Thematic Program in Partial Differential Equations:
Workshop on Patterns in Physics.

Global description of patterns far from onset: a case study.

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Outline:

I. Introduction: Rayleigh-Bénard experiment
II. The phase diffusion equation
III. Analytical results
IV. Introduction of twist: the case of the elliptic domain
V. Conclusion

References:

- N. M. Ercolani, R. Indik, A. C. Newell & T. Passot, The Geometry of the Phase Diffusion Equation, *J. Nonlinear Sci.*, **10**, 223 (2000).
- N. Ercolani, R. Indik, A.C. Newell & T. Passot
  Global description of patterns far from onset: a case study, *Physica D*, **184**, 127 (2003).

I. Introduction

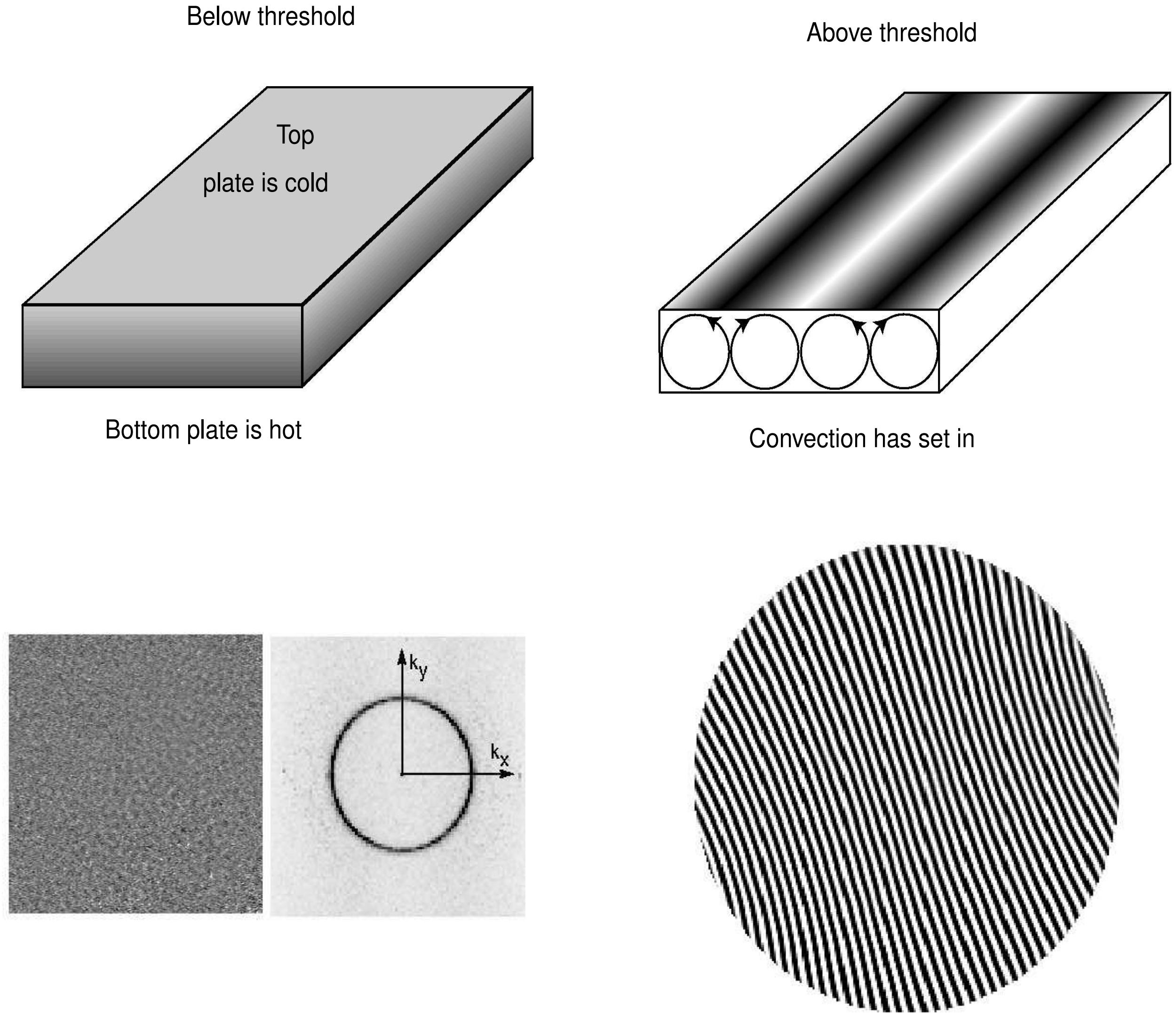


Figure 1: The Rayleigh-Bénard experiment (M. Wu, G. Ahlers, & D.S. Cannell, Phys. Rev. Lett. 75, 1743-1746 (1995); K.M.S. Bajaj, N. Mukolobwiez, N. Currier, & G. Ahlers, Phys. Rev. Lett. 83, 5282-5285 (1999))

Convection in a large box

Types of patterns (in Boussinesq fluids) :

◇ Straight rolls : with dislocations and amplitude grain boundaries $(R/R_C \leq 5)$; A becomes active at defect cores

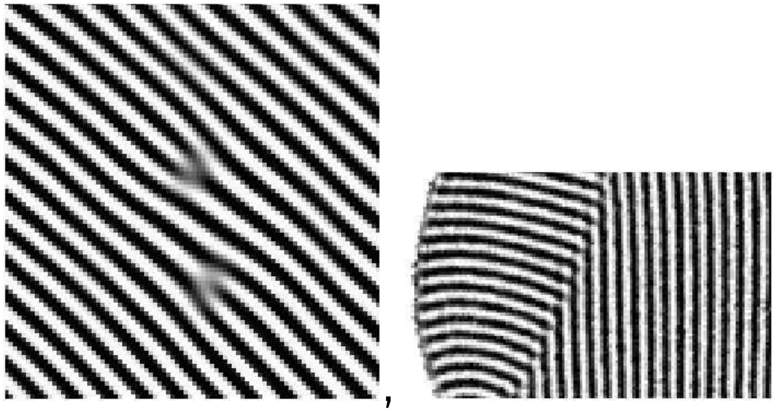


Figure 2: From J. Liu, K.M.S. Bajaj, and G. A., unpublished.

$\diamond$ Labyrinths : $(P \gg 1,\ R/R_C \gg 1)$; Phase grain boundaries (PGB) meet at concave and convex disclinations

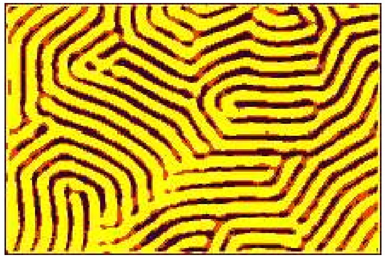


Figure 3: From M. Assenheimer and V. Steinberg, Europhysics News, 27, 125 (1996).

$\diamond$ Target patterns : $(P \geq 3,\ R/R_C \gg 1)$; mean flow is small;

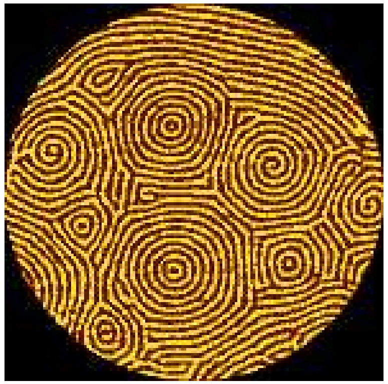


Figure 4: From M. Assenheimer and V. Steinberg, Phys. Rev. Lett. 70, 3888 (1993)

◇ Spirals : $(P \leq 3,\ R/R_C \gg 1)$; $\mathbf{V}$ becomes active

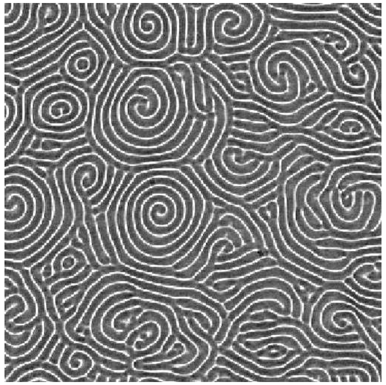


Figure 5: From J. Liu, K.M.S. Bajaj, and G. A., unpublished.

◇ Hexagons : $(P \geq 1.2,\ R/R_C \geq 2,\ k < k_c)$ with larger wavelength than that of coexisting rolls.

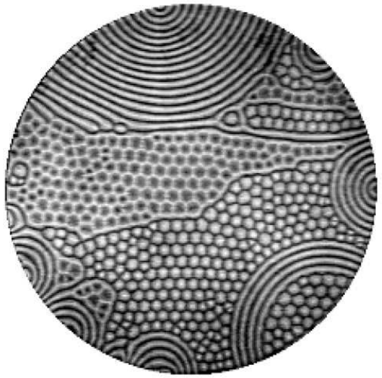


Figure 6: From Assenheimer and Steinberg, Phys. Rev. Lett. 76, 756. (1996)

Typical patterns can be described by three main order parameters

$\diamond$ local wavevector(s) $\mathbf{k_i} = \nabla\theta_i$ ($i > 1$ for multiphase planforms)

$\diamond$ amplitude A (slaved to k when $R/R_c \gg 1$)

$\diamond$ mean flow $\mathbf{V}$; advects the phase contours ; disappears at infinite Prandtl number

Convective patterns : several approaches

- Modulational description :

(Newell-Whitehead-Segel ; Ginzburg-Landau)

$$A_T - (\frac{\partial}{\partial X} - \frac{i}{2k_c}\frac{\partial^2}{\partial Y^2})^2 A = A - A^2 A^*$$

(i) Removes fast spatial and temporal scales ; order parameter = envelope of the rolls (complex variable): A

(ii) Asymptotics with distance to threshold as expansion parameter

(iii) Limited to a neighborhood of straight parallel rolls of a given direction

(iv) Describes the formation of dislocations ; core structure not exact

- Large-scale horizontal dynamics :

(Swift-Hohenberg)

$$w_t = -(1+\Delta)^2 w + Rw - w^3,$$

(i) Removes fast time ; Galerkin expansion in the vertical direction ; no scaling on the horizontal ones

(ii) Order parameter = vertical velocity (real variable): w

(iii) Expansion close to threshold ; necessity to simplify the equations ; in particular nonlinearities are “localized” in real space

$\Longrightarrow$ description no longer quantitative

(iv) Isotropic description ; describes the formation of all defect types.

- Further reduction : the phase formalism

(Pommeau-Manneville)

$$\Theta_T - D_\perp(k_0)\Theta_{YY} - D_{||}(k_0)\Theta_{XX} = 0$$

(i) Get rid of the fast time scale associated with amplitude relaxation

(ii) Expressing the slaving of the amplitude to the wavevector in NWS, one obtains an equation for the phase (real order parameter)

(iii) Formalism still limited to a fixed direction, close to threshold

(iv) Cannot describe defect formation

- The phase diffusion equation

(Cross-Newell)

$$\tau(k)\Theta_T - \nabla \cdot (\mathbf{k}B(k)) = 0$$

(i) Direct derivation from the microscopic system ; small parameter = inverse aspect ratio

(ii) Description quantitatively valid far from onset

(iii) Preserves isotropy ; can describe all stationary defects with emphasis on topology and far field ; core structure reduced at the microscopic scale.

(iv) Cannot describe the formation of defects (up to now), only their stationary structure.

II. The phase diffusion equation

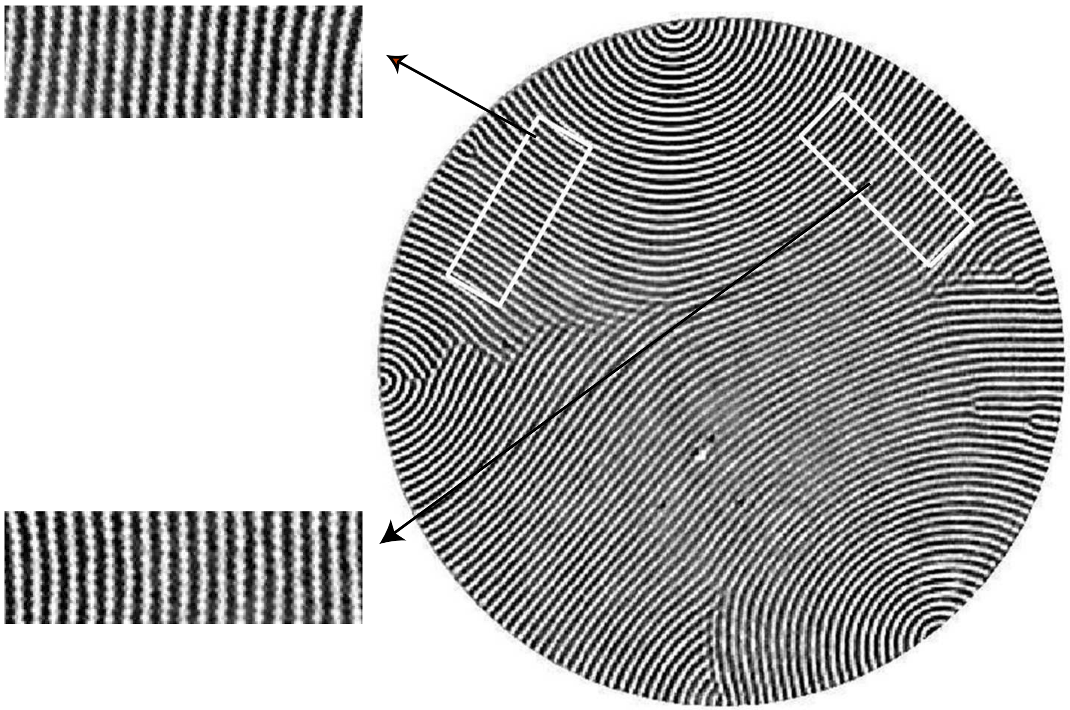


Figure 7: From Y.-C. Hu, R. Ecke, and G. Ahlers, Phys. Rev. E 51, 3263 (1995).

• Outline of the method :

Consider locally (spatially) periodic straight parallel rolls ; the wavevector $\mathbf{k}$ varies slowly over a distance ϵ^{-1}, which defines slow scales $\mathbf{X} = \epsilon \mathbf{x}$ and $T = \epsilon^2 t$. Each field is expanded in the form $w = f(\theta, z; A) + \epsilon w_1 + \epsilon^2 w_2 + \cdots$.

A slow phase is defined as $\Theta = \int \mathbf{k}(\mathbf{X}, T) d\mathbf{X} = \epsilon\theta$

Calculate $f(\theta, z; A)$: fully nonlinear solution, using Galerkin expansion. Leads to a relation $A(k)$: at sufficiently large value of R, the Rayleigh number, the roll amplitude is algebraically slaved to the wavenumber. Close to threshold, A becomes free.

The iterates w_i are calculated by linearization about $f \Longrightarrow$ solve inhomogeneous singular linear systems $\mathcal{L} w_i = R_i$.

(a) Translational invariance $\Longrightarrow \mathcal{L}\frac{\partial f}{\partial \theta} = 0$

(b) Pressure defined up to arbitrary constant P_s (mass conservation) $\Longrightarrow \mathcal{L}\frac{\partial f}{\partial P_s} = 0$

(c) For $k = k_l$ and $k = k_r$ only (the borders of the marginal stability band) $\mathcal{L}\frac{\partial f}{\partial A} = 0$

Solvability conditions $\langle w^A | R_i \rangle = 0$:

(a) $\Longrightarrow$ phase equation (at order ϵ)

(b) $\Longrightarrow$ mean flow equation (at order ϵ^2)

(c) $\Longrightarrow$ Partial differential equation for the amplitude close to onset (or near dislocation cores)

Difficulty : need to calculate w_1 exactly to get mean flow equation
$\longrightarrow$ use SVD : $\mathcal{L} = UDV^T$

System : phase diffusion / mean flow equations (with Souli, JFM **220**, 187 (1990))

$$\Theta_T + \rho(k)\mathbf{V}\cdot\nabla\Theta + \frac{1}{\tau(k)}\nabla\cdot\mathbf{k}B(k) = 0$$

$$\nabla\times\left\{\hat{k}\alpha(k)(\hat{k}\times\nabla\Psi)\cdot\hat{z}\right\}\cdot\hat{z} - \nabla\cdot\hat{k}\beta(k)\hat{k}\cdot\nabla\Psi =$$

$$\hat{z}\cdot\nabla\times\left\{\sigma\mathbf{k}\nabla\cdot\mathbf{k}A^2 - \frac{\hat{k}}{\tau_\alpha(k)}\nabla\cdot\mathbf{k}B_\alpha(k)\right\} - \nabla\cdot\hat{k}(\nabla\times\mathbf{k}B_\beta(k))\cdot\hat{z}$$

$$\Omega(k, A; R, P) = 0$$

where $\mathbf{V} = \nabla\times\Psi\hat{z}$ is the horizontal mean flow, $\hat{k} = \frac{\mathbf{k}}{k}$, $\sigma = P^{-1}$.

$\mathbf{V}$ is zero at infinite Prandtl number and in absence of curvature gradient.

$\underline{\text{When P} = \infty}$ one has

$$\boxed{\Theta_T - kD_\perp(k)\nabla\cdot\widehat{k} - D_{||}(k)\widehat{k}\cdot\nabla k = 0}$$

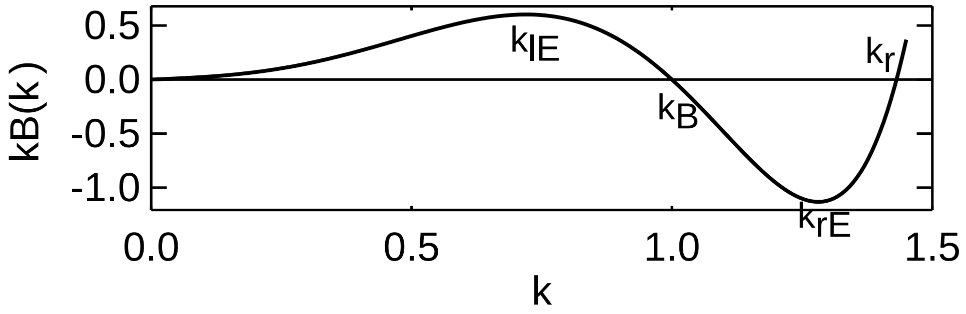
with

$D_{||}(k) = -\frac{1}{\tau}\frac{d}{dk}kB(k) = 0 \longrightarrow$ Eckhaus instability

$D_\perp(k) = -\frac{1}{\tau}B(k) = 0 \longrightarrow$ Zig-zag instability

- Results :

(i) The shape of $kB(k)$ is universal ; its zeros and extrema (possibly modified by the mean flow) give the frontiers of the Busse balloon relative to long-wave instabilities



(ii) Curvature selects the roll wavenumber k_B s.t. $B(k_B) = 0$; good agreement with experiments

(iii) Because of sidewall boundaries, patches of circular rolls dominate. Circular rolls are subject to a new instability named focus when the advection by the mean flow, generated by a target asymmetry, dominates over roll diffusion. This instability generates a temporal dependence with a low number of degrees of freedom inside the Busse balloon.

(iv) When the selected wavenumber k_B is outside the Busse balloon : defects are continuously created ; dynamics with a large number of degrees of freedom.

- Exact stationary solutions $(P = \infty)$:

$\diamond$ The system $\nabla \cdot \mathbf{k} B(k) = 0, \qquad \nabla \times \mathbf{k} = 0, \qquad \mathbf{k} = (f, g)$
is identical to that of the two-dimensional gas flow for $k < k_B$ with the essential difference that

$\star$ $\mathbf{k}$ is a director
$\star$ $B(k)$ changes sign .

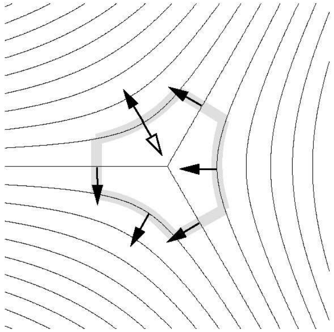
Shocks correspond to phase grain boundaries

$$\text{Jump conditions :} \begin{cases} s[f] + [g] = 0 \\ [fB] - s[gB] = 0 \end{cases}$$

where $s = \frac{dx}{dy}$ gives the direction of the shock line. If k is continuous across the shock, $k = k_B$ and the shock line separates the two patches at equal angles.

$\diamond$ Hodograph transform :

Consider the map $\mathbf{X} \to \mathbf{k} = (f = k\cos\phi, g = k\sin\phi)$. Its jacobian is $J = f_X g_Y - f_Y g_X$ and its winding number is the topological invariant called twist $T = \frac{1}{2}\int_C d\phi$ (with integration on the double cover where $\mathbf{k}$ is a vector field), also equal to $T = \frac{1}{2}\int_\Omega J dX dY$. Introduce $\hat{\theta}$, Legendre transform of θ s.t. $\theta(X,Y) + \hat{\theta}(f,g) = \mathbf{k}\cdot\mathbf{X}$.



We have $$k\frac{\partial}{\partial k}(kB\frac{\partial\hat{\theta}}{\partial k}) + \frac{\partial}{\partial k}(kB)\frac{\partial^2\hat{\theta}}{\partial\phi^2} = 0$$

This is a linear separable equation with a few exact solutions

- Target : $\hat{\theta} = c\int^k \frac{dk}{kB}$; $T = 2\pi$

$kB = \frac{c}{r}$ with $c = O(\epsilon)$, the core size.

- Convex disclination : $\hat{\theta} = (ck \int^k \frac{dk}{k^3 B}) \cos\phi$; $T = \pi$

$\theta = \frac{c}{kB} \cos\phi$ with $c = O(\epsilon)$; there exists a core region.

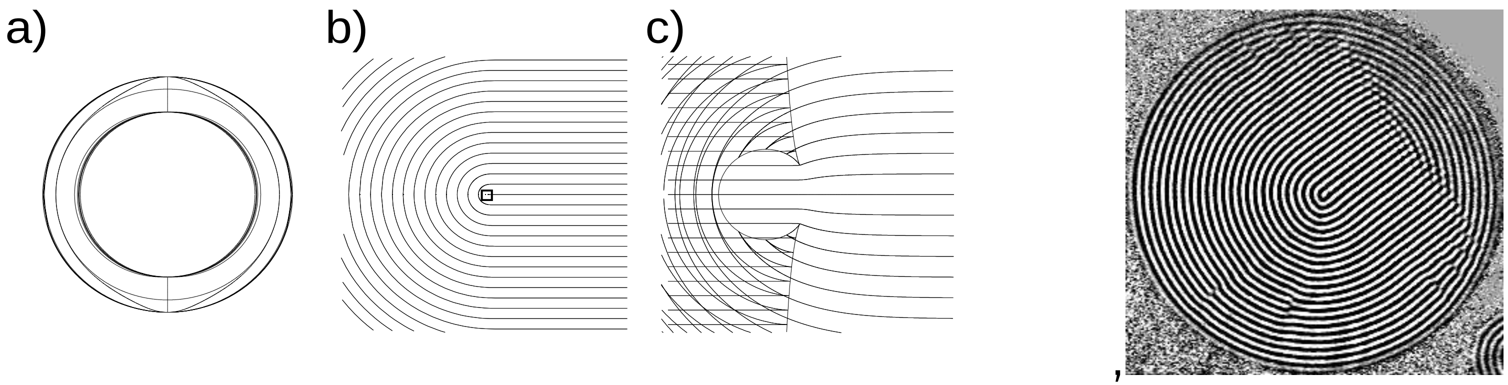


Figure 8: Right: from E. Bodenschatz

• Concave disclination : $\hat{\theta} = F(k)\cos 3\phi$; $T = -\pi$

$F(k) \simeq \ln(k_B^2 - k^2)$; there are multivalued regions.

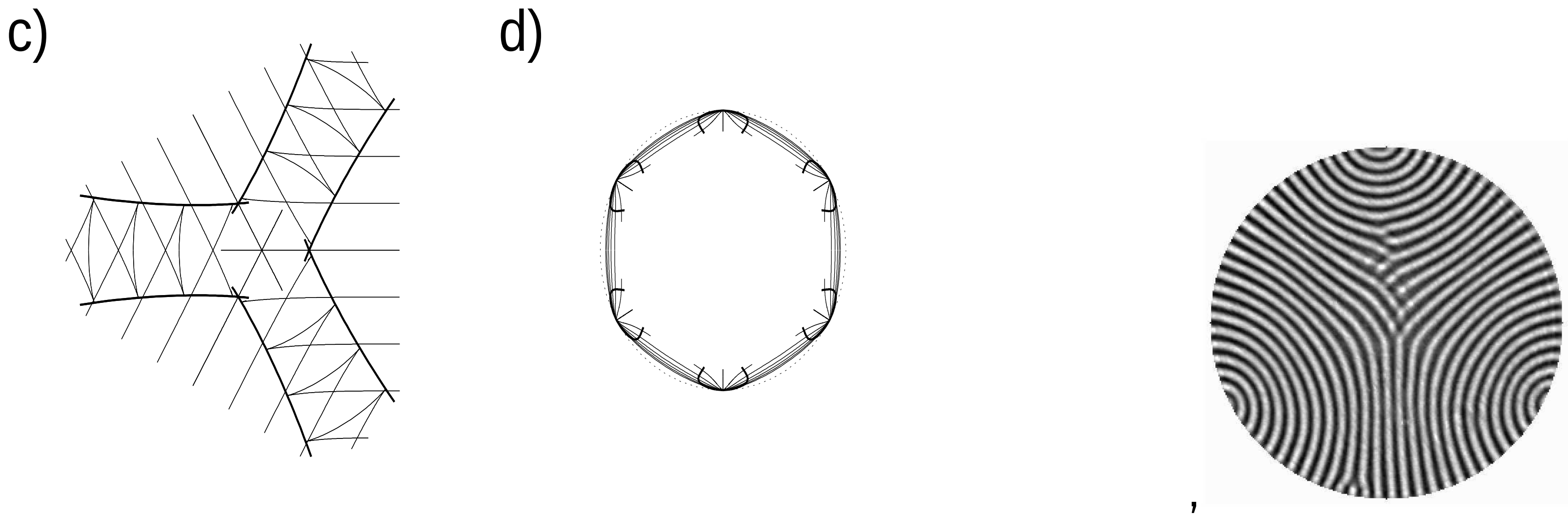


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Figure 9: Right: from J. Liu and G. Ahlers, Phys. Rev. Lett. 77, 3126 (1996).

Note : all these solutions not only capture the correct topology but also the correct energetics of defects, unlike harmonic solutions.

$\longrightarrow$ Need a regularization to put shocks and resolve the core region of convex disclinations.

• Regularization (Stationary case) :

Going to the next orders in the expansion leading to the PDE, one can identify the most important contribution, namely a term proportional to the biLaplacian of the phase.

$$\boxed{\tau(k)\Theta_T + \nabla \cdot \vec{k}B(k) + \epsilon^2\nabla^4\Theta = 0}$$

This equation provides a good model, also introduced in the context of thin film blistering (Ortiz & Gioia, J. Mech. Phys. Solids, **42**, 531, 1994).

It rewrites $\tau(k)\Theta_T = -\delta F/\delta\theta$ with

$$F = \int (\frac{1}{2}\underbrace{(\epsilon\nabla^2\theta)^2}_{\substack{\downarrow \\ \text{roll bending}}} + \underbrace{\frac{1}{2}G^2}_{\substack{\downarrow \\ \text{wavenumber mismatch}}})\, dxdy \qquad \text{and} \quad G^2 = -\int_{k_B^2}^{k^2} B dk^2$$

The bi-Laplacian of the phase, $\varepsilon^2\nabla^4\Theta$, provides the necessary bending resistance to arrest and saturate the roll bending due to the zig-zag instability and leads to a stationary line defect which is called a phase grain boundary.

III. Analytical Results

For k close to k_B, G^2 is approximated to second order by $(k^2 - k_B^2)^2$. Choosing $k_B = 1$, the RCN (regularized Cross Newell) free energy divided by ε becomes

$$E^\varepsilon[\Theta] = \int_\Omega \left(\varepsilon(\nabla \cdot \vec{k})^2 + \frac{1}{\varepsilon}(k^2 - 1)^2 \right) d\vec{X}. \qquad (1)$$

Question:

Asymptotic behavior as $\varepsilon \longrightarrow 0$ of the minimizers Θ^ε of $E^\varepsilon[\Theta]$ within the class

$$\mathcal{A}^\varepsilon = \left\{ \Theta \in H^2(\Omega);\ \Theta|_\Omega = \alpha^\varepsilon(s),\ \frac{\partial \Theta}{\partial n}|_\Omega = \beta^\varepsilon(s) \right\} \qquad (2)$$

The energy has the form of the Ginzburg-Landau functional except that the vector fields are gradients.

Theorem 1. *1. As $\varepsilon \longrightarrow 0$, the minimizers $\Theta^\varepsilon \longrightarrow \Theta^0$ in $H^1(\Omega)$ where Θ^0 solves the eikonal equation $|\nabla\Theta^0| = 1$. Defects are, therefore, supported on locally 1-dimensional sets which are a union of locally rectifiable curves. Let Σ denote this total defect locus.*

2. The asymptotic minimal energy is bounded:

$$\liminf_{\varepsilon\longrightarrow 0} E(\Theta^\varepsilon) \leq 1/3 \int_\Sigma |[\nabla\Theta^0]|^3 ds$$

where $[\nabla\Theta^0]$ is the jump in $\vec{k}^0$ across Σ and ds is the element of arclength.

3. In the class of cases when Σ is a single straight line segment, the previous inequality becomes an equality; i.e., the upper bound is tight.

Remark:

These one dimensional defect loci are $phase\ grain\ boundaries$. The bending term $\int_\Omega |\nabla\vec{k}|^2$ in this free energy will diverge as $1/\varepsilon$. This is a major increase in energetic cost compared to the $\log(1/\varepsilon)$ cost of the original Ginzburg-Landau problem whose defects are point vortices.

Hints of a demonstration:

• Analytical difficulties of RCN: 4^{th} order equation and thus it is difficult to calculate the minimizers.

Good approximate minimizers can be found by solving the self-dual problem

$$\varepsilon \nabla^2 \Theta = \pm\sqrt{G^2}$$

for which the free energy is equipartitioned between the wavenumber mismatch and the bending energy components.

The self-dual solutions are exact solutions provided the Hessian (proportional to the Gaussian curvature of the graph of Θ) vanishes; i.e.,

$$\Theta_{XX}\,\Theta_{YY} - \Theta_{XY}^2 = 0.$$

In the weak bending limit this equipartition is true in general; i.e., solutions of the associated self-dual equations were also solutions of the fourth order variational equations.

In the general case, these solutions nevertheless provide a good class of test functions for deriving uniform bounds on wavenumber fluctuations and curvature.

The class of admissible functions Θ must now satisfy satisfy boundary conditions $\Theta|_{\partial\Omega} = \alpha(s)$, independent of ε, and $\beta^{\varepsilon}(s) = \partial_\nu \Theta^{\varepsilon}_{SD}|_{\partial\Omega}$ where $\Theta^{\varepsilon}_{SD}$ is the solution of the self-dual equation corresponding to the boundary values $\alpha(s)$.

Moreover, it is easy to calculate their limit as $\varepsilon \longrightarrow 0$. In the $\varepsilon \longrightarrow 0$ limit, the curvature of Θ_{SD} concentrates in points.

The transformation

$$\Theta = \varepsilon \ln \Psi$$

linearizes the self-dual equation as the Helmholtz equation

$$\varepsilon^2 \nabla^2 \Psi - \Psi = 0.$$

Example of the "Knee" solution :

The straight roll solution is

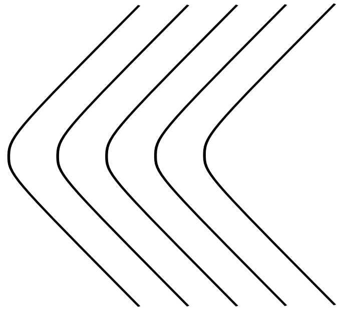
$$\Psi = e^{\vec{k}\cdot\vec{X}/\varepsilon}, \ k = 1$$

The regularized phase grain boundary (PGB) solution is simply the sum of two exponentials

$$\Psi = e^{\vec{k}_+\cdot\vec{X}/\varepsilon} + e^{\vec{k}_-\cdot\vec{X}/\varepsilon}$$

where $\vec{k_\pm} = (\cos\varphi, \ \pm\sin\varphi)$. That corresponds to a phase

$$\Theta = k_0 X + \varepsilon \ln 2 \cosh\left(\sqrt{1-k_0^2}Y/\varepsilon\right).$$



This PGB is also solution to the Cross-Newell equation since its Gaussian curvature is zero.

The energy of the PGB obeys $\lim_{\varepsilon\to 0} E^\varepsilon = \frac{8L}{3}\sin^3\varphi$. This coincides with the general result stated in the Theorem.

Theorem 2. *Suppose v_ϵ solves $\epsilon(\Delta v_\epsilon) + (1 - |\nabla v_\epsilon|^2) = 0$ on Ω with $v_\epsilon = \theta$ on the boundary of Ω where $|\theta(x) - \theta(y)| \leq a \operatorname{dist}(x, y)$ with $a < 1$. Then as $\epsilon \to 0$, v_ϵ converges uniformly on the closure of Ω to the unique viscosity solution of $|\nabla v|^2 - 1 = 0$ on Ω with $v = \theta$ on Ω.*

Prescription:

$$\mathbf{k} = \nabla v(\vec{X}) = -\frac{\vec{X} - \vec{X}(\bar{s})}{|\vec{X} - \vec{X}(\bar{s})|},$$

where

$$\left(\frac{\vec{X} - \vec{X}(\bar{s})}{|\vec{X} - \vec{X}(\bar{s})|} - \nabla v(\vec{X}(\bar{s})) \right) \cdot \vec{X}'(\bar{s}) = 0.$$

This result is due to Ercolani and Taylor (Physica D, in press) who have generalized the type of possible boundary conditions.

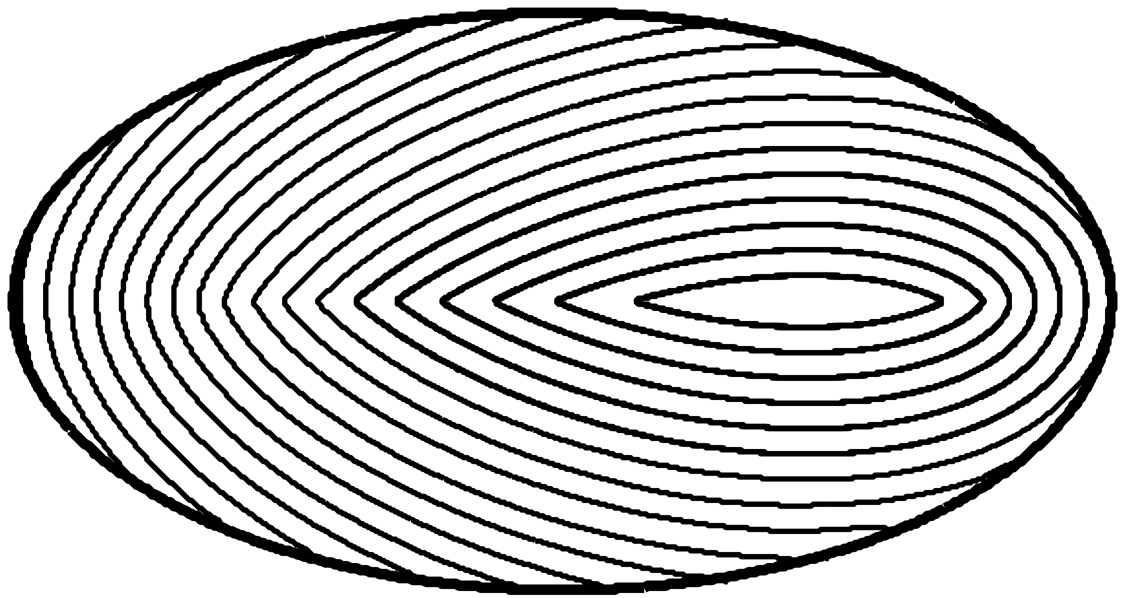


Figure 10: Eikonal solution with non-constant boundary conditions, and horizontal defect locus

Corollary 3. *There is a constant C, independent of ϵ, such that for domains Ω with generic defect locus Γ,*

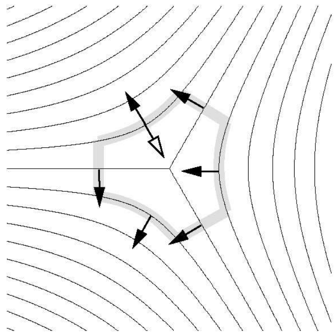
$$\begin{aligned} \int_\Omega |\nabla \mathbf{k}|^2 d\mathbf{x} &\leq C/\epsilon \qquad (3) \\ \int_\Omega (1-k^2)^2 d\mathbf{x} &\leq C\epsilon. \qquad (4) \end{aligned}$$

From (4) we may conclude that $|\nabla\Theta^\epsilon|^2 \to 1$ in $L^2(\Omega)$. It follows that there is a subsequence $\Theta^{\epsilon_j} \rightharpoonup \bar{\Theta}$ in $H^1(\Omega)$. This sequence converges strongly to $\bar{\Theta}$ in $L^2(\Omega)$.

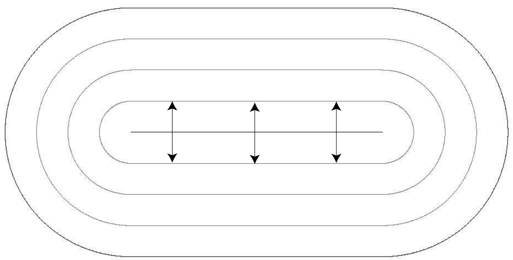
Recent results (Ambrosio, DeLellis, Mantegazza, DeSimone, Kohn, Mller, Otto) allow to prove strong convergence in $H^1(\Omega)$.

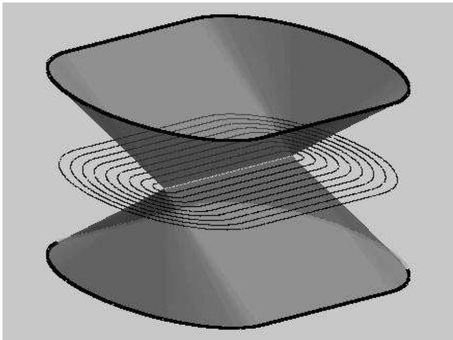
IV. Presence of twist

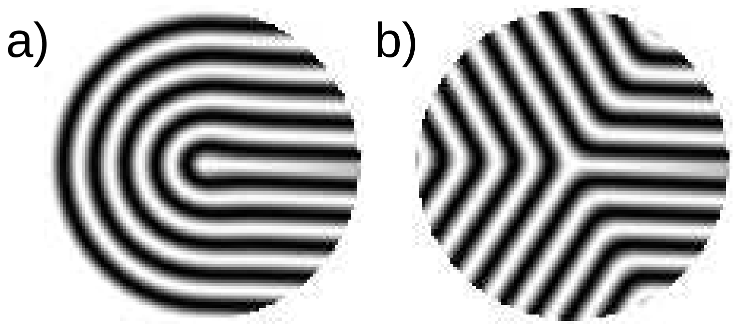
The wavevector is a director field:



To include such double-valued fields one can consider single-valued vector fields on Riemann surfaces:







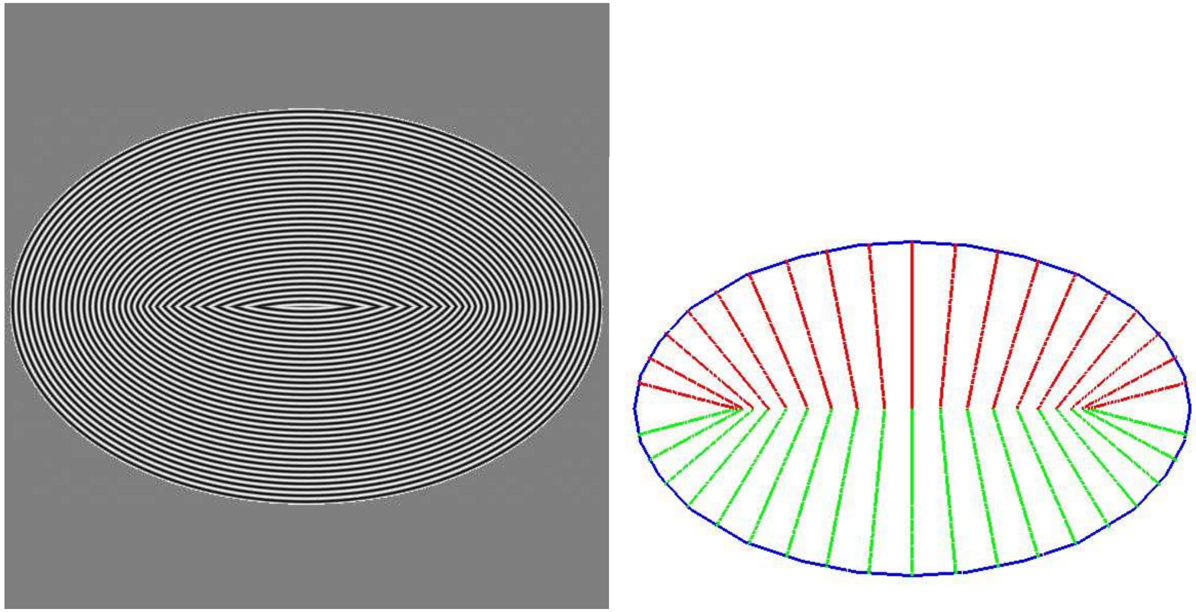
a) Convex disclination b) Concave disclination numerically calculated as solutions of the RCN equation.

The previous theorem involves minimization over vector fields. What happens with director field perturbations?

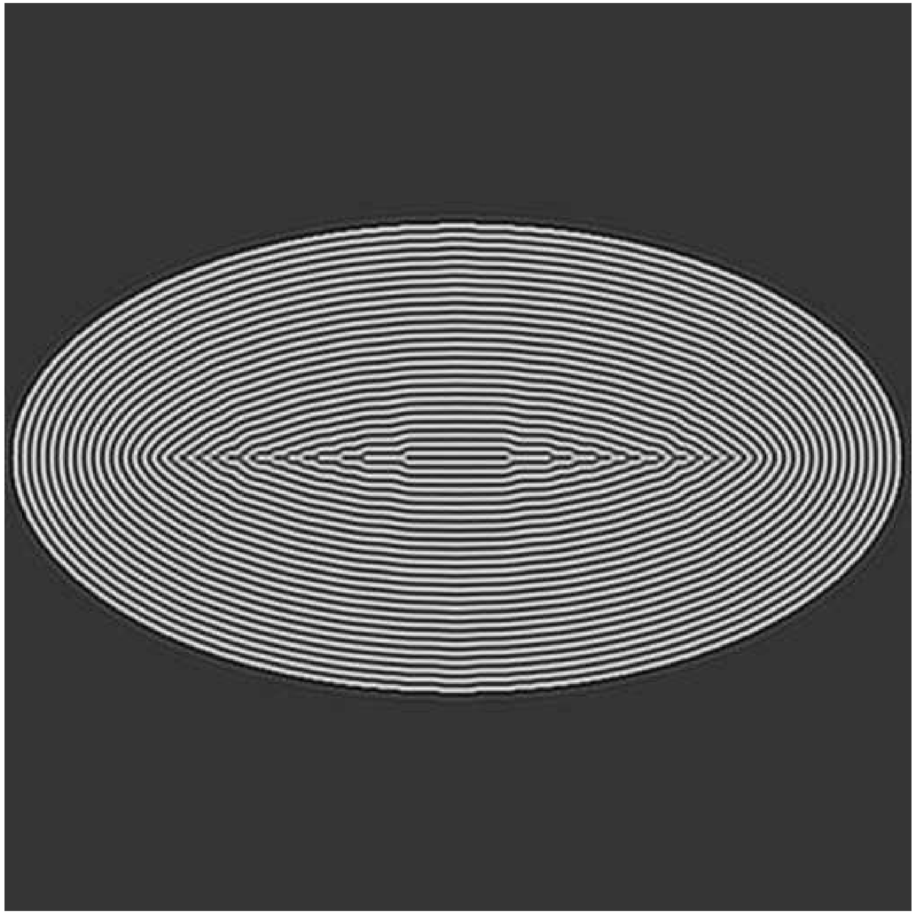
In particular the energy cost associated with the sign reversal of $\mathbf{k}$ should be discounted.

Consider a test case: the ellipse container.

The weak solution is



It is used as initial condition in a Swift-Hohenberg code



In the central regions of the PGB where the rolls bend sharply the computed solution shows a string of dislocations which can also be viewed as convex and concave disclinations pairs.

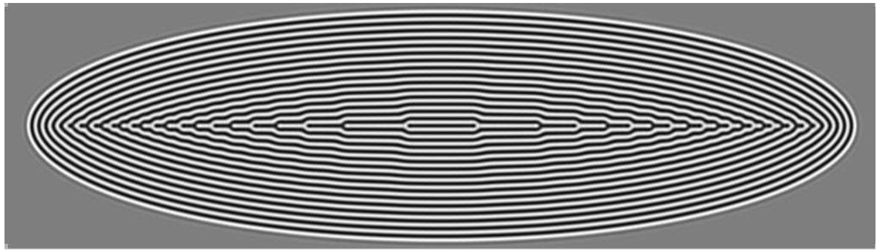
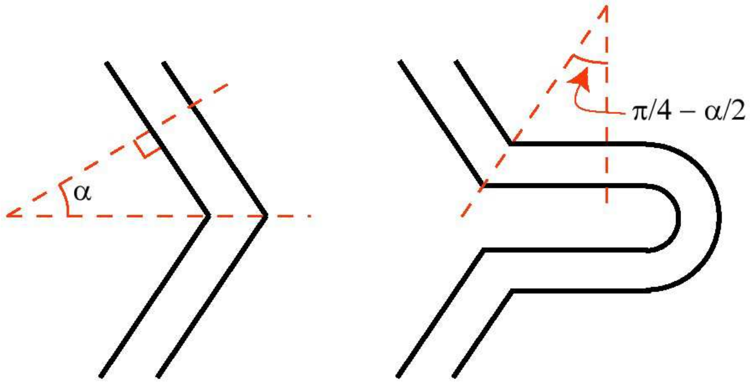


Figure 11: Rolls from numerical simulation of Swift-Hohenberg with an ellipse whose major axis is 4 times longer than its minor axis.

Their spacing gets closer further out and are then replaced by the eikonal PGB.



$\frac{8}{3}\sin^3\alpha$ $\qquad$ $\frac{8}{3}(1-\sin\alpha)$

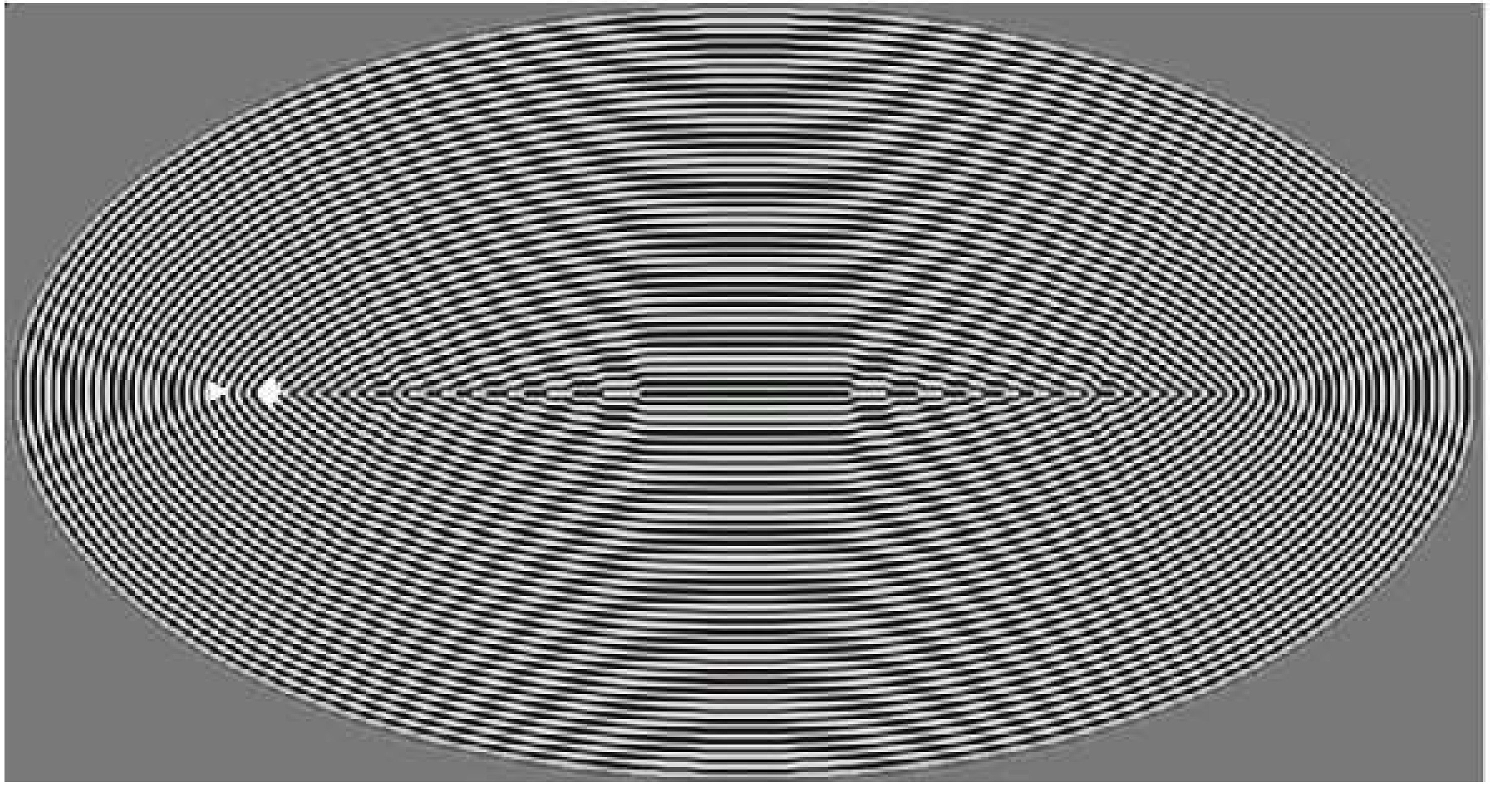
Energy cost per unit length of grain boundary

The eneregy of the circular part of the convex disclination, proportional to $\epsilon \ln \frac{1}{\epsilon}$ is negligible.

The convex-concave disclination pair is energetically preferred when $\alpha > 43^o$.

Experiment with Swift-Hohenberg:

The first protuberance indeed appears close to the critical angle ($\phi \approx 43^o$).



Triangle: curvature center Diamond: critical transition

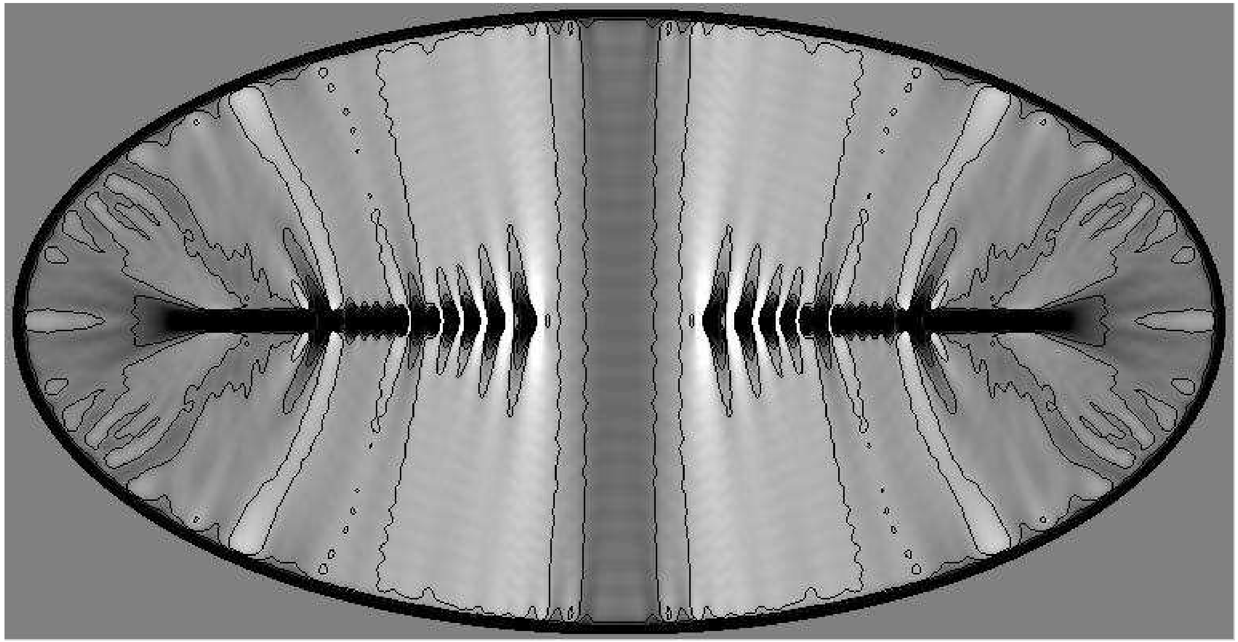
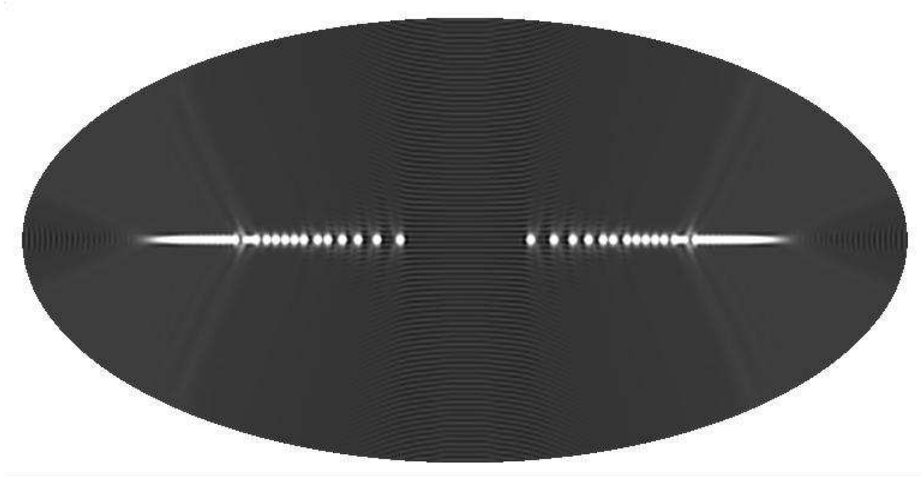


Figure 12: Local wavenumber magnitude. Lighter grays correspond to higher values of k. The contours shown are $k = .995$, $k = 1$ and $k = 1.005$.



Energy density (smoothed to remove features at the roll wavelength).

Tightly spaced dislocations reproduce weak roll bending, while widely spaced ones replace sharply bent rolls.

Comparison with Experiments

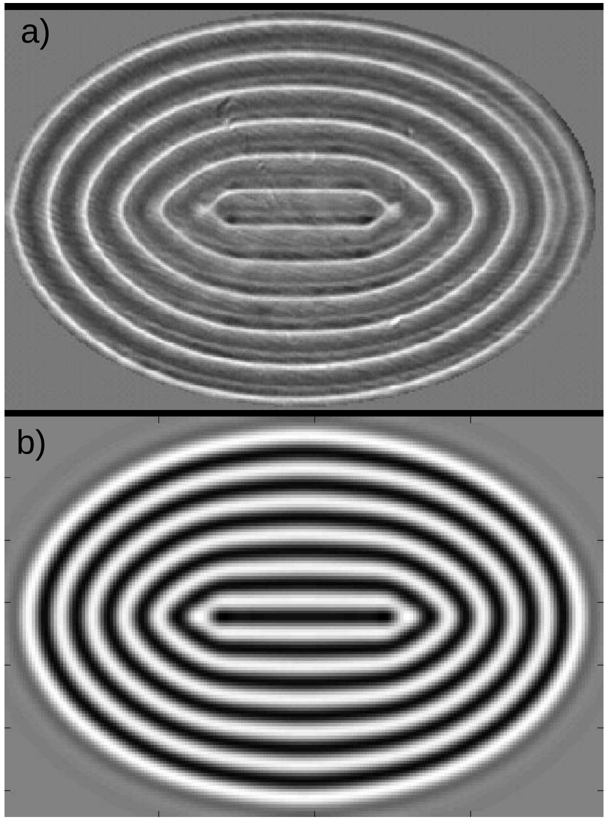


Figure 13: a) Image of convection rolls from an experiment with ethanol at a Prandtl number of 14.7 (courtesy of Meevasana and Ahlers) b) Numerical simulation of Swift-Hohenberg with similar geometry

In addition, it is found in the experiments that the size of the inner straight roll decreases as the stress parameter is increased. This particular result is not found with the SH equation. This behavior is likely to be related to the decrease of the selected wavenumber in Oberbeck-Boussinesq as the Rayleigh number increases.

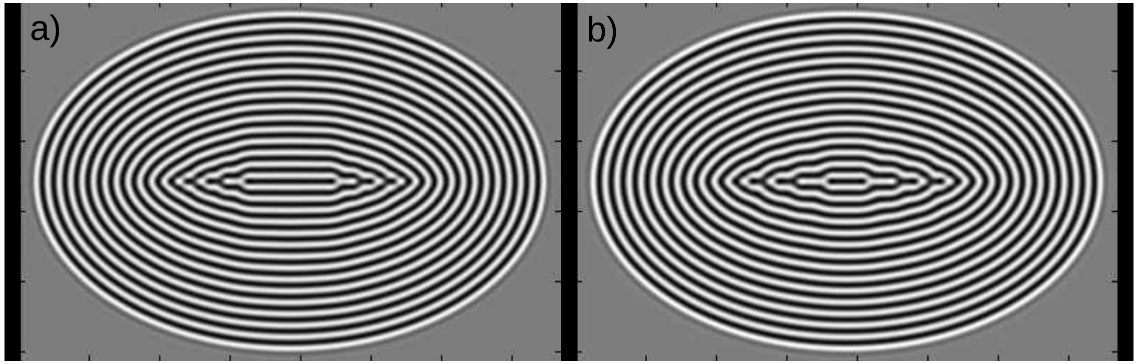
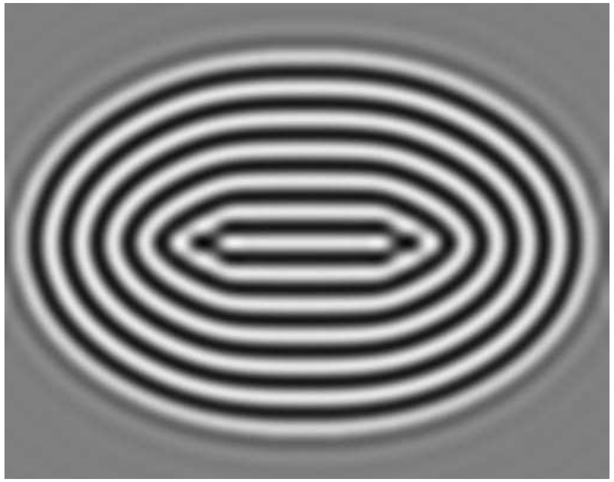
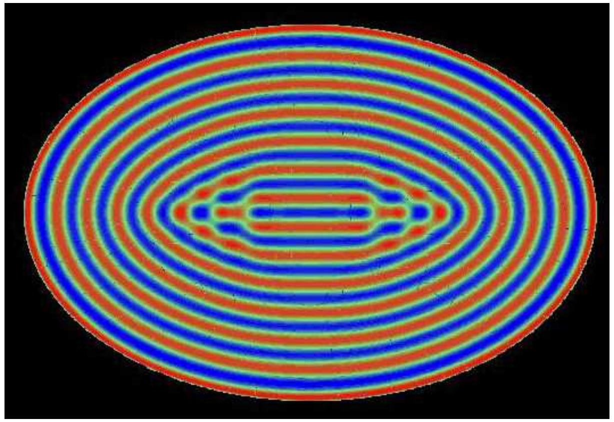


Figure 14: Result of integrating Swift-Hohenberg using $k_B = 1$. This was used as the initial condition for b) which was Swift-Hohenberg for $k_B = 0.95$

Comparison with other simulations





Swift-Hohenberg simulation

Boussinesq simulation

(courtesy of Mark Paul)

There is an explicit formula for a string of dislocations whose character is quite similar to the dislocations seen in the numerical experiments. For example, a string of dislocations located along the x-axis, at positions $\pm x_n$ is

$$\theta = y - \mathsf{sign}(y)\epsilon \log\left(1 + \sum_{n=1}^{N}\left(\frac{e^{n\pi} - e^{(n+1)\pi}}{2}\right)\mathsf{erf}\left(\frac{x - x_n}{\sqrt{2\epsilon|y|}}\right)\right. \\ \left. - \sum_{n=1}^{N}\left(\frac{e^{n\pi} - e^{(n+1)\pi}}{2}\right)\mathsf{erf}\left(\frac{x + x_n}{\sqrt{2\epsilon|y|}}\right)\right). \tag{5}$$

This is an exact solution of the phase equation with a "weak bending" assumption. In fact, if a multi-dislocation with the same spacing as that seen in the numerical solution is patched to the outer portion of the eikonal solution, this initial condition settles to a solution of the same form with the position of the dislocations essentially unchanged. (The only real changes are along the interface where the solutions are patched together.)

V. Conclusion

• Variational model for patterns far from threshold based on a regularized Cross-Newell phase-diffusion equation.

• Variations must be made over a class of vector fields which are only constrained to be locally gradient.

• The energy should be modified to discount the bending energy cost associated with sign reversal of the local wavevector.

Major difficulty: minimization must be made on the vector field as well as on the geometry (type and location of defects).