suppose the conclusion is false, then for some $c_0 \leq \frac{1}{2}$, there exists a sequence ε_k, Q_k, v_k satisfying

$$(17)\ \frac{\varepsilon_k}{|Q_k|^{\frac{1}{2}}} \geq 1, \qquad \frac{1}{|Q_k|^2}\int_{Q_k} v_k^2 \to 0, \qquad \frac{1}{|Q_k|}\int_{Q_k} \varepsilon_k^2|\nabla\nabla v_k|^2 + (1-|\nabla v_k|^2)^2 < c_0.$$

Rescaling as before, (17) gives

$$\int_{Q_1} u_k^2 \to 0, \qquad \int_{Q_1} \left(\frac{\varepsilon_k}{\lambda_k}\right)^2 |\nabla\nabla u_k|^2 + (1-|\nabla u_k|^2)^2 < c_0.$$

Since $\frac{\varepsilon_k}{\lambda_k} \geq 1$, we are now in the same situation as case 1 in the proof of Lemma 4.

We now have all the necessary tools.

Proof of Theorem 1: We argue by contradiction. If the assertion of the theorem is false, then there exists a sequence v_k, ε_k such that

$$(18)\ \left(\int_{Q_1} \varepsilon_k|\nabla\nabla v_k|^2 + {\varepsilon_k}^{-1}(1-|\nabla v_k|^2)^2\right)\left(\int_{Q_1} v_k^2\right)^{\frac{1}{2}} + \int_{Q_1} \varepsilon_k^2|\nabla\nabla v_k|^2 + (1-|\nabla v_k|^2)^2 \to 0.$$

Without loss of generality, we may assume the functions v_k are Q_1-periodic with mean value 0. In fact, since the L^2 norm is minimized when the mean value is zero, if we can prove Theorem 1 for functions whose mean value on Q_1 is zero, the general case follows immediately. We separate the argument into three cases.

Case 1: Suppose ε_k stays bounded away from 0. Then the second term in (18) gives

$$\int_{Q_1} |\nabla\nabla v_k|^2 \to 0, \quad \text{and} \quad \int_{Q_1} |\nabla v_k|^2 \to 1.$$

But Poincare's inequality and the hypothesis of periodicity gives

$$\int_{Q_1} |\nabla v_k|^2 \leq C\int_{Q_1} |\nabla\nabla v_k|^2 \to 0,$$

which is a contradiction.

Case 2: Suppose $\liminf_k \varepsilon_k = 0$ but $\int_{Q_1} v_k^2$ stays bounded away from 0. Passing to a subsequence if necessary, we may suppose that $\varepsilon_k \to 0$. Now the first term in (18) gives

$$\int_{Q_1} \varepsilon_k|\nabla\nabla v_k|^2 + \varepsilon_k^{-1}(1-|\nabla v_k|^2)^2 \to 0$$

while Lemma 2 gives

$$\liminf_k \int_{Q_1} \varepsilon_k|\nabla\nabla v_k|^2 + \varepsilon_k^{-1}(1-|\nabla v_k|^2)^2 > 0.$$

This is a contradiction.

Case 3: Suppose $\liminf_k \varepsilon_k = 0$ and $\liminf_k \int_{Q_1} v_k^2 = 0$. Passing to a subsequence if necessary, we may assume that $\int_{Q_1} v_k^2 \to 0$. If along this subsequence ε_k stays bounded away from 0, we get a contradiction as in Case 1. Therefore (passing to a further subsequence) we may suppose that $\varepsilon_k \to 0$.

Our plan is to derive a contradiction to (18) using Proposition 5. We apply Propositon 5 for a fixed value of c_0. To simplify notation we drop the subscript k, writing $v = v_k$, and setting

$$\delta = \left(\int_{Q_1} v^2 \right)^{1/2}.$$

For any integer $N > 1$, we may partition the cell Q_1 into N^2 squares of sidelength $\omega = 1/N$. The appropriate choice of N will be made presently. If

$$\int_{Q_\omega} v^2 \leq c_1 \omega^4,$$

apply Proposition 5 to Q_ω we obtain

$$\int_{Q_\omega} \varepsilon |\nabla\nabla v|^2 + \varepsilon^{-1}(1 - |\nabla v|^2)^2 \geq c_0 |Q_\omega|^{\frac{1}{2}} \qquad \text{if } \omega \geq \varepsilon;$$

or

$$\int_{Q_\omega} \varepsilon |\nabla\nabla v|^2 + \varepsilon^{-1}(1 - |\nabla v|^2)^2 \geq c_0 \varepsilon^{-1} |Q_\omega| \qquad \text{if } \varepsilon \geq \omega.$$

The proper choice of N and $\omega = 1/N$ depends on the relation between ε and δ.

First alternative: Suppose $\varepsilon \gg \delta$. Then we choose N so that $\omega \approx \sqrt{\varepsilon\delta}$. Notice that $\varepsilon \gg \omega \gg \delta$. Consider the N^2 squares Q_ω obtained as above. We say $Q_\omega \in \mathcal{A}$ if $\int_{Q_\omega} v^2 \geq c_1 w^4$, and we write $|\mathcal{A}|$ for the number of squares in $\mathcal{A}$. Since

$$\sum_{Q_\omega \in \mathcal{A}} \int_{Q_\omega} v^2 \leq \int_{Q_1} v^2 = \delta^2,$$

we have

$$|\mathcal{A}| c_1 \omega^4 \leq \delta^2,$$

i.e. $|\mathcal{A}| \leq \frac{\delta^2}{c_1 \omega^4} \ll \frac{1}{\omega^2}$. Therefore on most squares (more than $N^2/2$ when $\delta \ll 1$), we have

$$\int_{Q_\omega} v^2 \leq c_1 \omega^4.$$

Since $\varepsilon \gg \omega$, for $Q_\omega \notin \mathcal{A}$, Proposition 5 gives

$$\int_{Q_\omega} \varepsilon^2 |\nabla\nabla v|^2 + (1 - |\nabla v|^2)^2 \geq c_0 |Q_\omega|$$

Summing over all these squares, we obtain

$$\begin{aligned} \int_{Q_1} \varepsilon^2 |\nabla\nabla v|^2 + (1 - |\nabla v|^2)^2 &\geq \sum_{Q_\omega \notin \mathcal{A}} \int_{Q_\omega} \varepsilon^2 |\nabla\nabla v|^2 + (1 - |\nabla v|^2)^2 \\ &\geq c_0 \sum_{Q_\omega \notin \mathcal{A}} |Q_\omega| \gtrsim 1. \end{aligned}$$

This contradicts (18).

Second alternative: Suppose $\delta \gtrsim \varepsilon$. Then we choose N and $\omega = 1/N$ so that $\omega = M\delta$, where M is a constant to be chosen later in the argument. As before, we consider the N^2 squares Q_ω and the subset $\mathcal{A}$ of Q_ω's such that $\int_{Q_\omega} v^2 \geq c_1 w^4$. Since

$$\sum_{Q_\omega \in \mathcal{A}} \int_{Q_\omega} v^2 \leq \int_{Q_1} v^2 = \delta^2$$

we have

$$|\mathcal{A}| \leq \frac{\delta^2}{c_1 \omega^4} = \frac{1}{M^2 c_1} \frac{1}{\omega^2}.$$

We now choose M: it should be large enough that $M^2 c_1 \geq 2$. This insures that $|\mathcal{A}| \leq \frac{1}{2}\frac{1}{\omega^2}$, so at least half the Q_ω's are not in $\mathcal{A}$.

Now recall that $\omega \gtrsim \varepsilon$. So for each $Q_\omega \notin \mathcal{A}$ we can apply Proposition 5 to the associated Q_ω to get

$$\int_{Q_\omega} \varepsilon|\nabla\nabla v|^2 + \varepsilon^{-1}(1-|\nabla v|^2)^2 \geq c_0 |Q_\omega|^{\frac{1}{2}}.$$

Summing over all these squares gives

$$\begin{aligned} \fint_{Q_1} \varepsilon|\nabla\nabla v|^2 + \varepsilon^{-1}(1-|\nabla v|^2)^2 &\geq \sum_{Q_\omega \notin \mathcal{A}} \int_{Q_\omega} \varepsilon|\nabla\nabla v|^2 + \varepsilon^{-1}(1-|\nabla v|^2)^2 \\ &\geq c_0 \frac{1}{2\omega^2} |Q_\omega|^{\frac{1}{2}} \gtrsim \frac{1}{\omega}. \end{aligned}$$

Therefore

$$\left(\int_{Q_1} \varepsilon|\nabla\nabla v|^2 + \varepsilon^{-1}(1-|\nabla v|^2)^2\right)\left(\int_{Q_1} v^2\right)^{\frac{1}{2}} \gtrsim \frac{\delta}{\omega} \gtrsim 1.$$

This contradicts (18). The proof is now complete. □

3 Upper bounds on the coarsening rate

As explained in the Introduction, Theorem 1 leads immediately to a time-averaged upper bound on the coarsening rate, by using the framework of [KO].

Theorem 6 *For any $0 \leq \theta \leq 1$ and $r < 3$ satisfying $\theta r > 1$ and $(1-\theta)r < 2$, there is a constant C (depending only on θ and r) with the following property. For any square $Q \subset \mathbb{R}^2$, and any Q-periodic solution of (1), the energy per unit area $E(t)$ and the standard deviation $L(t)$ satisfy*

$$(19)\quad \fint_0^T E^{\theta r} L^{-(1-\theta)r} dt \geq \frac{1}{C} \fint_0^T (t^{-\frac{1}{3}})^r dt \qquad \text{provided } T \geq C L^3(0) \text{ and } E(0) \leq \frac{1}{C}.$$

Proof of Theorem 6: Lemma 3 of [KO] shows that (19) follows by an ODE argument once we know the two relations

$$EL \gtrsim 1 \text{ for } E \ll 1$$

and

$$\dot{L}^2 \leq -\dot{E}.$$

The first relation is precisely the assertion of Theorem 1, and the second is an elementary consequence of the PDE's steepest-descent character – see (6)–(8). □

We noted in the introduction that anisotropic analogues of (1) are also sometimes considered as models of epitaxial growth. Our upper bounds extend to a broad class of such models with no extra work.

Theorem 7 *Suppose the evolution equation for u is steepest descent for the anisotropic energy*

$$(20)\qquad E = \frac{1}{2}\fint_Q |\nabla\nabla u|^2 + W(\nabla u)$$

rather than the isotropic energy (2). Assume

$$(21)\qquad W(\xi) \geq C(1-|\xi|^2)^2$$

for some $C > 0$ (This holds, for example, if (a) $W \geq 0$ grows quartically at ∞, (b) W vanishes only at finitely many points ξ_i on the unit circle, and (c) the Hessian at each ξ_i is strictly positive.) Then the conclusion of Theorem 6 remains valid.

Proof of Theorem 7: The anisotropic energy still satisfies

$$EL \gtrsim 1 \text{ for } E \ll 1,$$

as an immediate consequence of Theorem 1 and (21). And it still satisfies the dissipation relation

$$\dot{L}^2 \leq -\dot{E}$$

by the same proof as before. So Lemma 3 of [KO] still applies. □

Though not particularly natural for epitaxial growth, one can also consider steepest descent for an energy of the form (20) with less symmetry. For example, suppose $W \geq 0$ vanishes at finitely many points ξ_i, but the ξ_i don't have the same norm. Then the proof of Theorem 7 does not work, however the time-averaged $t^{-1/3}$ lower bound is still valid. This can be shown by combining the methods of [KO] with those of [B, FT, S]. We refer readers to [KY] for details.

4 Some open problems

Our accomplishment is relatively modest: just a time-averaged lower bound for E, and no upper bound at all for L. It would be nice to prove pointwise bounds for both E and L. The same issue arises in the work of [KO] on phase separation.

Among anisotropic problems with energy (20), it is natural to consider the case when W is minimized at the vertices of a regular N-gon. Our method gives the same result for every N, but numerical simulations suggest the case $N = 4$ is different – it coarsens more slowly. The origin of this effect is explained in [MG]. Briefly: the valleys form a sort of lattice with defects. Therefore there are *two* physical length scales – the spacing of the lattice of valleys, and the distance between defects in this lattice. We wonder whether this effect can be captured using an energy-based argument similar to that of the present paper.

Another interesting class of models are the ones without slope selection. A typical example [G] is steepest descent for

$$E = \frac{1}{2} \fint |\nabla \nabla u|^2 - \ln(1 + |\nabla u|^2).$$

Since $-\ln(1 + |\nabla u|^2)$ is unbounded below, the order parameter ∇u grows indefinitely in time. We wonder whether the viewpoint of this paper can help explain the coarsening exponents calculated in [G].

Most epitaxial growth models neglect desorption, leading to the conservation law $\frac{d}{dt} \int u = 0$. A different model was recently considered by Šmilauer, Rost and Krug [SRK]:

$$u_t = -\Delta^2 u - 2\nabla \cdot ((1 - |\nabla u|^2)\nabla u) + V(|\nabla u|).$$

The source term $V(|\nabla u|)$ is designed to capture the effects of desorption near peaks. Numerical simulation suggests that it drastically changes the coarsening law: for isotropic continuum equation, coarsening is initially very slow ($L \sim t^{1/4}$) but after a while it becomes very fast ($L \sim t^{1/2}$). We wonder whether the viewpoint of this paper can be extended to equations of this kind.

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