Energy-Driven Pattern Formation

Robert V. Kohn

Courant Institute, NYU

ICM2006, Madrid

Perspective

Key insight: upper bound on coarsening rate is universal.

Key approach: two ways to measure length scale: a neg norm (L) and perimeter (E); linked by interpolation and energy ineqs.

Generalizes: to multiple phases, Mullins-Sekerka dynamics, Ostwald ripening, epitaxial growth

Open questions: similar results have *not* been shown for motion by curvature, grain growth, or Ginzburg-Landau vortices.

(1) Bounds on coarsening rates

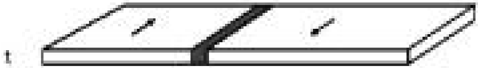
(2) Structure of a cross-tie wall

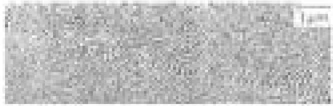
tools	Optimal lower bound via inspired integration by parts
work by	Alouges, Rivière, & Serfaty, COCV 2002
version here	DeSimone, Kohn, Müller & Otto 2005

(3) Pathways of thermally-activated switching

Cross-tie wall

This is a special type of domain wall seen in "soft," thin ferromagnets (not too thin!)





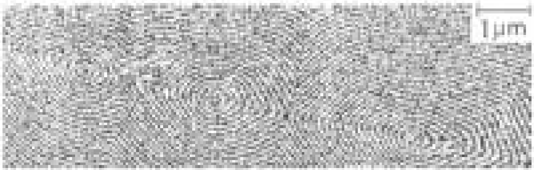
Question: Why this particular pattern?

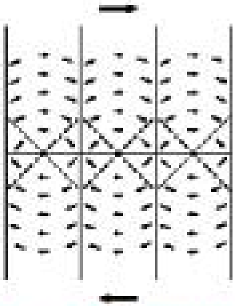
Answer: It minimizes the total energy.

Main steps:

- Identify an appropriate class of patterns
- Learn how to calculate the energy of a pattern
- Understand what pattern corresponds to the experiments
- Prove a lower bound that's sharp for this pattern

Elaborating on the question





The magnetization $m = (m_1, m_2)(x_1, x_2)$ is piecewise smooth & divergence-free (even across discontinuities). Also $|m| = 1$.

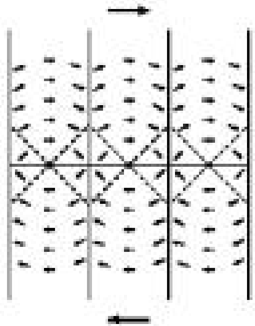
This permits a "simple" 180-deg wall, where m jumps across the axis.

Instead the film chooses a mixture of lower-angle walls. Why?

Note: the pattern is fully-determined (constant in some regions, circles in others) except for its internal length scale.

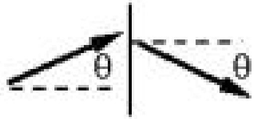
Magnetization patterns and their energies

A magnetization pattern is a piecewise smooth vector field $m = (m_1, m_2)(x_1, x_2)$ such that div $m = 0$ (weakly, even across discontinuities) and $|m| = 1$. We call the discontinuities walls.



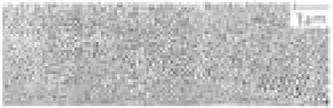
The energy of a pattern is the sum of the energies of its walls.

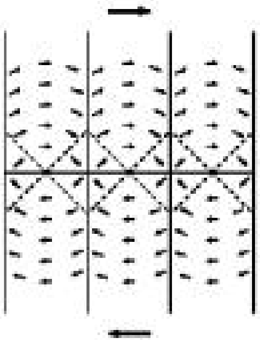
For a wall with total angle 2θ, energy $= (\sin\theta - \theta\cos\theta) \times$ length.



Remark: A more primitive starting point is micromagnetics. Our framework corresponds to "thick-film Néel walls". Comes from micromagnetics when film thickness $>>$ exchange length.

Refining the question





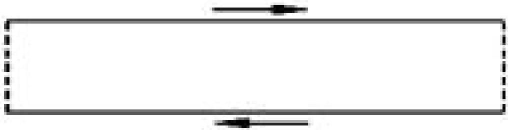
Energy density $\sin\theta - \theta\cos\theta$ is very nonlinear. Small angles are much cheaper than large.

The proposed pattern achieves energy/length $\sqrt{2} - 1$. Much better than a 180-deg wall, for which energy/length = 1.

But to know this is optimal, we must prove a geometry-independent lower bound, showing no other pattern can do better.

Strategy of the lower bound

Consider rectangular domain, with periodic bc at sides and $m = (\pm 1, 0)$ at top/bottom:



When all else fails, integrate by parts! Look for an entropy $\Sigma(m) = (\Sigma_1(m), \Sigma_2(m))$ such that

- for m smooth, $|m| = 1$ and $\operatorname{div} m = 0$ imply $\operatorname{div} \Sigma(m) = 0$
- at a wall with half-angle θ, $|[\Sigma(m) \cdot \nu]| \leq \sin\theta - \theta\cos\theta$

Every such Σ gives a lower bound, since

$$\text{bdry data} = \left| \int_{\text{bdry}} \Sigma \cdot n \right| \leq \int_{\text{interior}} |\operatorname{div} \Sigma| \leq \text{total wall energy}$$

Finding the good entropy

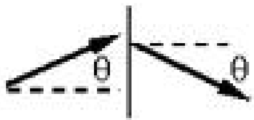
First pass (wrong but informative):

$$\Sigma(m) = \tfrac{1}{2}(\theta m + m^{\perp}) \quad \text{when} \quad m = e^{i\theta}$$

First condition: $\operatorname{div} m = 0 \Rightarrow \operatorname{div} \Sigma(m) = 0$ for θ smooth, since

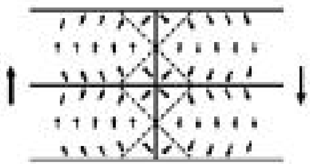
$$\operatorname{div} \Sigma(m) = \tfrac{1}{2}\theta \operatorname{div} m.$$

Second condition: $|[\Sigma \cdot \nu]| \le \sin\theta - \theta\cos\theta$. Holds *with equality*!



$\nu = (1,0)$, $m = (\cos\theta, \pm\sin\theta) \Rightarrow$
$[\Sigma \cdot \nu] = \Sigma_1^R - \Sigma_1^L = \sin\theta - \theta\cos\theta$.

Problem: θ isn't well-defined,
because the walls contain vortices.



Finding the good entropy – continued

Successful choice is similar in each quadrant:

$$\begin{array}{lll} \theta m + m^\perp + (0, -\sqrt{2}) & \text{for} & -\pi/4 \le \theta \le \pi/4 \\ (\pi/2 - \theta)m - m^\perp + (-\sqrt{2}, 0) & \text{for} & \pi/4 \le \theta \le 3\pi/4 \\ (\theta - \pi)m + m^\perp + (0, \sqrt{2}) & \text{for} & 3\pi/4 \le \theta \le 5\pi/4 \\ (3\pi/2 - \theta)m - m^\perp + (\sqrt{2}, 0) & \text{for} & 5\pi/4 \le \theta \le 7\pi/4 \end{array}$$

This gives a continuous $\Sigma : S^1 \to R^2$ satisfying both our requirements. In particular: at a div-free discontinuity,

$$|[\Sigma(m) \cdot \nu]| \le \text{wall energy density}$$

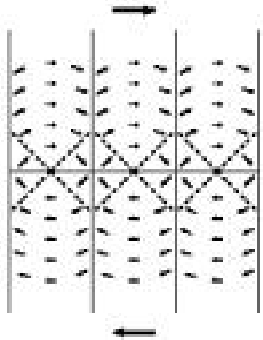
with equality when total angle is $\le$ 90 deg.

Our pattern achieves the bound because it uses only discontinuities $\le$ 90 deg. (No arithmetic needed!)

Comments

Internal length scale is set by higher-order effects. Can be explained using micromagnetics:

- *anisotropy* prefers the far-field values of m, so favors small length scale;
- *finite thickness/exchange ratio* gives walls tails that repel, favoring large length scale



Is our cross-tie pattern unique? (Defining feature: achieves net 180-deg wall, using discontinuities of angle $\leq$ 90 deg.)

There's a cross-tie pattern for each wall angle $>$ 90 deg
(A simple discontinuity is optimal for wall-angles $<$ 90 deg)

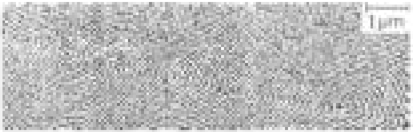
Outline

What is energy-driven pattern formation? Hard to define, but "you know it when you see it." So I'll discuss three examples:

(1) Bounds on coarsening rates
(2) Structure of a cross-tie wall
(3) Pathways of thermally-activated switching

Unifying theme: challenges to nonlinear PDE and calc of varns, coming from physics and materials science.

Perspective



Key achievement: Explain the cross-tie wall by proving an optimal lower bound for the associated variational problem.

Key approach: Integration by parts, using an "entropy" $\Sigma(m)$.

Related ideas: Argument resembles (a) use of null-Lagrangians to estimate relaxed energies, and (b) use of "calibrations" to study minimal surfaces.

Open questions: Were we lucky? Or did there *have* to be an integration-by-parts-based argument?

(1) Bounds on coarsening rates

(2) Structure of a cross-tie wall

(3) Pathways of thermally-activated switching

tools	Action minimization, sharp-interface limit
framework	Kohn, Otto, Reznikoff, & Vanden-Eijnden, CPAM 2006
1D analysis	Kohn, Reznikoff, & Tonegawa, Calc. Var. PDE 2006

Thermal switching

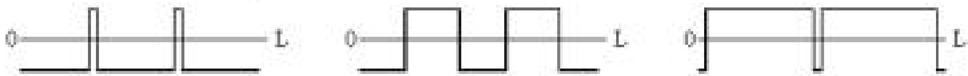
Focus on the functional

$$E = \int_\Omega \frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{4\varepsilon}(u^2-1)^2.$$

Its only local minima are $u \equiv 1$ and $u \equiv -1$ (for Ω convex, or periodic boundary conditions).

Question: What are the pathways of thermally-activated switching?

Answer (1D periodic): $N \geq 1$ "seeds" nucleate; walls propagate at constant velocity, then annihilate.



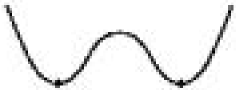
Start by explaining the question ...

Importance of thermal fluctuations

Nature finds local not global minima

- water can be heated $>$ 100 deg C
- most foams are metastable (e.g. beer)

Systems escape from local minima via thermal fluctuations



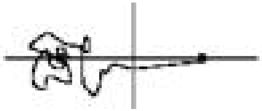
- $dz = -\nabla E(z)\,dt +$ noise
- small noise $\Rightarrow$ escape is rare

Events can be rare and yet very important

- reliability of complex systems
- failure of a computer's hard drive

Action minimization

Think, for example, of
$E(z) = (z_1^2 - 1)^2 + z_2^2$



$$dz = -\nabla E\, dt + \sqrt{2\gamma}\, dw$$

Transitions are rare, yet also predictable via

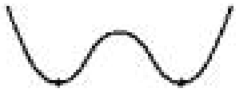
Large deviation principle: Given that transition takes time $\leq T$, it occurs (with very high probability) by approx the pathway that minimizes the action:

$$\min_{\substack{z(0)=(1,0)\\ z(T)=(-1,0)}} \frac{1}{4}\int_0^T |z_t + \nabla E|^2\, dt.$$

Note: the integrand is equation error.

Large vs small switching times

As time allowed for switching $T \to \infty$, action-min path is simple:



- go uphill to lowest mtn pass
- go downhill from there

$$\frac{1}{4}\int_0^{\tau} |z_t + \nabla E|^2 = \frac{1}{4}\int_0^{\tau} |z_t - \nabla E|^2 + \int_0^{\tau} \langle z_t, \nabla E\rangle$$
$$= \text{nonnegative} + (E(\tau) - E(0)).$$

Assertion follows, using τ = time of arrival at ridge. Therefore "classical nucleation theory" is all about saddle points.

Situation is different when T is fixed:

- The optimal pathway *need not* go through a saddle.
- Note that fixing T is natural – early failures, though extremely rare, may be the ones we care about most.

Simplest infinite-dimensional case

Ginzburg-Landau $\quad E = \int \frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{4\varepsilon}(u^2-1)^2$

SDE becomes a stochastic PDE. Hard to interpret except in 1D. Focusing on action minimimization avoids this issue.

Steepest descent is $\varepsilon u_t = -\nabla E = \varepsilon \Delta u - \varepsilon^{-1}(u^3 - u)$, after scaling t so velocity has order 1. Sharp interface limit is motion by curvature.

Action functional (suitably scaled) is

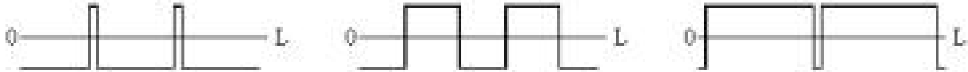
$$\frac{1}{4}\int_0^T \int_\Omega |\varepsilon^{1/2} u_t + \varepsilon^{-1/2}\nabla E|^2 \, dx \, dt$$

Goal is to minimize action subject to $u \equiv -1$ at $t = 0$ and $u \equiv 1$ at $t = T$, in the sharp-interface limit $\varepsilon \to 0$.

The sharp-interface limit

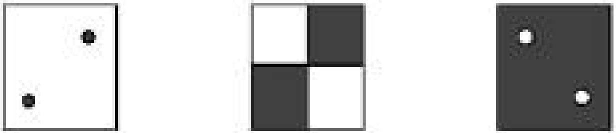
1D (periodic) case (rigorous)

Optimal pathway nucleates $2N$ walls (N equispaced seeds) then propagates them at constant velocity.



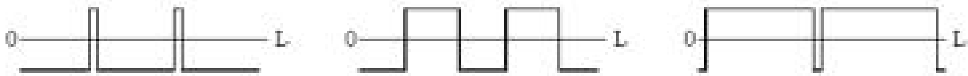
2D case (still only formal)

Similar; but nucleation can be cost-free (if seeds are points), and propagation can be cost-free (motion by curvature).



$$\min_{\text{trajectories}} [\text{nucl cost, if any}] + \int\int (v + \kappa)^2$$

Discussion



(1) Nucleation events involve appearance of new walls or seeds. Not associated with saddle point or "critical nucleus."

(2) Heart of rigorous 1D analysis is a structure theorem: as $\varepsilon \to 0$, action integrand converges for a.e. t to a measure with point masses (at walls), varying continuously in t.

(3) Action minimization is closely related to:

- steepest descent: $\varepsilon u_t = \varepsilon \Delta u - \varepsilon^{-1}(u^3 - u)$
- DeGiorgi's conjecture: $\varepsilon^{-1} \int |\varepsilon \Delta u - \varepsilon^{-1}(u^3 - u)|^2$

Hints toward the analysis

(1) Action controls the energy, e.g. jumps in energy cost action:

$$\int_{t_1}^{t_2}\int |\varepsilon^{1/2}u_t + \varepsilon^{-1/2}\nabla E|^2 = \int_{t_1}^{t_2}\int |\varepsilon^{1/2}u_t - \varepsilon^{-1/2}\nabla E|^2 + 4\int_{t_1}^{t_2}\int \langle u_t, \nabla E\rangle$$
$$= \text{pos} + 4(E(t_2) - E(t_1))$$

(2) Action controls wall profile and velocity: arguing as above, and using that $E = 0$ when $u \equiv \pm 1$:

$$\int_0^T\int |\varepsilon^{1/2}u_t + \varepsilon^{-1/2}\nabla E|^2 = \int_0^T\int \varepsilon u_t^2 + \varepsilon^{-1}|\nabla E|^2$$

(3) Propagation cost is of order 1: $\iint \varepsilon u_t^2$ is bounded below via

$$\frac{4}{3}|\Omega| = \int_0^T\int u_t(1-u^2) \le \left(\iint \varepsilon u_t^2\right)^{1/2}\left(\iint \varepsilon^{-1}(u^2-1)^2\right)^{1/2}$$

(1) Bounds on coarsening rates

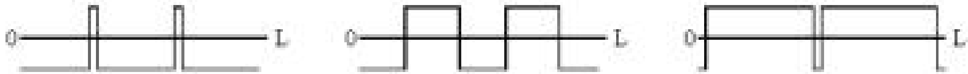
tools Interpolation and energy inequalities

work by Kohn & Otto, CMP 2002

(2) Structure of a cross-tie wall

(3) Pathways of thermally-activated switching

Perspective



Physical idea: Focus on thermally-activated switching in fixed time T. Though rare, such events may nevertheless be very important.

Mathematical idea: Action minimization offers a new challenge in the analysis of sharp-interface limits.

Wide open: Rigorous analysis complete only for 1D Ginzburg-Landau. How about more complex models from condensed matter physics (e.g. magnetic switching)?

What is energy-driven pattern formation?

Today's examples were:

- Bounds on coarsening rates via energy & interpoln ineqs
- Cross-tie wall structure via optimal geometry-indep bound
- Thermal switching via sharp-interface limit, action min

Other areas of recent progress include: twinning due to martensitic transformation; domain patterns in ferromagnets; vortex patterns in type-II superconductors.

Some common themes:

- Questions from physics, answers from analysis
- Energy-driven, but not necessarily at equilibrium
- Focus on examples; unity will emerge in due course

References and credits

Bounds on coarsening rates

Presented here Kohn and Otto, CMP 2002
Closely related Kohn-Yan; Pego-Dai; Conti, Niethammer & Otto
Numerical figs Puri, Bray, Lebowitz, PRE 56 (1997)

Cross-tie wall structure

More general Alouges, Rivière & Serfaty, COCV 2002
Version here DeSimone, Kohn, Müller & Otto, review article, 2005
Experimental fig Nakatani et al, Jap. J. Appl. Phys. 28 (1989)

Thermal switching

Framework Kohn, Otto, Reznikoff & Vanden-Eijnden, CPAM 2006
1D analysis Kohn, Reznikoff & Tonegawa, Calc Var PDE 2006

For more detail and a 4th example (branching of domains) see my ICM Proceedings article (on my web page).

Thanks to NSF for its generous support of this work

Coarsening

$t = 1$ $t = 2$ $t = 10$

Focus for simplicity on motion by surface diffusion

$$v_{\mathrm{nor}} = \Delta_\Gamma \kappa \quad \Gamma(t) = \text{evolving curve}$$

Common belief, for random initial data:

- length scale coarsens, $\ell(t) \sim t^{1/4}$
- solution is statistically self-similar

Evolution is energy-driven:

$$\frac{d}{dt}\mathrm{Perimeter} = \int_\Gamma \kappa v_{\mathrm{nor}} = -\int_\Gamma |\nabla_\Gamma \kappa|^2$$

Why is this difficult?

- Conjectured self-similarity might be wrong.

  Not even clear what it means!

- Assertion that $\ell(t) \sim t^{1/4}$ says
  - (1) Solution never stops coarsening.
    False e.g. for spheres. Therefore subtle.
  - (2) Solution doesn't coarsen faster.
    True without exception. Therefore accessible.

Recent progress: A weak version of (2), showing (very roughly)

$$\ell(t) \le Ct^{1/4}$$

Getting started

Two very different methods for defining local length scale $\ell(t)$:

Represent spatial structure by $\chi(x) = \pm 1$. Assume:

- spatially periodic (so averaging is easy)
- equal vol fractions (for simplicity only)

Method 1: Perimeter per unit volume

$$E = \fint |\nabla \chi| \qquad \text{scales like } 1/\ell(t)$$

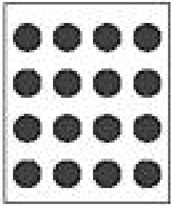
Method 2: A negative Sobolev norm

$$L = \max_{|\nabla g| \leq 1} \fint g\chi \qquad \text{scales like } \ell(t)$$

Norm defining L is dual to $W^{1,\infty}$. Hence we write (heuristically)

$$L = \fint |\nabla^{-1} \chi|$$

Thinking about E and L



Consider 2D system of size R, with inclusions on length scale ℓ. Number of inclusions is $N \sim (R/\ell)^2$. Take $\chi = 1$ in black phase, $\chi = -1$ in white.

Clearly E = perimeter/area = $\sim N\ell/N\ell^2 \sim 1/\ell$.

To see why $L = \max_{|\nabla g| \leq 1} \fint \chi g \sim \ell$, argue that

- optimal $g \sim \ell$ at inclusion centers
- optimal $g \sim -\ell$ far from inclusions

so $\chi g \sim \ell$, whence $L \sim \ell$.

Key observation

E and L are related by

- interpolation inequality: We always have

$$EL \geq \text{const.}$$

Proof makes no use of evolution law. Essentially:

$$\fint |\chi| \leq C \left(\fint |\nabla \chi|\right)^{1/2} \left(\fint |\nabla^{-1} \chi|\right)^{1/2}$$

- energy inequality: Solutions of the evolution law satisfy

$$dE/dt \leq 0 \quad \text{and} \quad (dL/dt)^2 \leq 2E|dE/dt|$$

Intuition why dE/dt controls dL/dt: coarsening requires motion, which dissipates energy. Proof is simple (like most energy inequalities).

These are sufficient (sort of)!

The available information

$$EL \geq C, \quad dE/dt \leq 0, \quad (dL/dt)^2 \leq 2E|dE/dt|$$

does not imply

$$L(t) \leq Ct^{1/4} \quad \text{or} \quad E(t) \geq Ct^{-1/4},$$

but it does imply a time-averaged version of the latter:

$$\frac{1}{T}\int_0^T E^3(t)\,dt \geq \frac{1}{T}\int_0^T \left(t^{-1/4}\right)^3 dt$$

provided $T \gg L^4(0) \gg 1 \gg E(0)$. Proof is an ODE argument (like Gronwall's inequality).