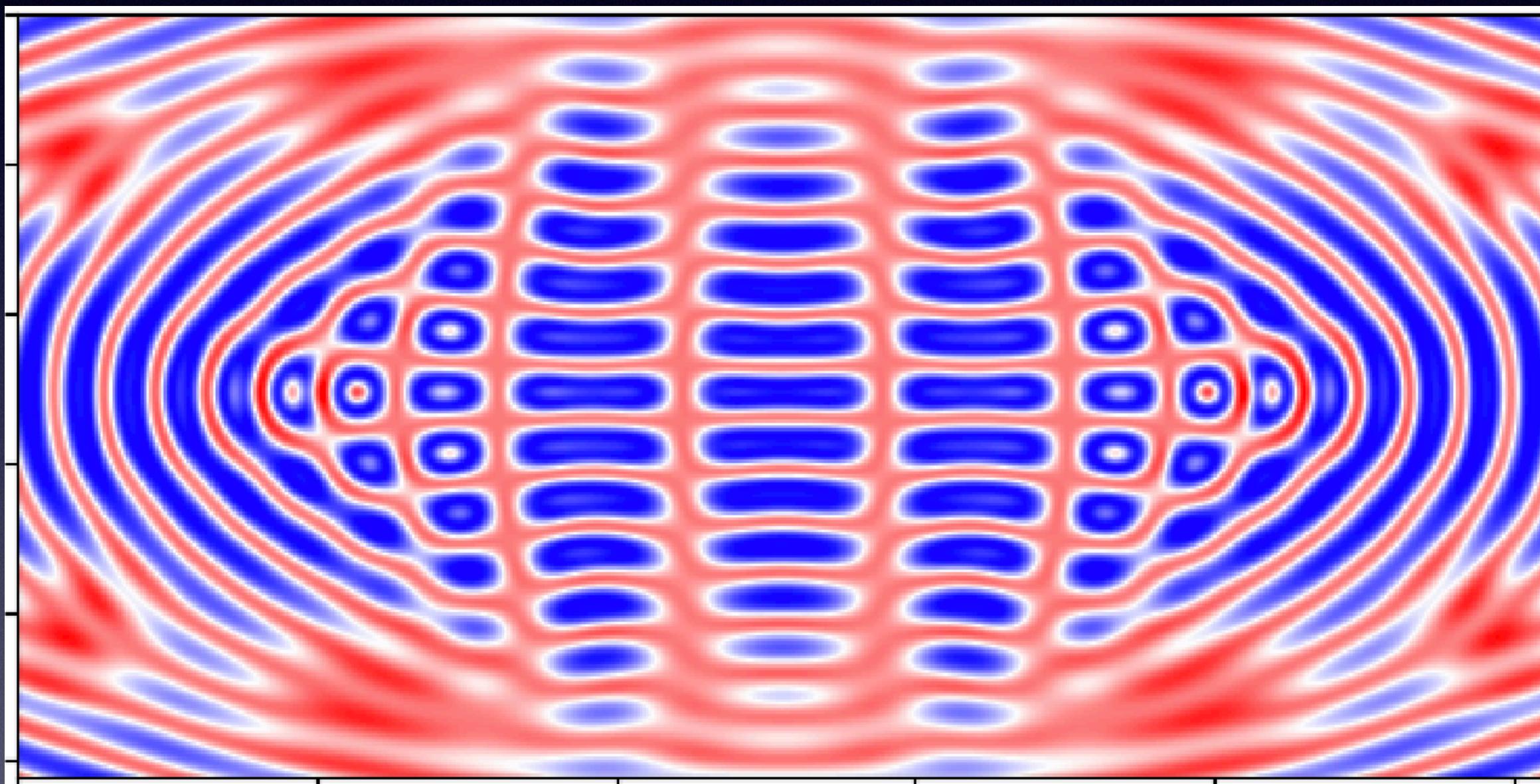
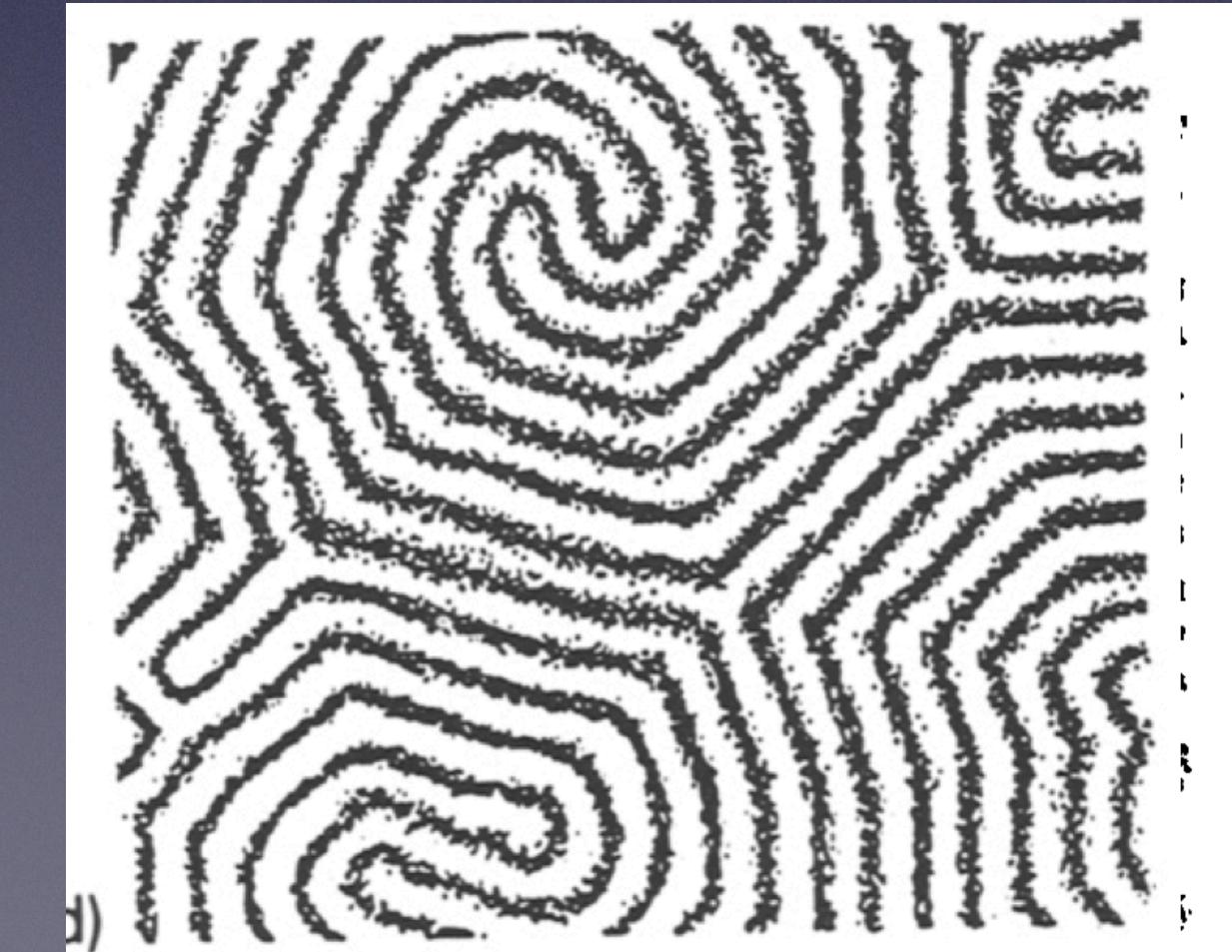
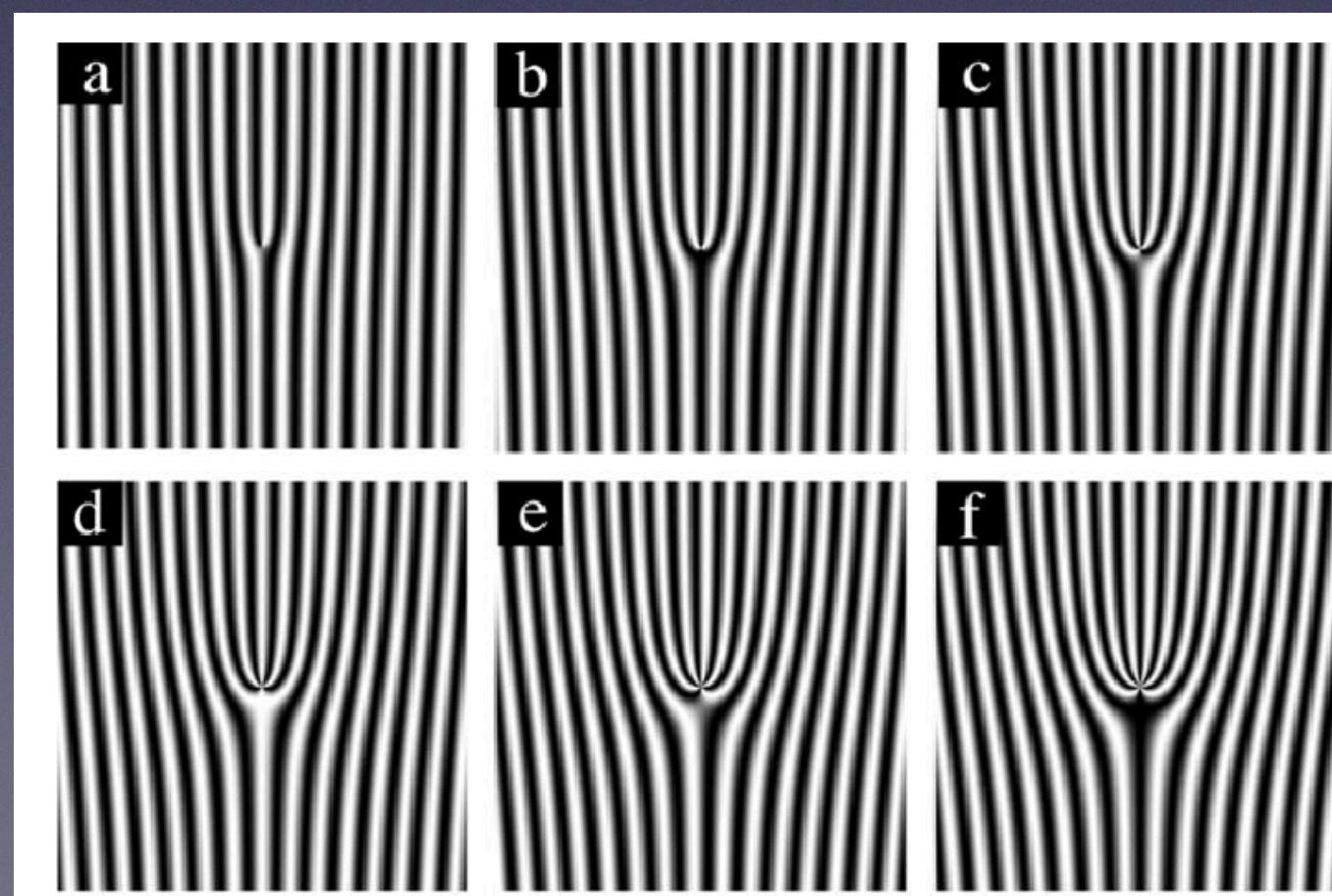
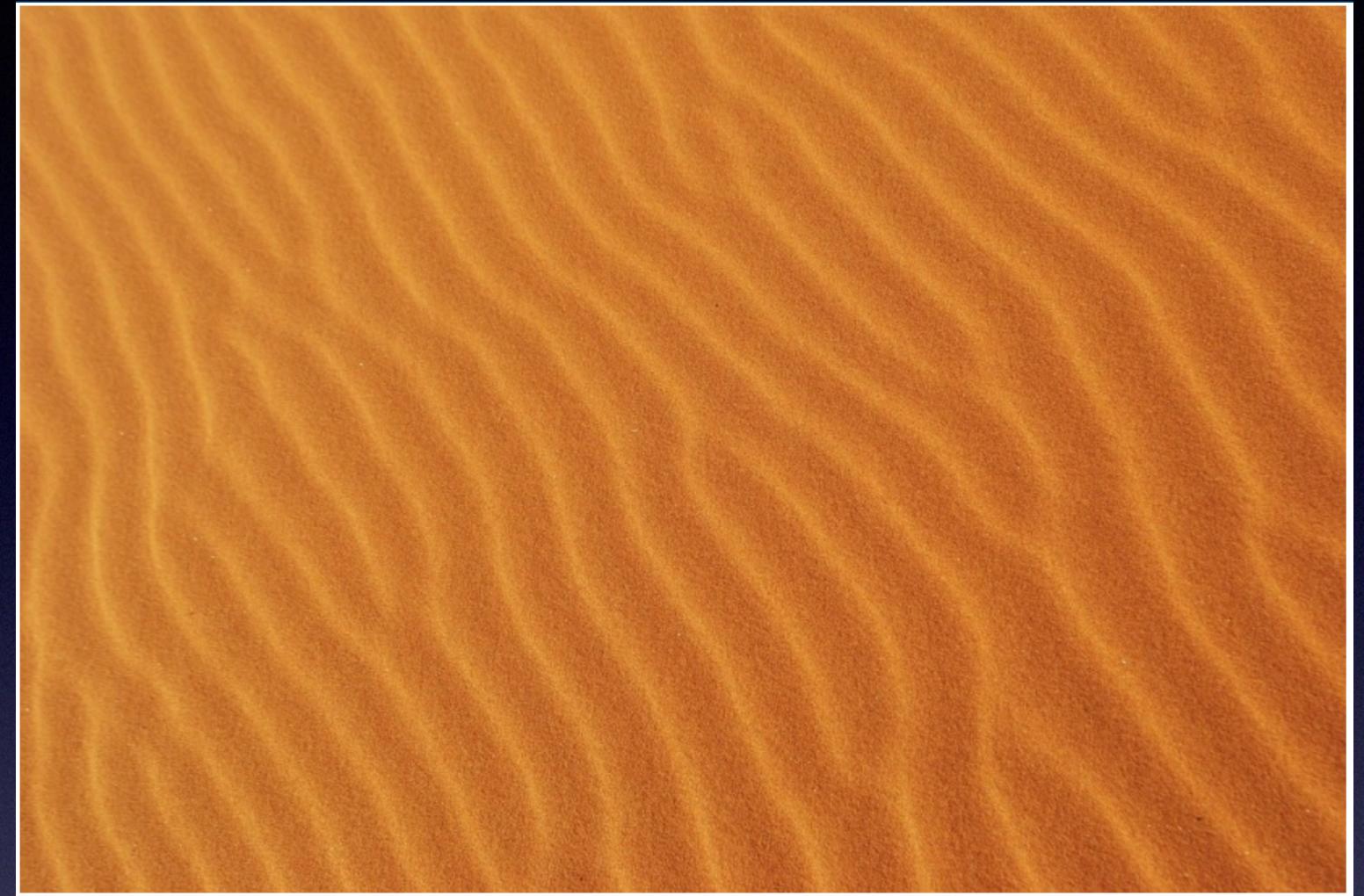
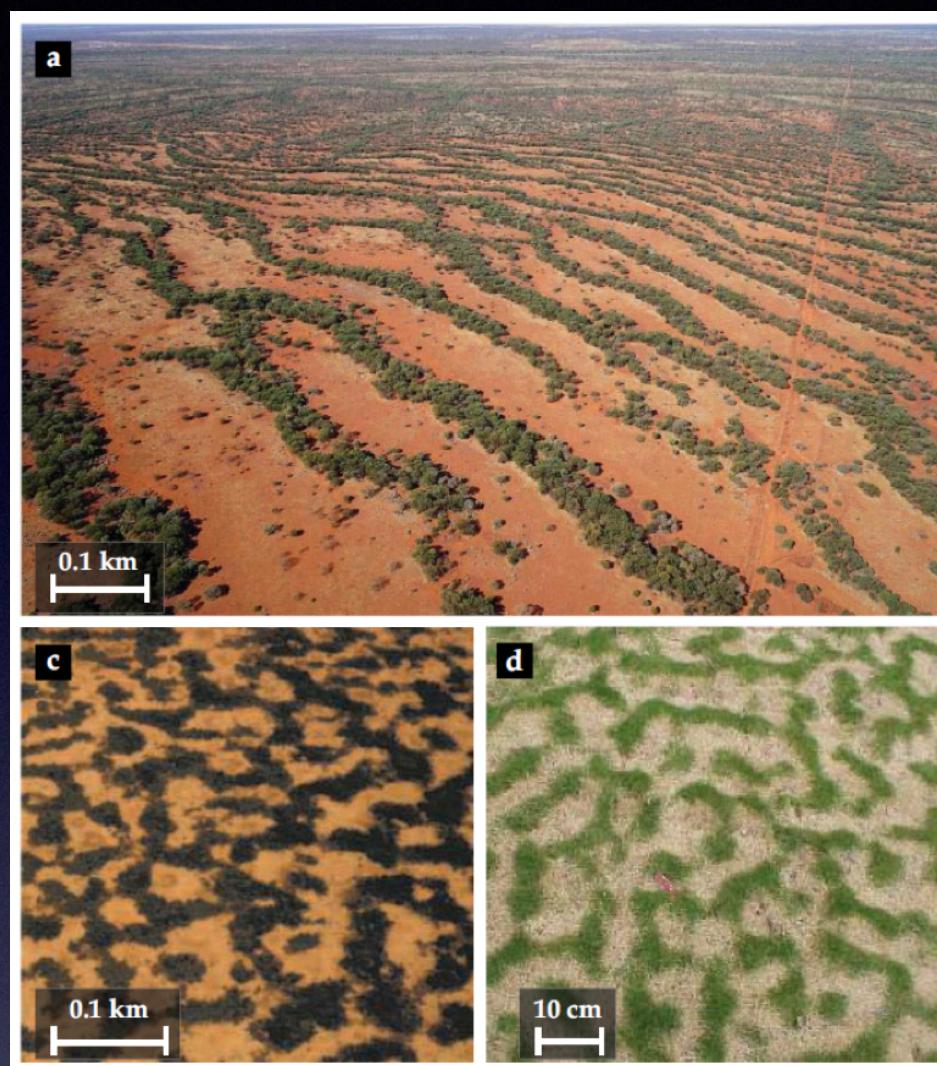
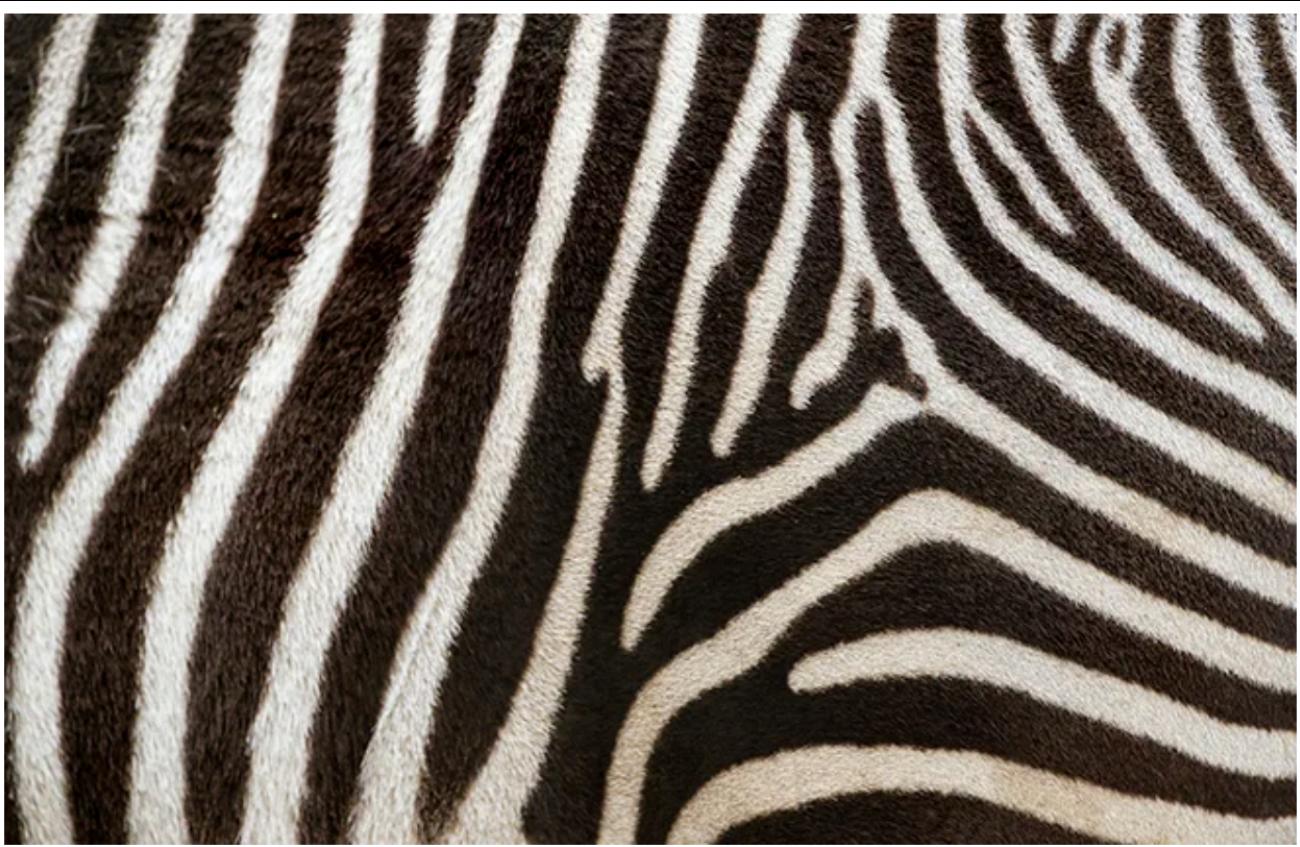


The Theory of Natural Stripe Patterns



Edward McDugald
University of Arizona

Natural Stripe Patterns are Ubiquitous



Canonical “Microscopic” Mathematical Model: Swift Hohenberg

- Can be derived from the Oberbeck-Bousinesq approximation for heat transfer in fluids. For striped patterns, $R > 0$
- The generalizable quality of SH is that it is rotationally and translationally invariant, and it is a gradient flow.
- Difficult to deduce qualitative descriptions from SH

$$u_t = -(\nabla^2 + 1)^2 u + R u - u^3$$

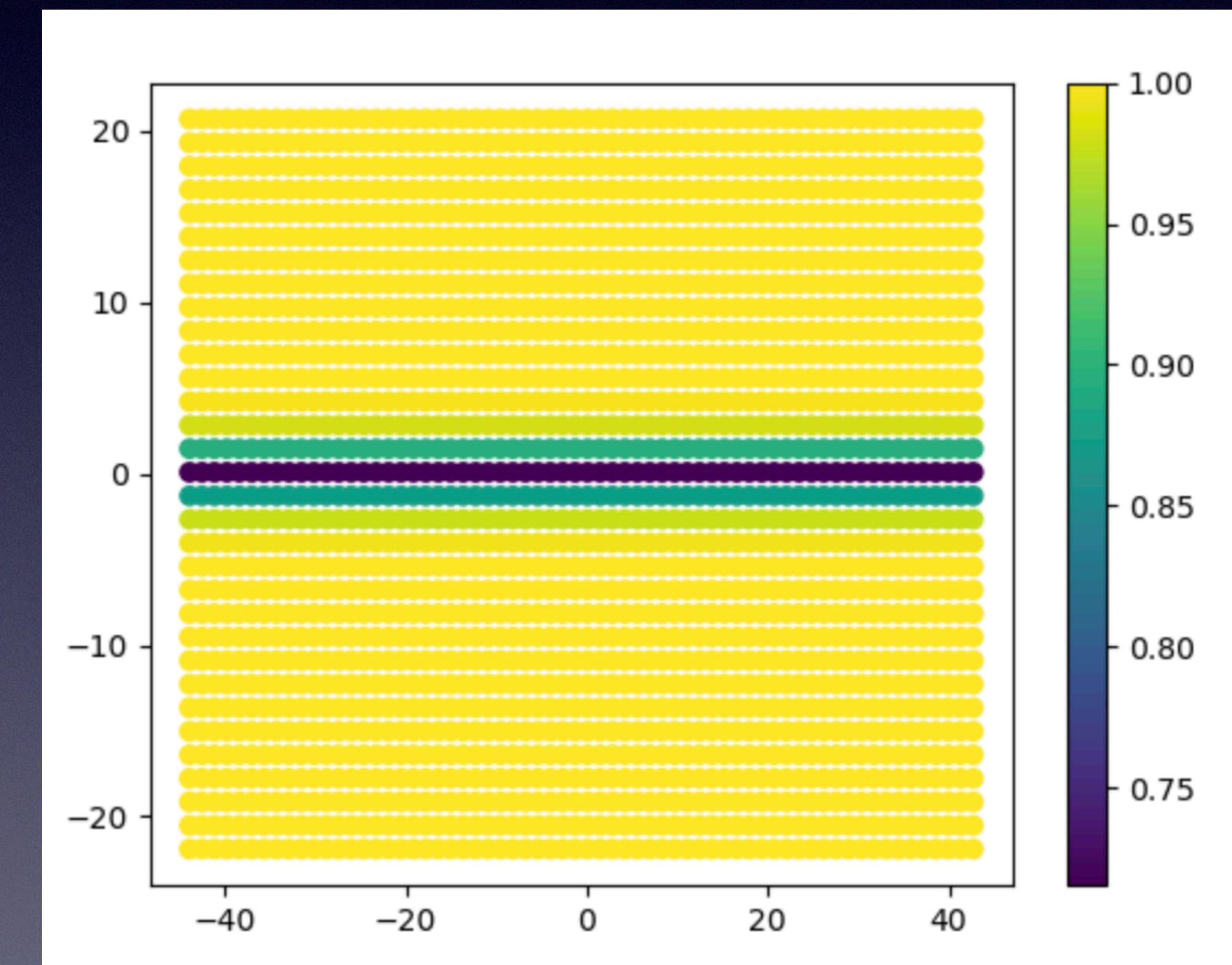
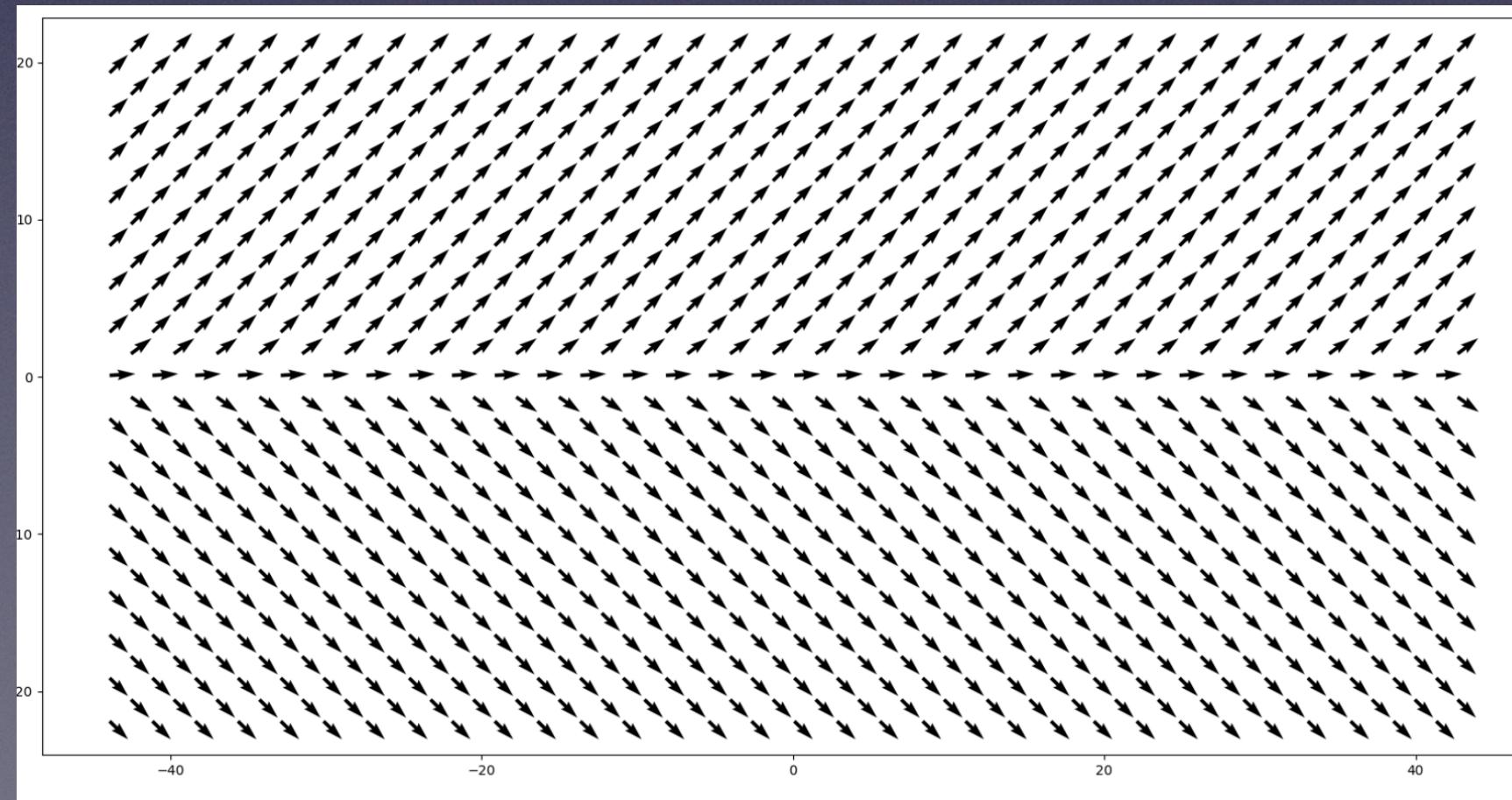
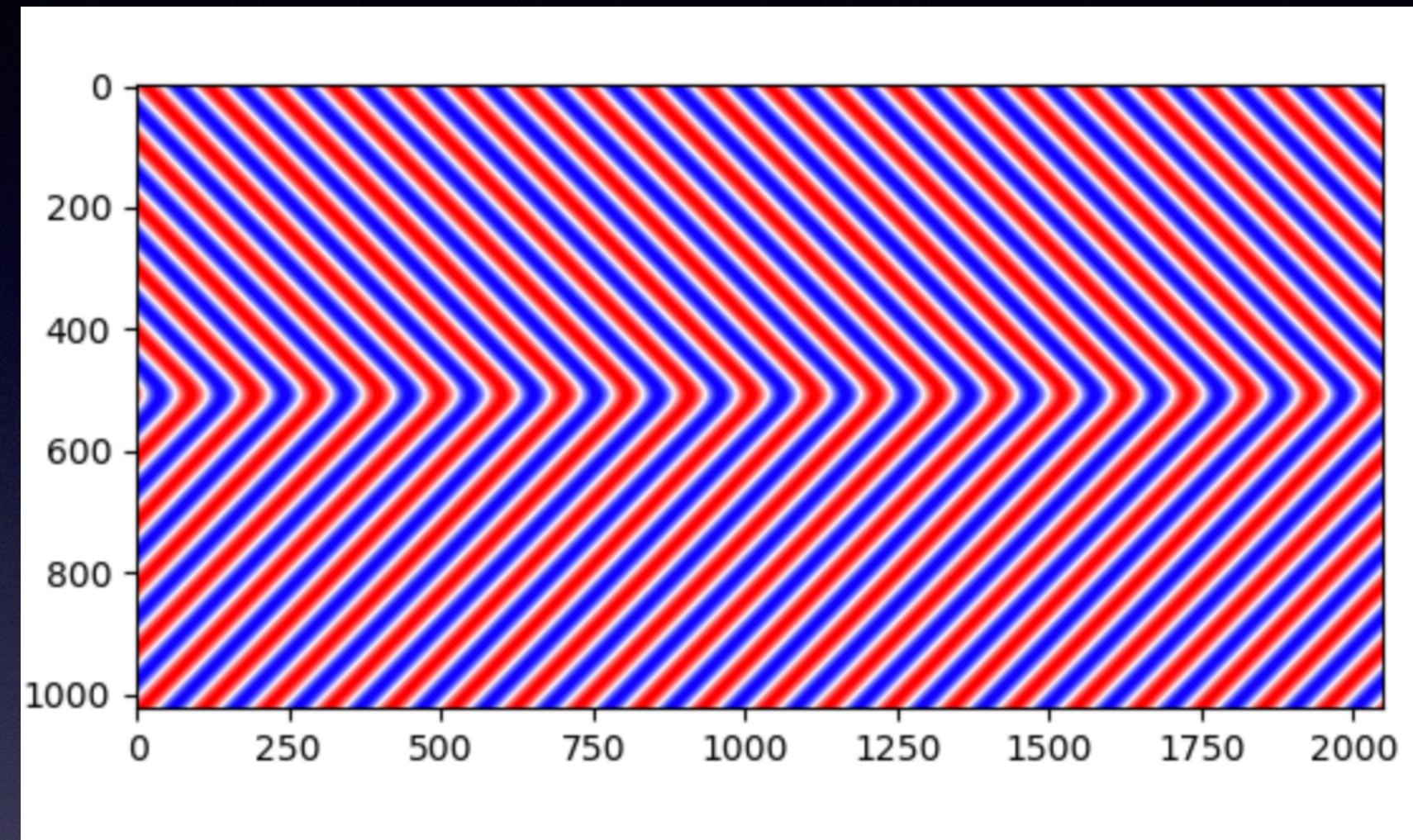
$$u_t = -\frac{\delta E}{\delta u}$$

$$E = \int ((\nabla^2 + 1)u)^2 - \frac{1}{2}R u^2 + \frac{1}{4}u^4$$

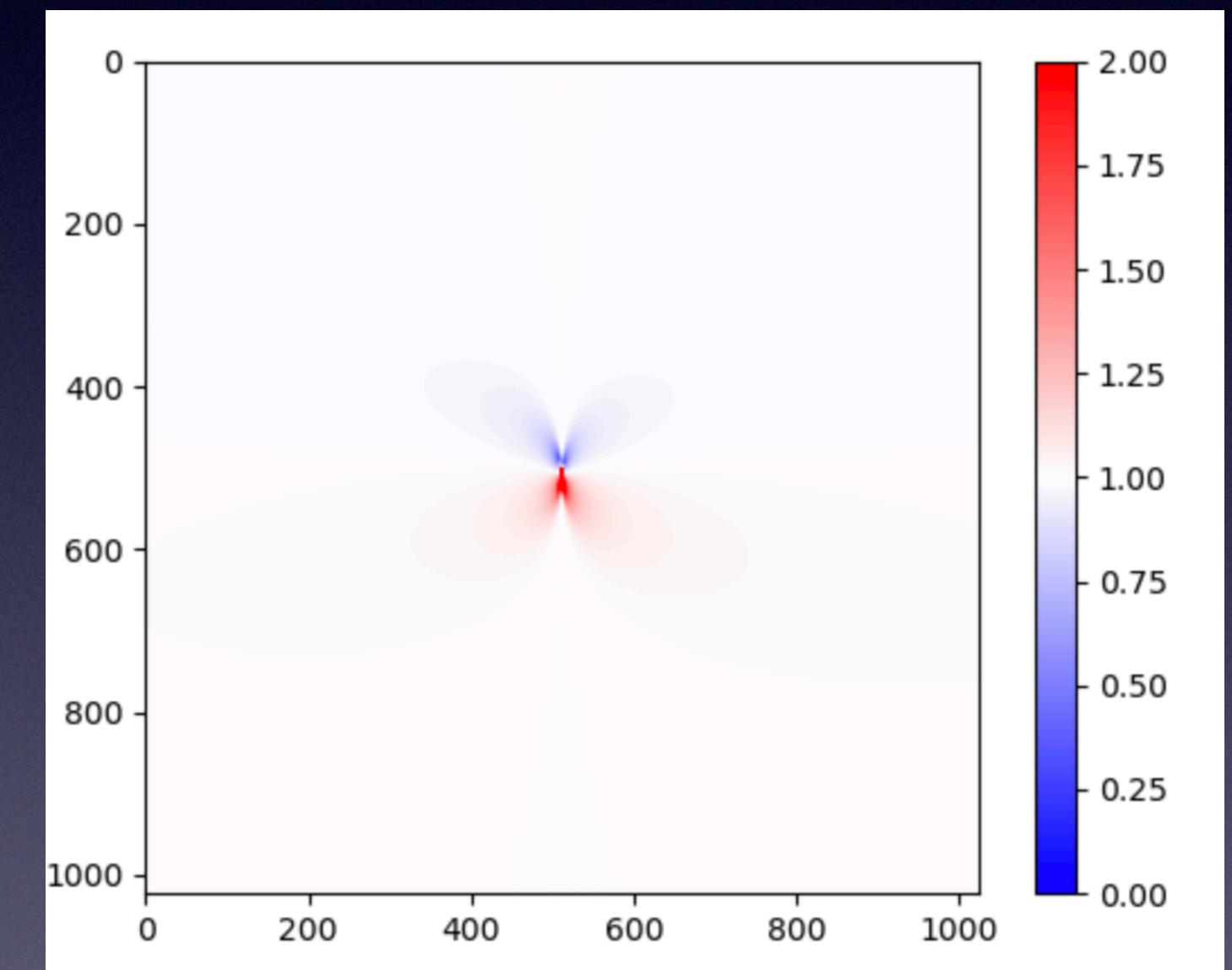
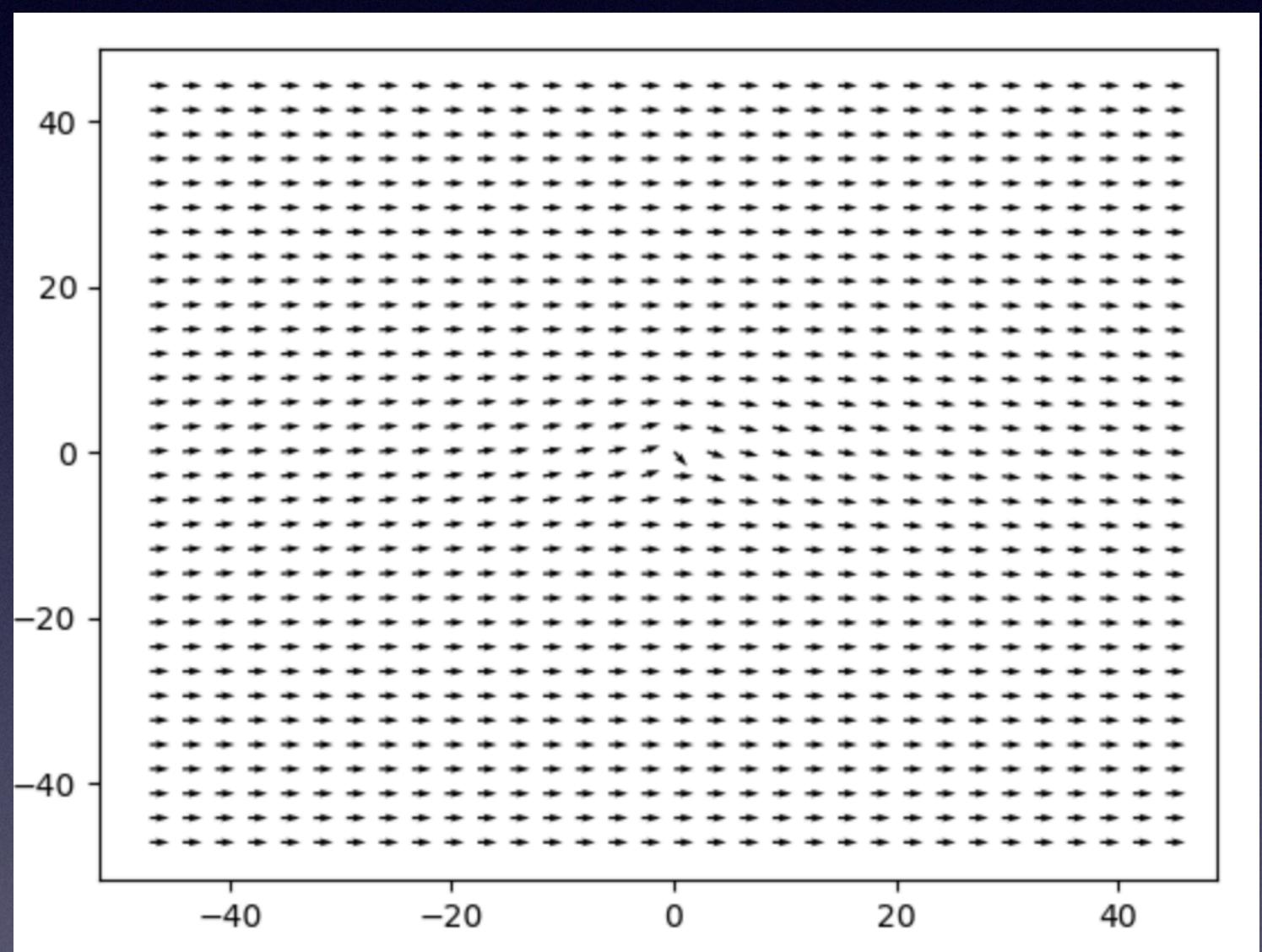
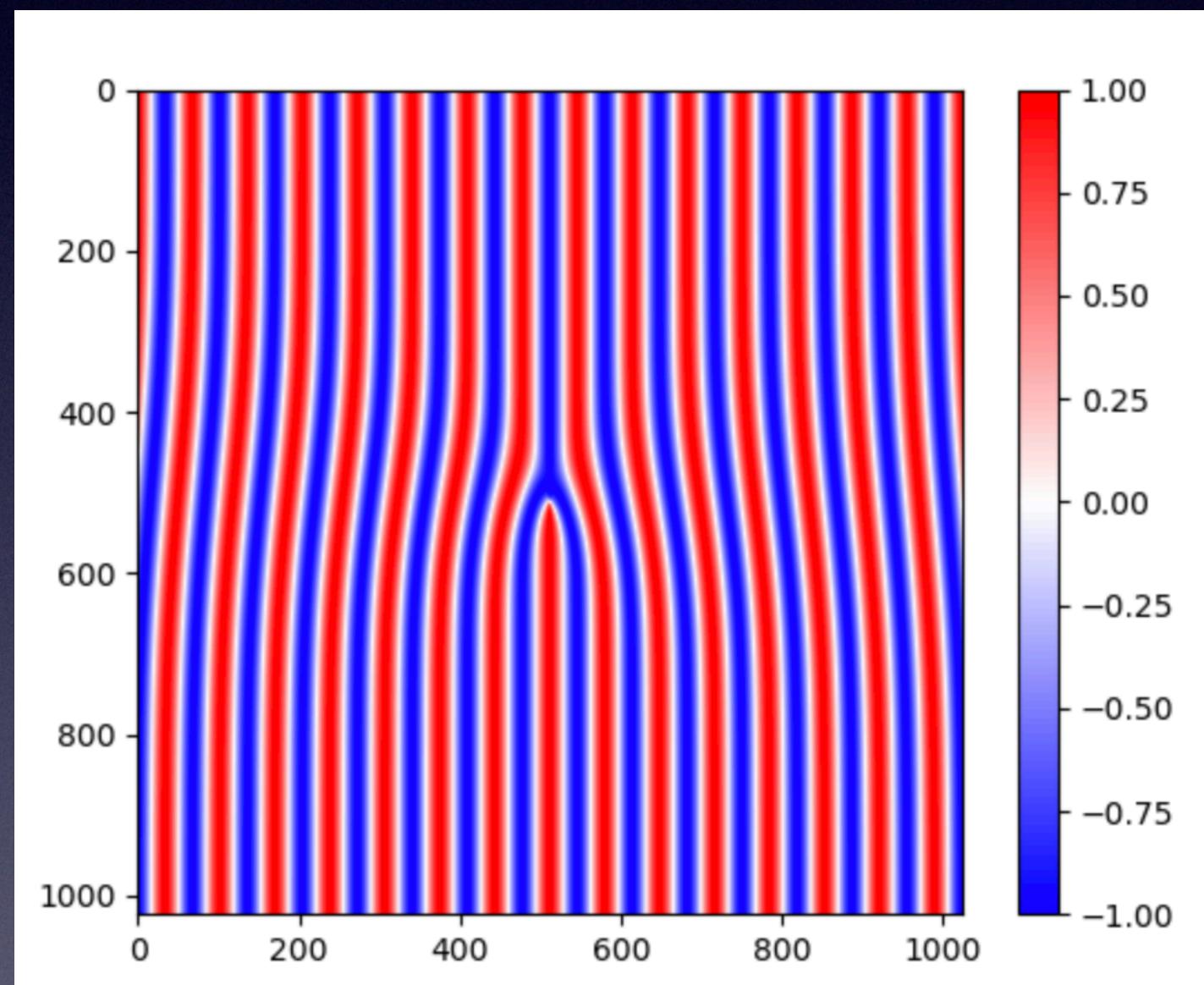
Observation: Existence of a local Wave Vector

- SH admits steady solutions of the form $u = \sum_n A_n(k^2) \cos n\theta$
- The fields are periodic, and locally resemble a plane wave almost everywhere. Moreover, the wave vector changes slowly compared to the underlying field. This motivates both an ansatz in terms of a phase, $\theta = \vec{k} \cdot \vec{x}$, where $\vec{k} = \nabla \theta$ and an introduction of slow space and time scales.
- We will commonly refer to the wave number, which is $k = |\vec{k}| = |\nabla \theta|$

Wave Vector Field near a Phase Grain Boundary



Wave Vector Field near a Dislocation



Deriving a Macroscopic Equation via Method of Multiple Scales and Averaging

- Define slow variables: $\vec{X} = \epsilon \vec{x}$, $T = \epsilon^2 t$, $\Theta = \epsilon \theta$
- This change of variables yields: $\partial_t = \epsilon \Theta_T \partial_\theta + \epsilon^2 \partial_T$, $\nabla_x = \vec{k} \partial_\theta + \epsilon \nabla_{\vec{X}}$
- Option 1: Write $u = u(\theta; X, Y, T) = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \dots$, and substitute into SH. At each order of ϵ , one will obtain solvability conditions that give PDEs for Θ
- Option 2: Write $u = u(\theta; , X, Y, T)$, and substitute into the SH *energy*, average over θ , and compute variations in terms of the amplitude and phase variables.

Easiest Example: Averaging the Complex SH Energy (1)

- The SH energy is: $E[u, u^*] = \int (\nabla^2 + 1)u(\nabla^2 + 1)u^* - \frac{1}{2}Ru u^* + \frac{1}{2}u^2(u^*)^2$
- The Ansatz is: $u = A(k^2; \vec{X}, T)e^{i\theta(\vec{x}, t)}$
- The variations in u, u^* are $\frac{\delta E}{\delta u} = (\nabla^2 + 1)^2 u^* - Ru^* + u^2 u^*$ and $\frac{\delta E}{\delta u^*} = (\nabla^2 + 1)^2 u - Ru + (u^*)^2 u$
- The first and second order spatial derivatives are:
$$\nabla_{\vec{x}} u = e^{i\theta}(i\vec{k} + \epsilon \nabla_{\vec{X}})A$$
$$\nabla_{\vec{x}} u^* = e^{-i\theta}(-i\vec{k} + \epsilon \nabla_{\vec{X}})A$$
$$\nabla_{\vec{x}}^2 u = e^{i\theta}(-k^2 + i\epsilon(2\vec{k} \cdot \nabla_{\vec{X}} + \nabla_{\vec{X}} \cdot \vec{k}) + \epsilon^2 \nabla_{\vec{X}}^2)A$$
$$\nabla_{\vec{x}}^2 u^* = e^{-i\theta}(-k^2 - i\epsilon(2\vec{k} \cdot \nabla_{\vec{X}} + \nabla_{\vec{X}} \cdot \vec{k}) + \epsilon^2 \nabla_{\vec{X}}^2)A$$

Easiest Example: Averaging the Complex SH Energy (2)

- The averaged energy is now written (the averaging in θ occurs automatically):

$$\bar{E} = \bar{E}_0 + \epsilon^2 \bar{E}_2 = \int \left((k^2 - 1)A^2 - RA^2 + \frac{1}{4}A^4 + K \right) d\vec{x} + \epsilon^2 \int \left((2\vec{k} \cdot \nabla A + \nabla \cdot \vec{k}A)^2 + 2(1 - k^2)A \nabla^2 A \right) d\vec{x}$$

- The variations in u, u^*, A, θ are related by: $\delta E = \frac{\delta E}{\delta u} \delta u + \frac{\delta E}{\delta u^*} \delta u^* = -2A_t \delta A - 2A^2 \Theta_t \delta \theta$

- $\frac{\delta E_0}{\delta A} = 2A((k^2 - 1)^2 - R + A^2)$, and $A_t = \epsilon^2 A_T$, so $A^2 = R - (k^2 - 1)^2$.

- Then $E_0 = \int \left(-\frac{A^4}{4} + K \right) d\vec{x} = \int \left(-\frac{1}{2}(A^2(k^2))^2 \right) d\vec{x}$ and $\frac{\delta E_0}{\delta \theta} = A^2(k^2) \frac{dA^2(k^2)}{dk^2} 2\nabla \cdot \vec{k}$

- Then $A^2 \theta_t + A^2 \frac{dA^2}{dk^2} \nabla \cdot \vec{k} = A^2 \theta_t + B(k^2) \nabla \cdot \vec{k} = 0$.

- First Order Phase Equation: $A^2 \Theta_T + \nabla_{\vec{X}} \cdot \vec{k} B(k^2) = 0$

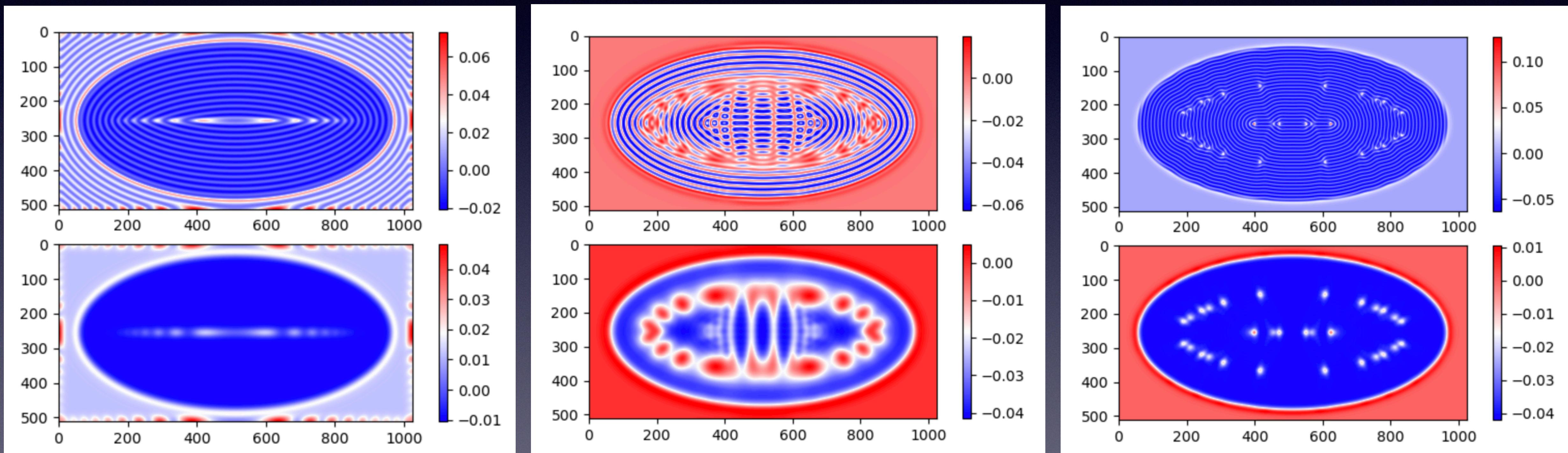
Easiest Example: Averaging the Complex SH Energy (3)

- In stripe patterns having a slowly varying wave vector, there is a preferred wave number k_B . It turns out that the leading order phase diffusion is ill-posed for wave numbers $k < k_B$. This state occurs at bends in the pattern, and we go to the second order energy term for regularization.
- We use the simplification $\bar{E}_2 \approx \int A^2(k_B^2)(\nabla \cdot \vec{k})^2 d\vec{x}$.
- And obtain the Regularized Cross Newell Equation:
$$A^2(k_B^2)\Theta_T + \nabla \cdot B(k^2) + \epsilon^2 A^2(k_B^2) \nabla^4 \Theta = 0$$
- We can define the constant of integration K in the leading order energy to write
$$\bar{E} = \int \left(\left(\frac{d}{dk^2} B(k^2) \right)_{k_B^2} (k^2 - k_B^2) + \epsilon^2 (\nabla \cdot \vec{k})^2 A^2(k_B^2) \right) d\vec{x}$$
. The first and second terms are called the “strain” and “bending” energies respectively.

A Few Notes

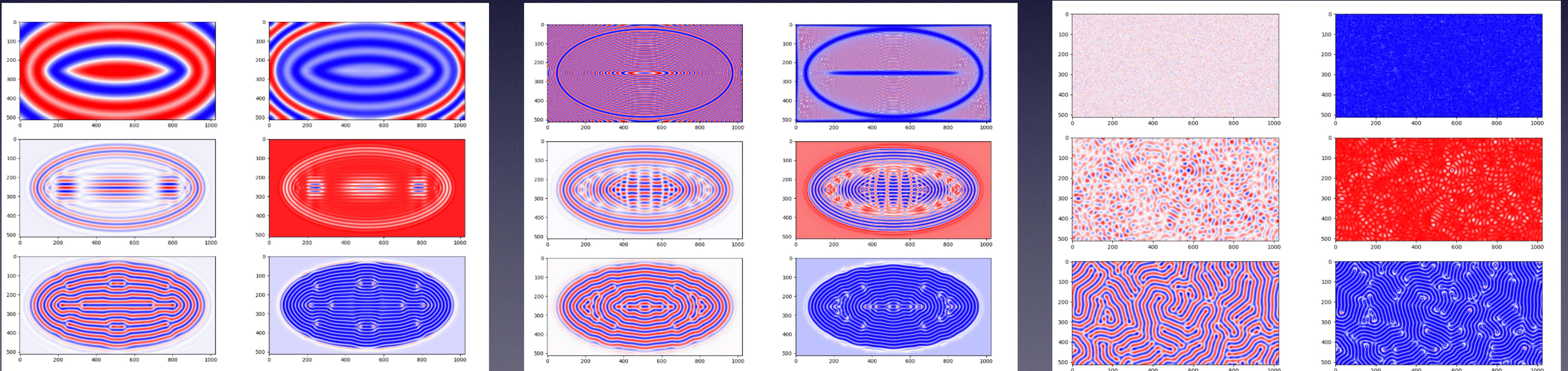
- For complex fields, the $e^{i\theta}, e^{-i\theta}$ terms cancel and eliminate any dependence on θ in the energy functional. For real fields, this is not the case.
- We also have a more difficult Ansatz for real fields: $u = \sum_n A_n(k^2) \cos(n\theta)$. It turns out that the even harmonics are 0, and $A_1 \gg A_3 \gg A_5 \dots$
- The assumption $A = A(k^2)$ is a statement that the amplitudes are slaved to the wave number. Note that in the RCN, we evaluate the amplitude at the dominant wave number. However, near defects, the wave number changes, and thus the amplitudes will change.
- The RCN is derived in terms of slow variables, under an assumption that the wave number changes slowly. It is unclear how much error to expect in regions where the wave number is changing rapidly.
- For real fields, the RCN is written: $\langle w_\theta^2 \rangle_{k_B} \Theta_T + \nabla \cdot \vec{k} B(\vec{k}) + 2\epsilon^2 \langle w_\theta^2 \rangle_{k_B} \nabla^4 \Theta = 0$ with $B(k^2) = -2 \frac{dE_0}{dk^2}$ and $E_0(k^2) = \left\langle \frac{1}{4} \langle w^4 \rangle \right\rangle_{k^2}^{k_B^2}$
- In both cases, the macroscopic energy is a function of $|\vec{k}| = |\nabla \theta|$ and $\nabla \cdot \vec{k} = \Delta \theta$

Macroscopic Equations as a Smoothed Gradient Flow



Analysis of the RCN (1)

- The leading order energy is minimized when $k = k_B$. This explains why the pattern rapidly adjusts itself to consist of stripes of wave number k_B .
- One may say that $k = |\vec{k}| = |\nabla\theta|$ is an order parameter for the system.



Analysis of the RCN (2)

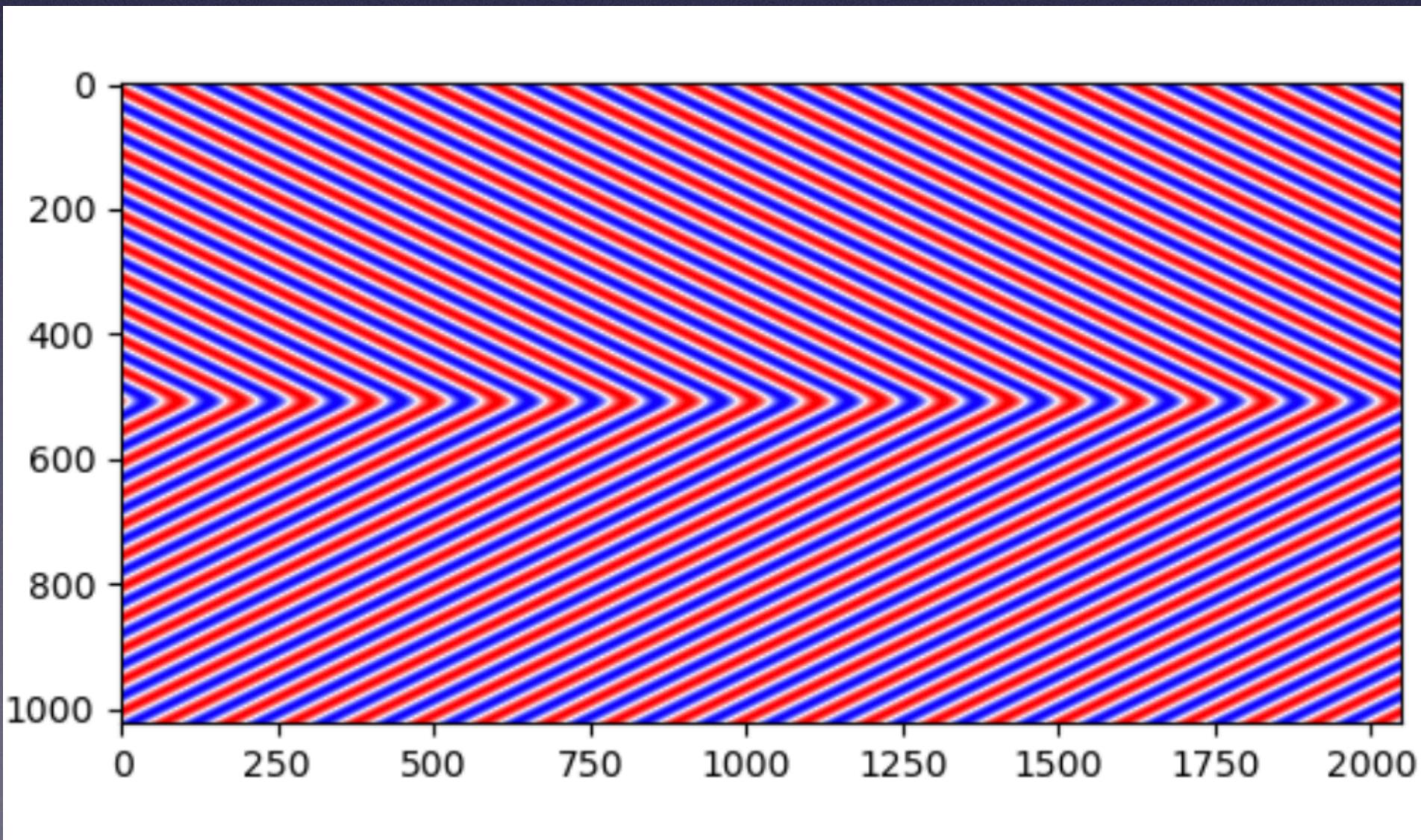
- The *stationary* RCN may be written: $\eta \nabla^4 \theta + \nabla \cdot \vec{k}B = -\frac{\delta \bar{E}}{\delta \theta} = 0$ with $\bar{E} = \int \left(\frac{1}{2} \eta |\nabla^2 \theta|^2 + \frac{\alpha}{2} G^2 \right) d\vec{x}$, where $G^2 = -\frac{1}{\alpha} \int_{k_B^2}^{k^2} B dk^2$
- Analysis may be simplified by seeking *self dual* solutions: $\sqrt{\alpha}G = \pm \sqrt{\eta} \nabla^2 \theta$. These are solutions where the stress and strain energies are in balance.
- α is a normalizing constant, determined by requiring that $G^2 = (k^2 - k_B^2)^2$ at leading order.
- If \hat{J} is the Jacobian matrix from (x, y) to (k_x, k_y) , it can be shown that for $\vec{k} \cdot \vec{k} \approx k_B^2$, $\hat{J}\vec{k} = 0$.
- This allows the RCN to be linearized!

Analysis of RCN (3)

- Let $\beta = \sqrt{\frac{\alpha}{\eta}}$, $s = \pm 1$. Consider the perturbed self-dual equation $\nabla^2\theta = \beta s G + s\chi$.
- Let $\theta = \frac{1}{\beta s}\psi$ and $\chi = \psi\nu$.
- Using the fact that $\hat{J}\vec{k} = 0$ almost everywhere, and the first order approximation $G^2 = (k^2 - k_B^2)^2$, we obtain:
$$\begin{aligned}\nabla^2\psi - (\beta^2 k_B^2 + \beta\chi)\psi &= 0 \\ \nabla^2\nu - (\beta^2 k_B^2 + \beta\chi)\nu &= -4\beta\psi^{-1}J\end{aligned}$$
- Note that if $J = 0$, then $\chi = 0$, and we just have the Helmholtz equation.
- If J is similar to a delta function, then the equation pair can be handled perturbatively.

Simple RCN Solutions

- The simplest solutions are sums of exponentials: $\psi = \sum_{i=1}^N \exp(\beta \vec{k}_j \cdot x), |\vec{k}_j| = k_B$
- Phase Grain Boundaries: arise when $N = 2$, and has wave vector field
$$\vec{k} = \frac{1}{2}(\vec{k}_1 + \vec{k}_2) + \frac{1}{2}s(\vec{k}_1 + \vec{k}_2)\tanh\left(\frac{1}{2}(\vec{k}_1 + \vec{k}_2) \cdot \vec{x}\right)$$



The Stationary Dislocation Solution

- Seek solutions of the form $\psi = \exp(\beta k_B x) F(x, y)$, such that

$$\psi = \exp(\beta k_B x) F(x, y)$$

$$2\beta k_B F_x + F_{yy} = 0$$

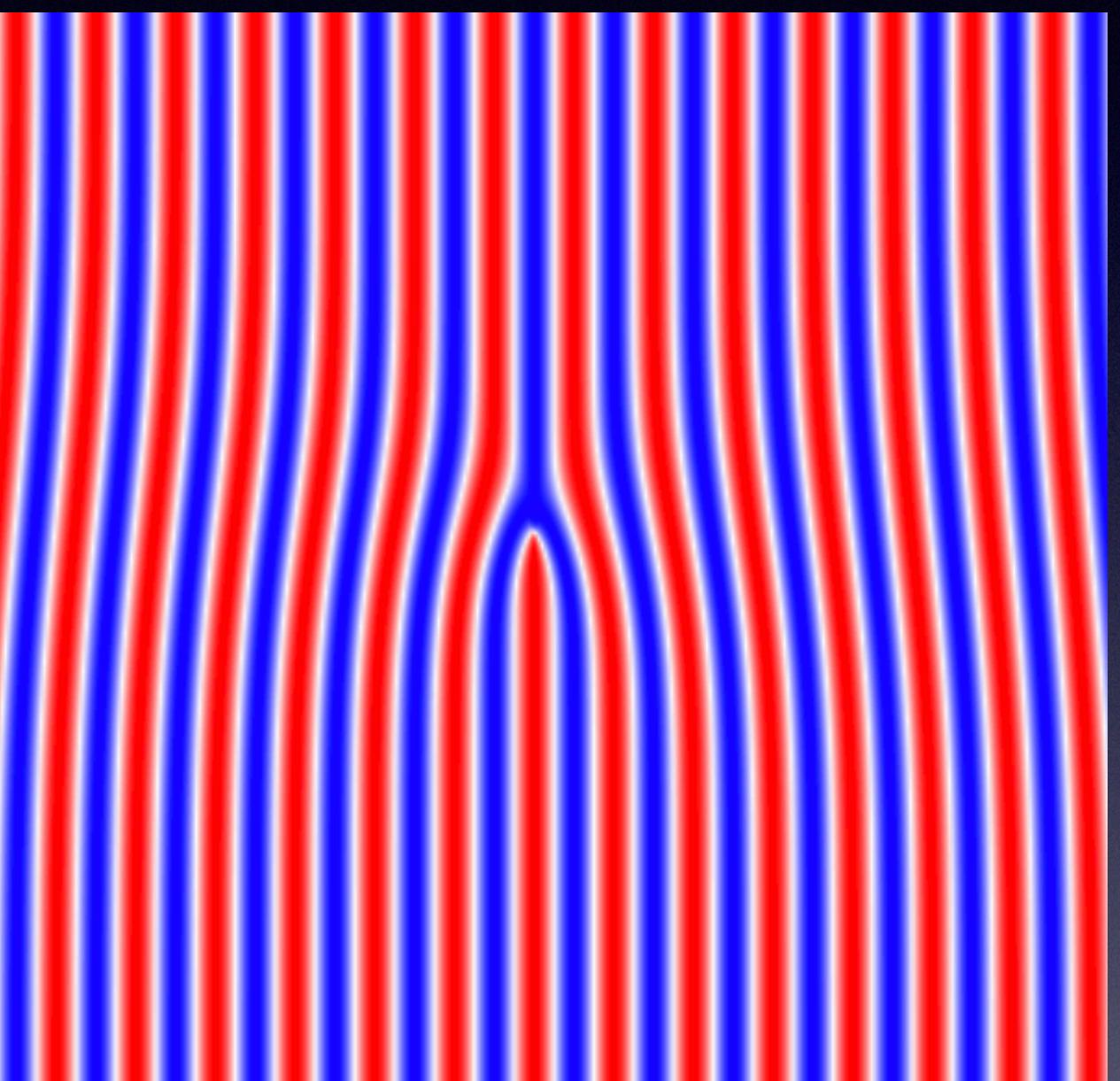
$$\theta(-x, y) = \theta(x, y)$$

$$\theta(x, y) = k_B x, y >> 1$$

$$\theta(x, y) = k_B x + \pi sgn(x), y << -1$$

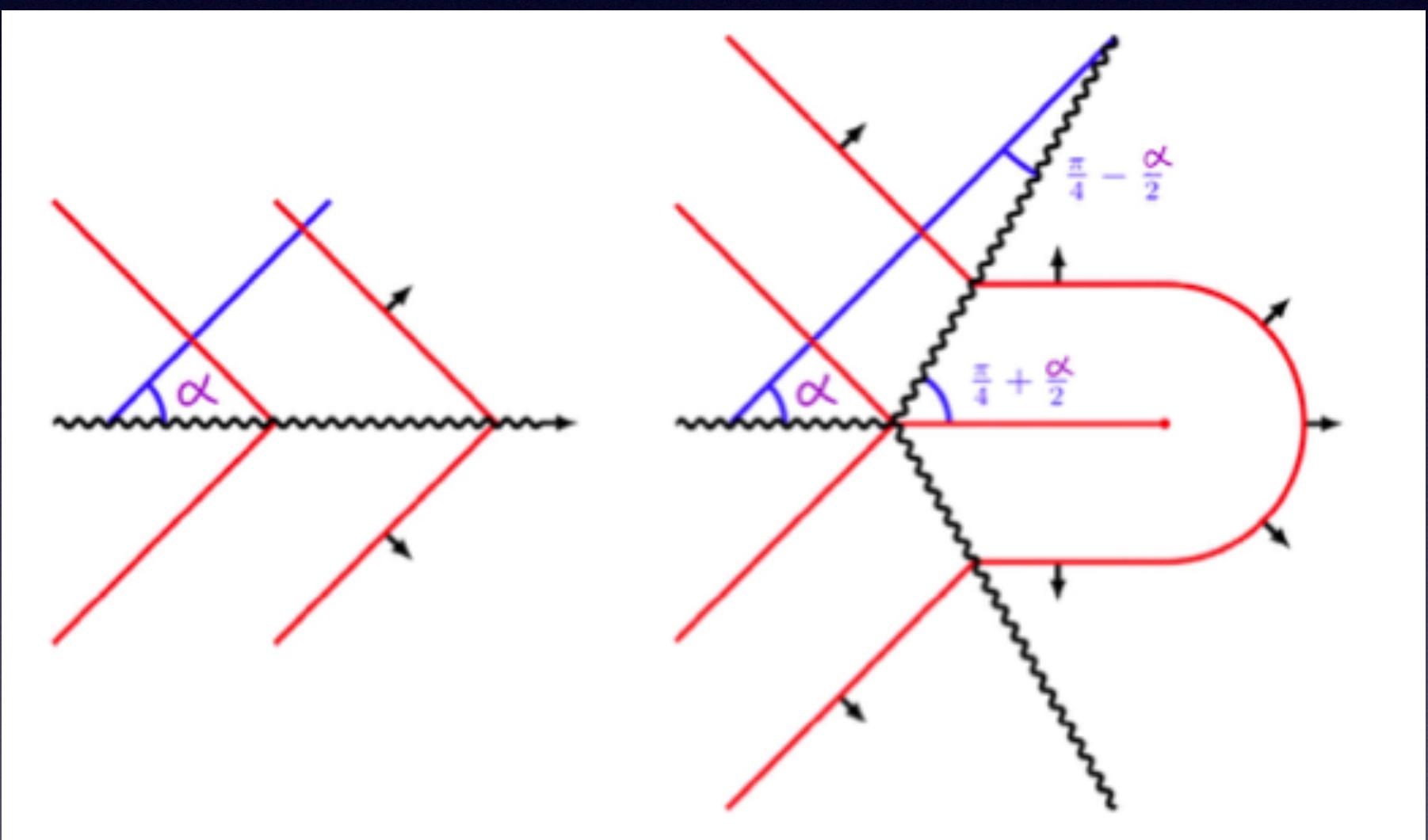
- You get

$$\theta(x, y) = k_B x + \frac{1}{\beta} \ln \left\{ \frac{1}{2} (1 + \exp(\beta \pi sgn(x))) + \frac{1}{2} (1 - \exp(\beta \pi sgn(x))) \operatorname{Erf}(\sqrt{\beta k_B}) \frac{y}{\sqrt{|x|}} \right\}$$



An argument for the creation of VX Pairs

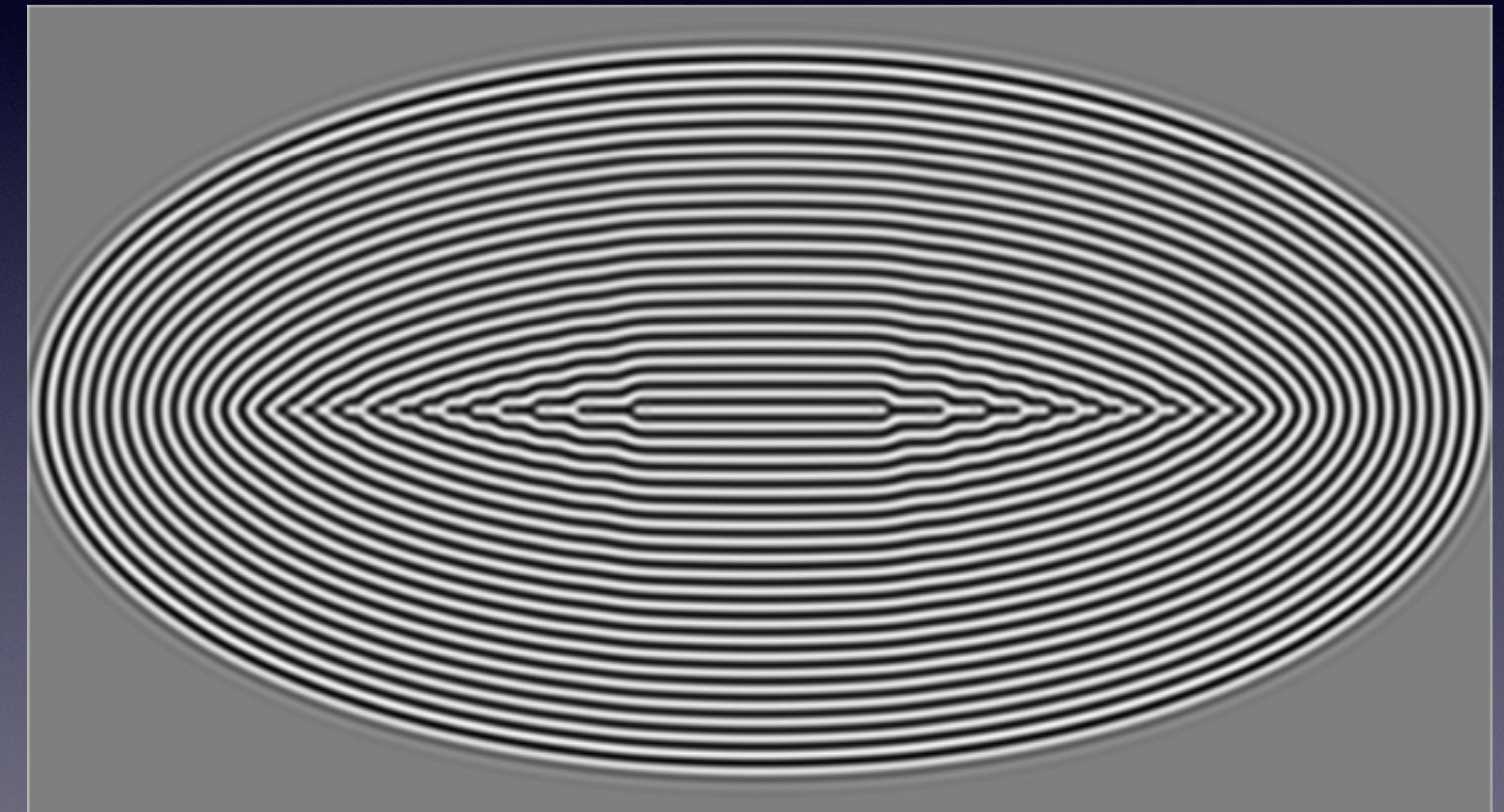
- The PGB can be parameterized such that $\vec{k}_1 \cdot \vec{k}_2 = \cos(2\alpha)$, where α is the angle \vec{k} makes with the PGB.
- The energy cost per unit length is proportional to $\sin^3(\alpha)$. But, as $\alpha \rightarrow \frac{\pi}{2}$, the stripes are parallel, implying there should be no energy cost. This suggests that as α increases, the PGB becomes unstable, to a new state that is described by a director field.
- The director field state has energy proportional to $1 - \sin(\alpha)$.
- Thus, PGBs become VX pairs when $\sin^3(\alpha) > 1 - \sin(\alpha)$, ie $\alpha \approx .24\pi$



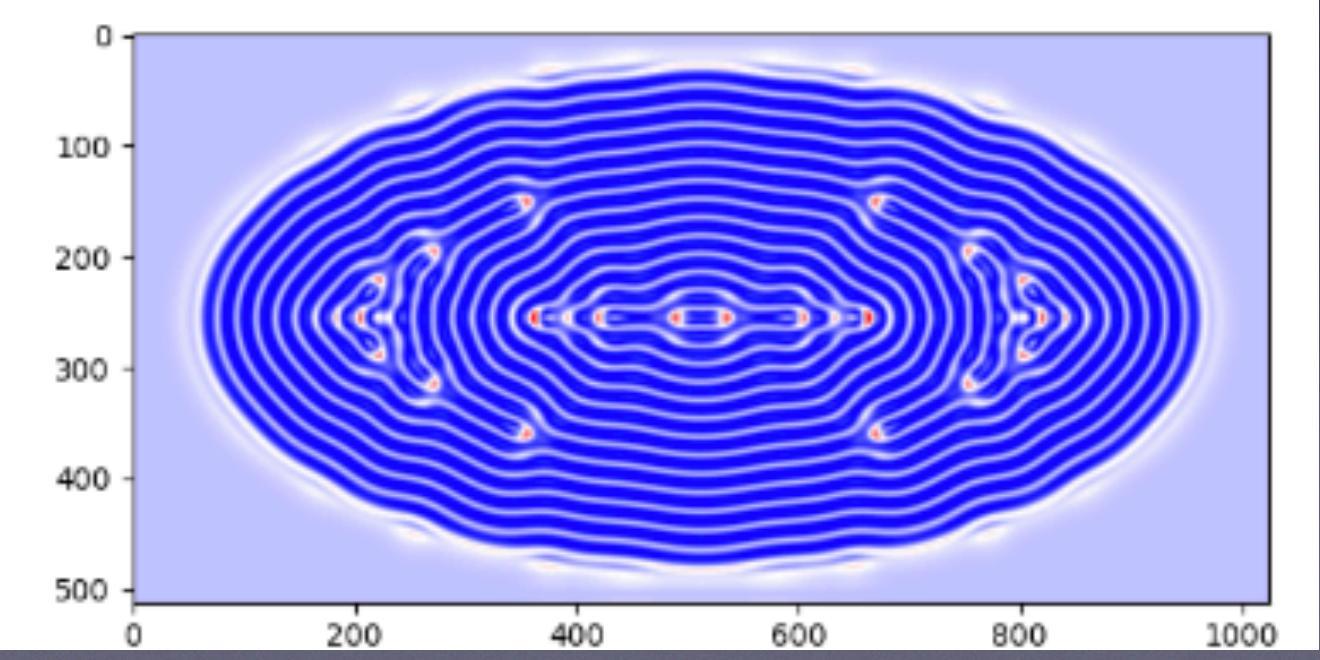
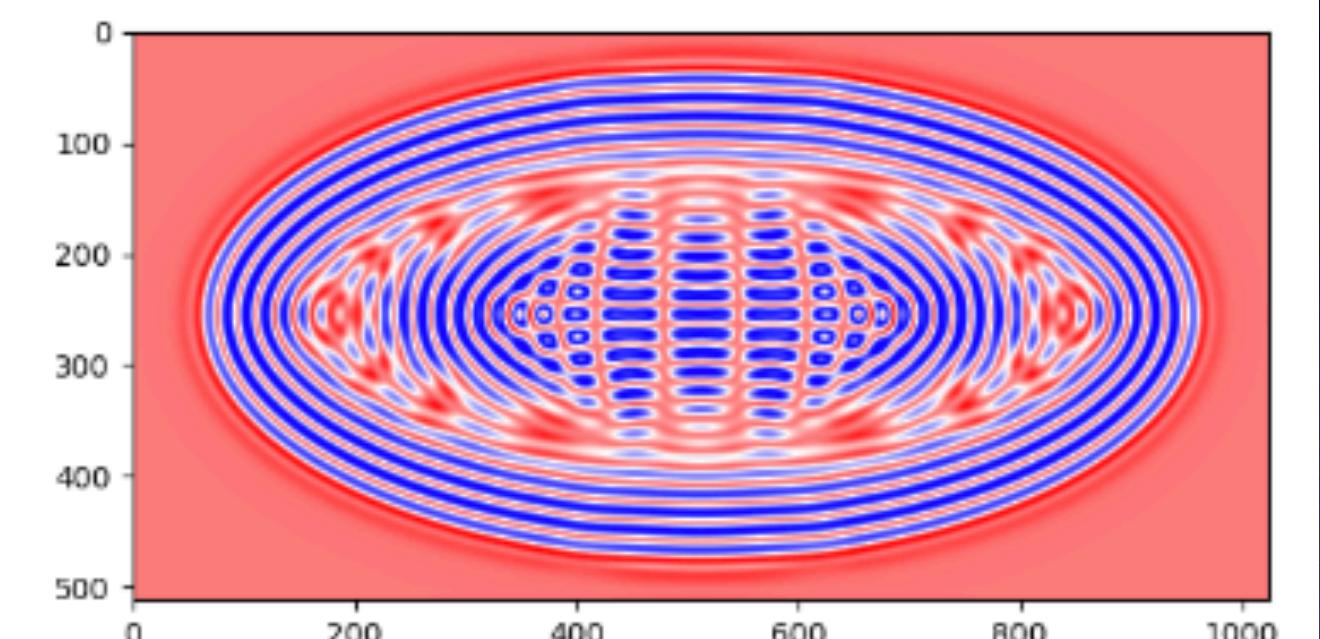
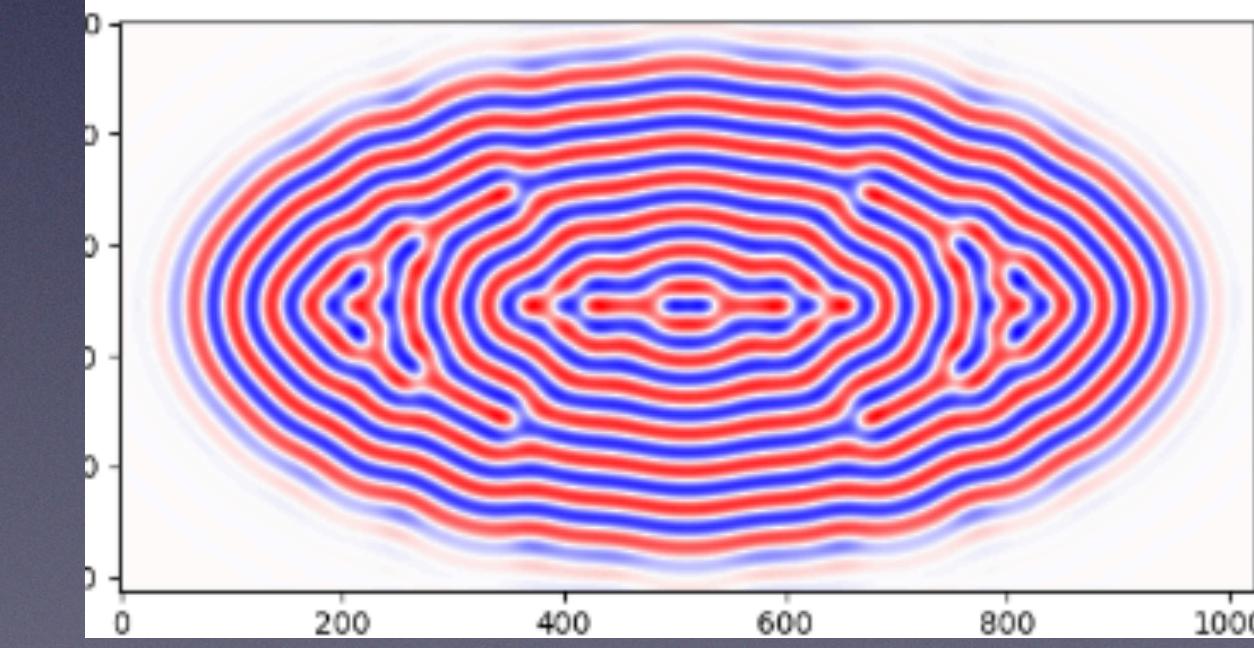
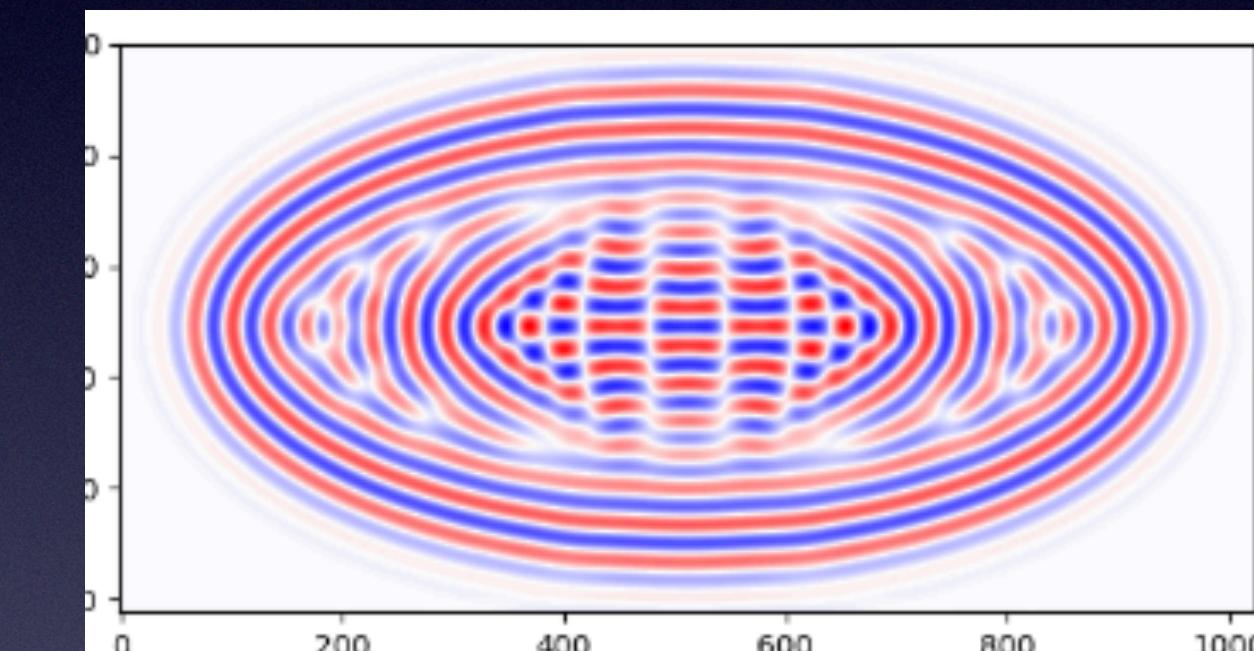
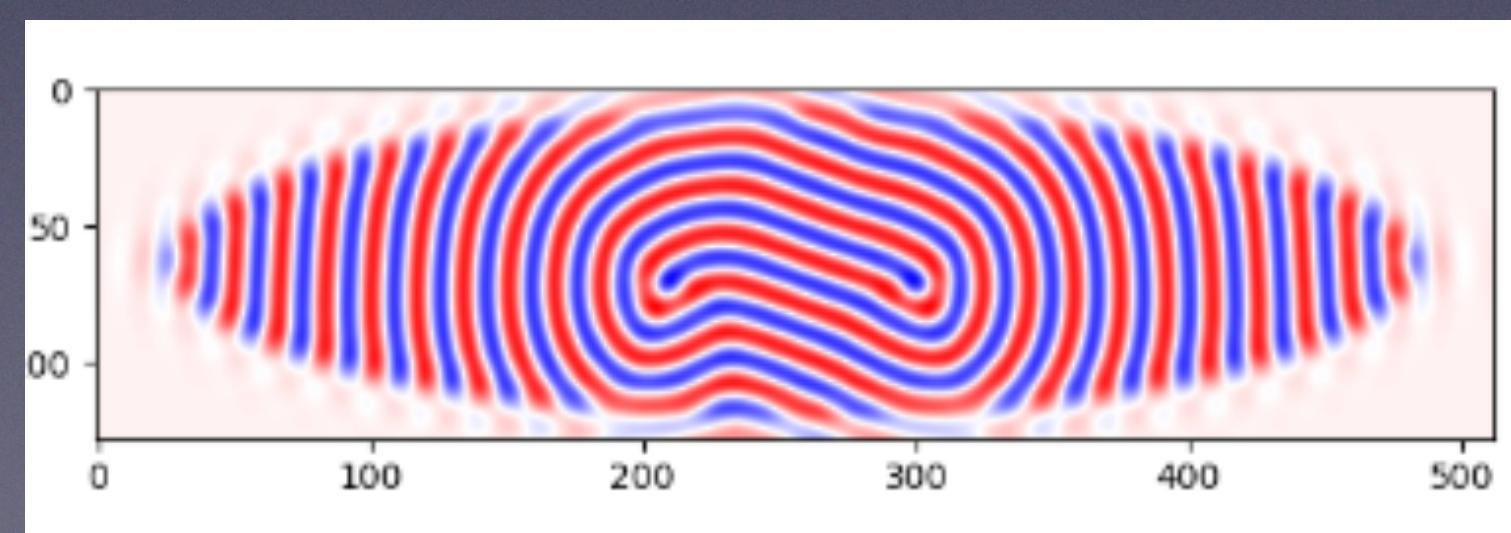
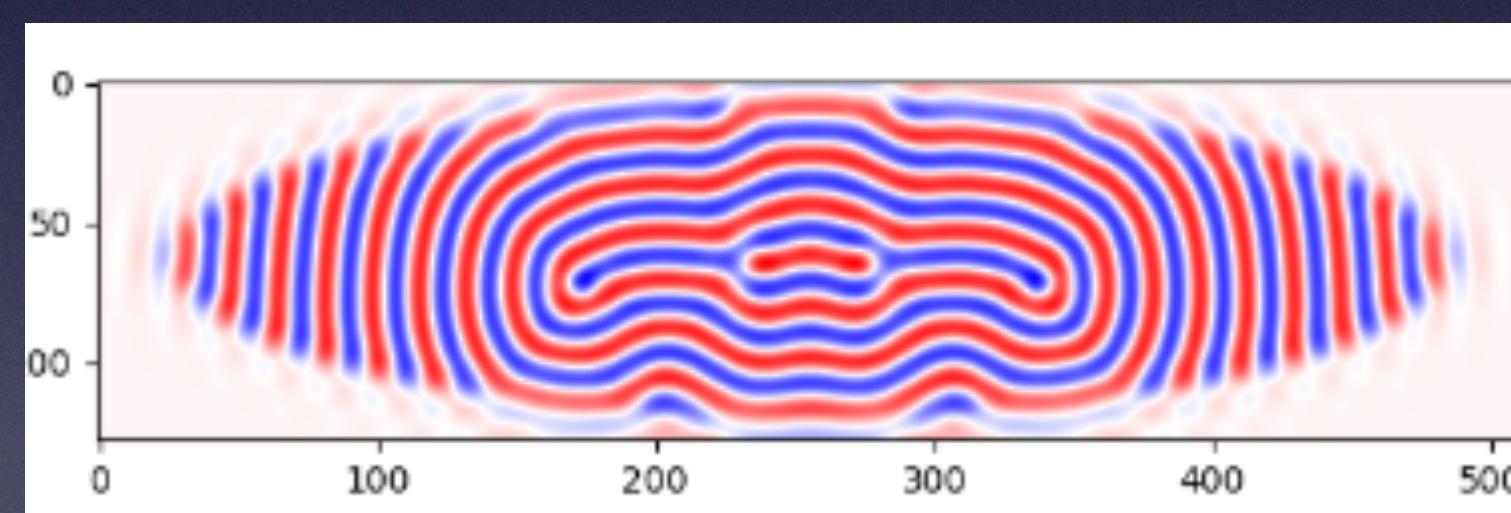
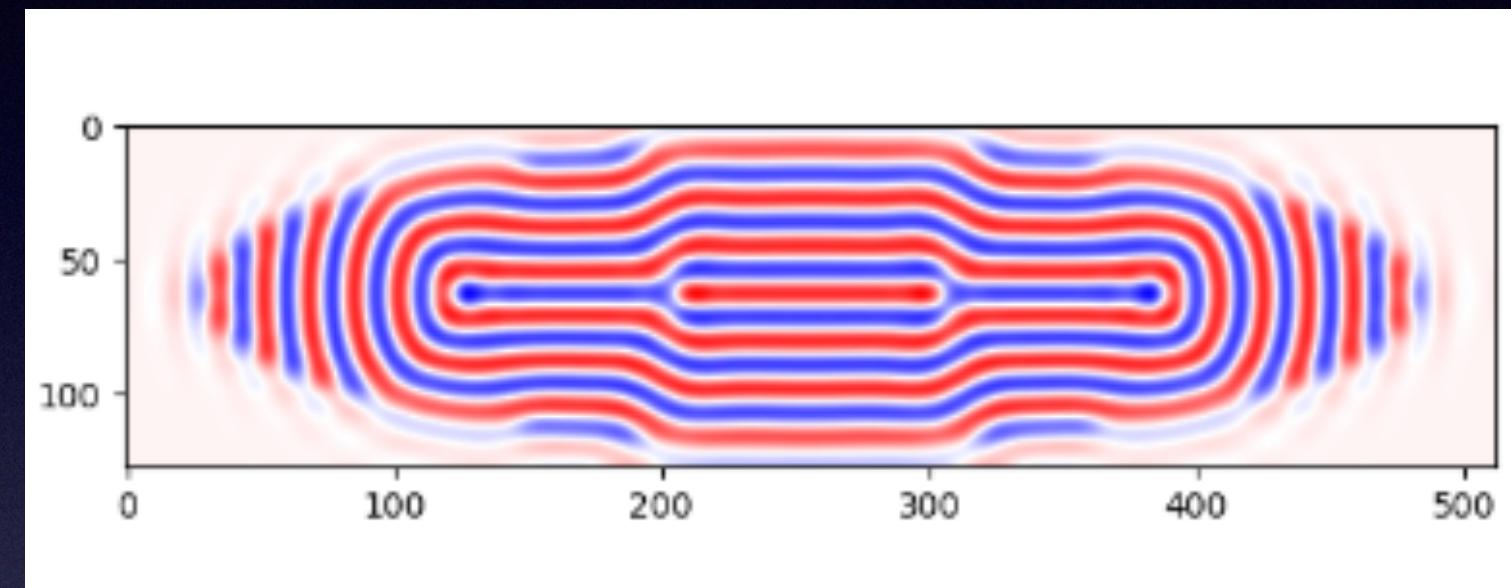
More on VX Pairs

- Ercolani NM, Kamburov N, Lega J. 2018 <http://dx.doi.org/10.1098/rsta.2017.0193>. Showed the Knee Solutions arise when solving the stationary RCN in a function space of single-valued phases. Ie \vec{k} is a vector field.
- Ercolani, N.M., Venkataramani, S.C. 2009 <https://doi.org/10.1007/s00332-008-9035-9>. Showed that VX pairs should be found in function spaces of multi-valued phases. Ie \vec{k} is a director field.
- What is the actual difference between a VX pair and a dislocation?

An open problem: How do lines of multi-dislocations emerge?

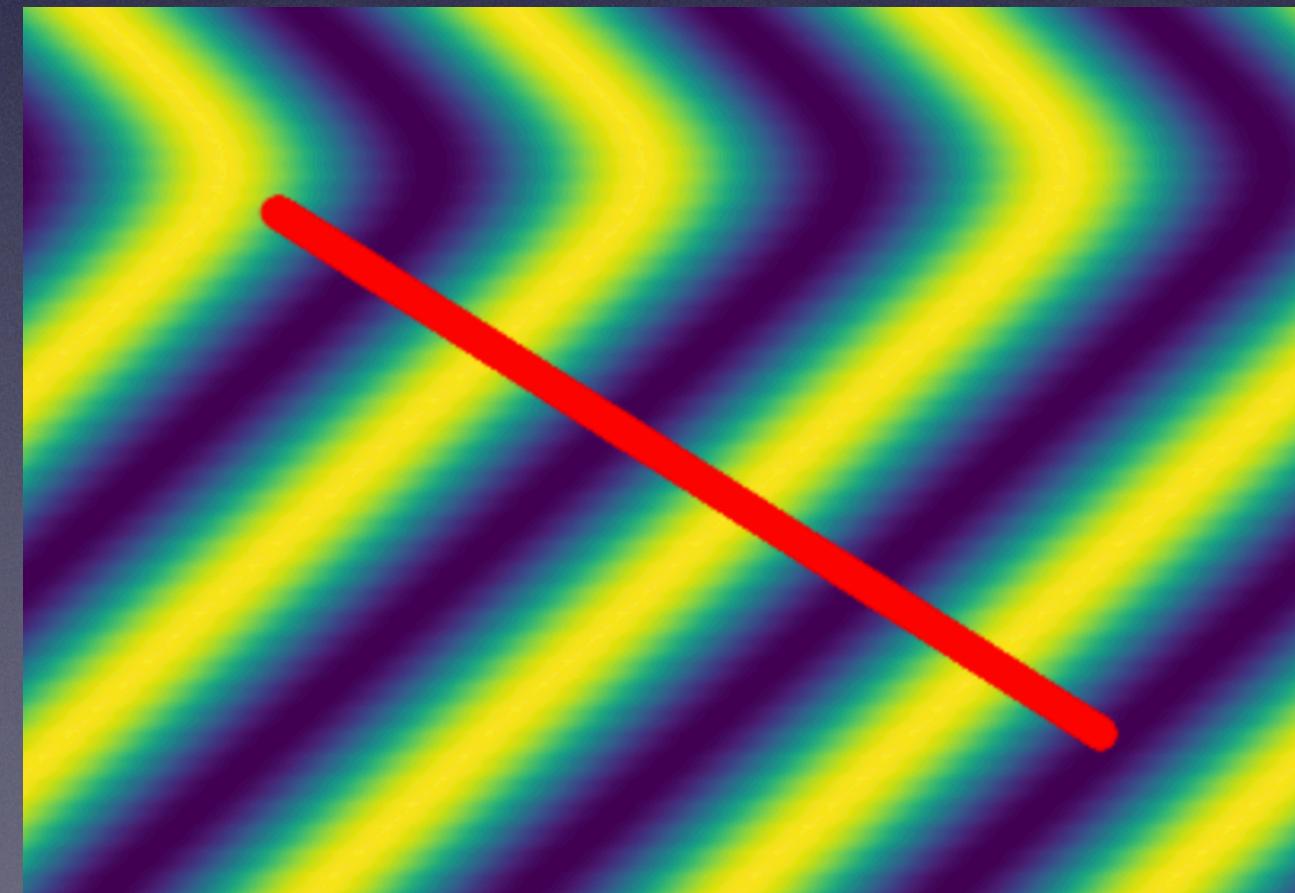
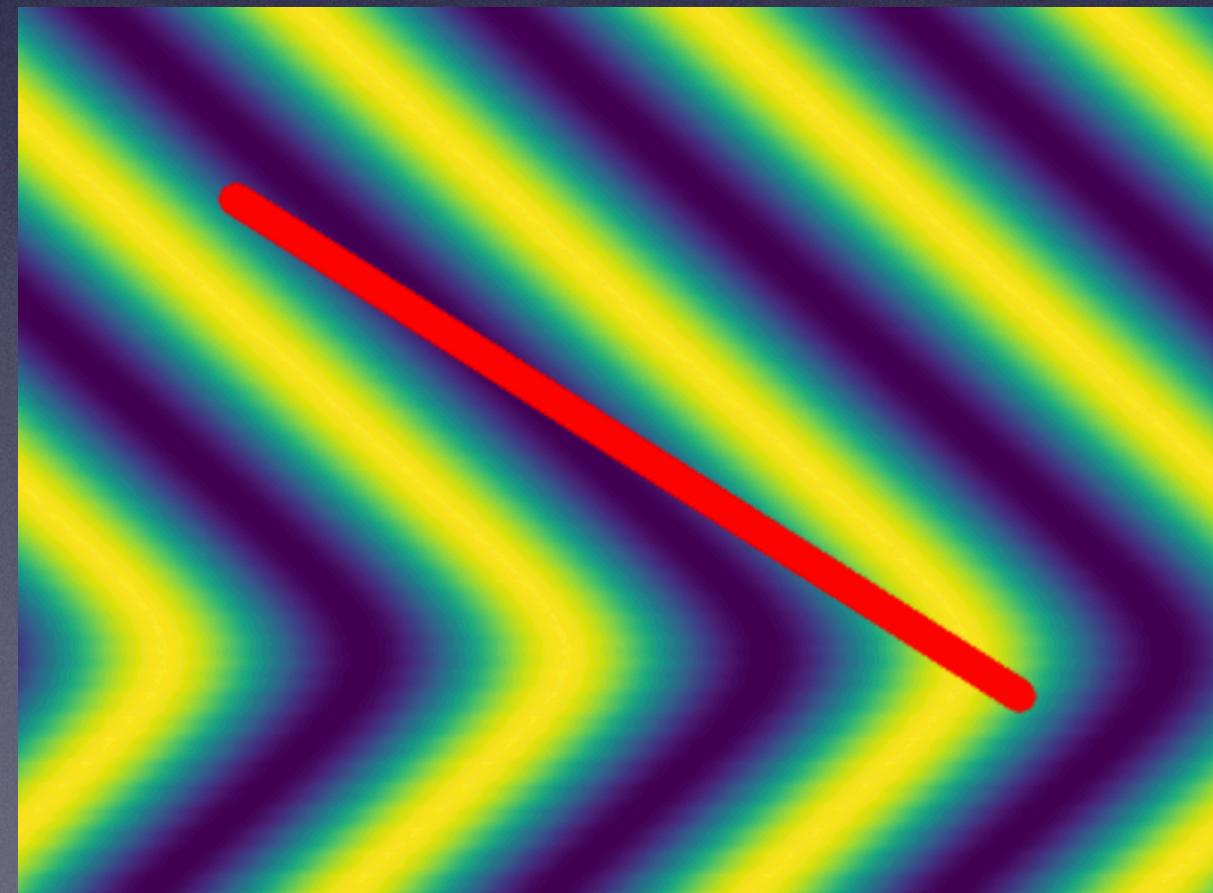
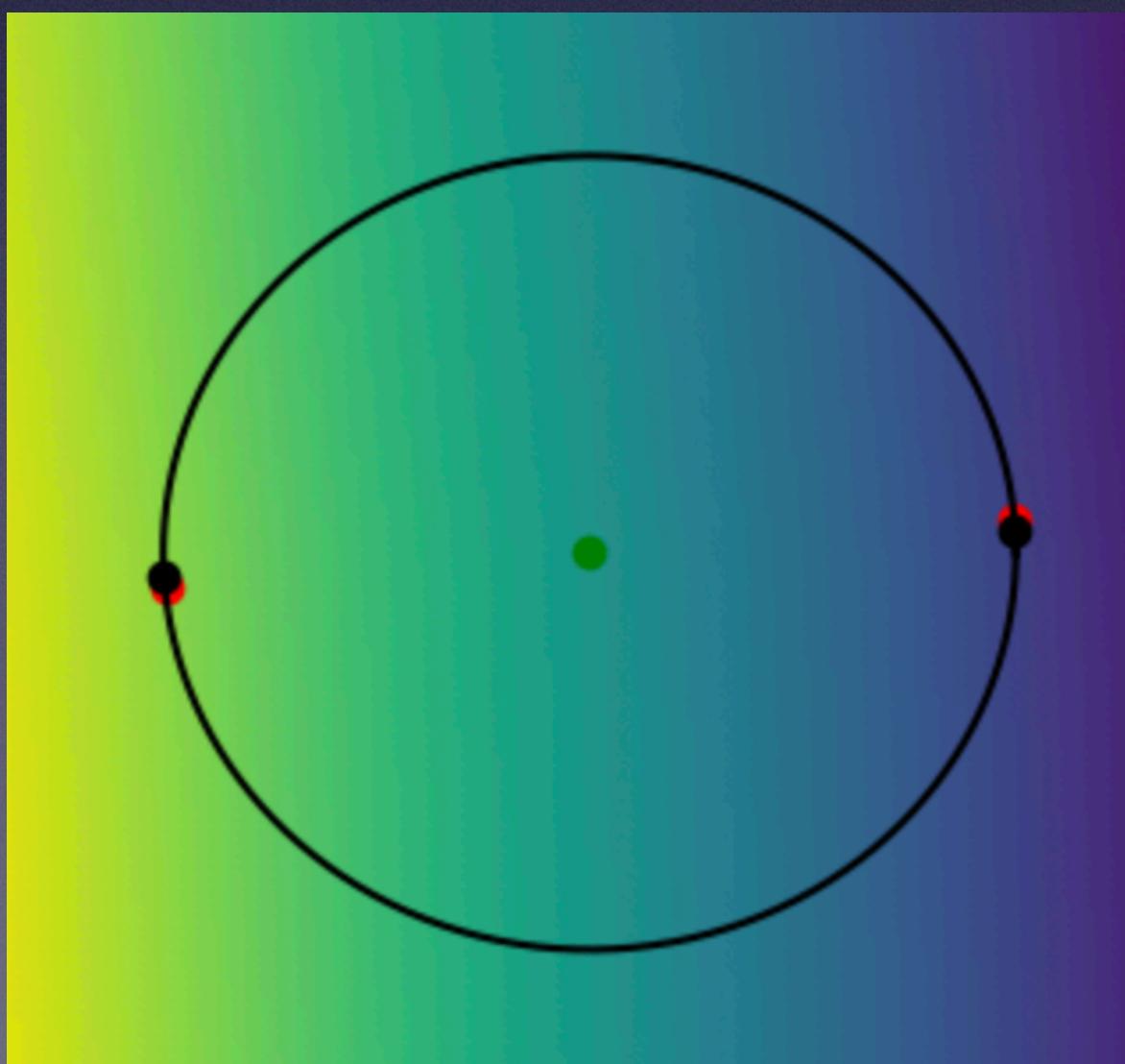


More Generally: There are many evolutions that are not qualitatively understood.



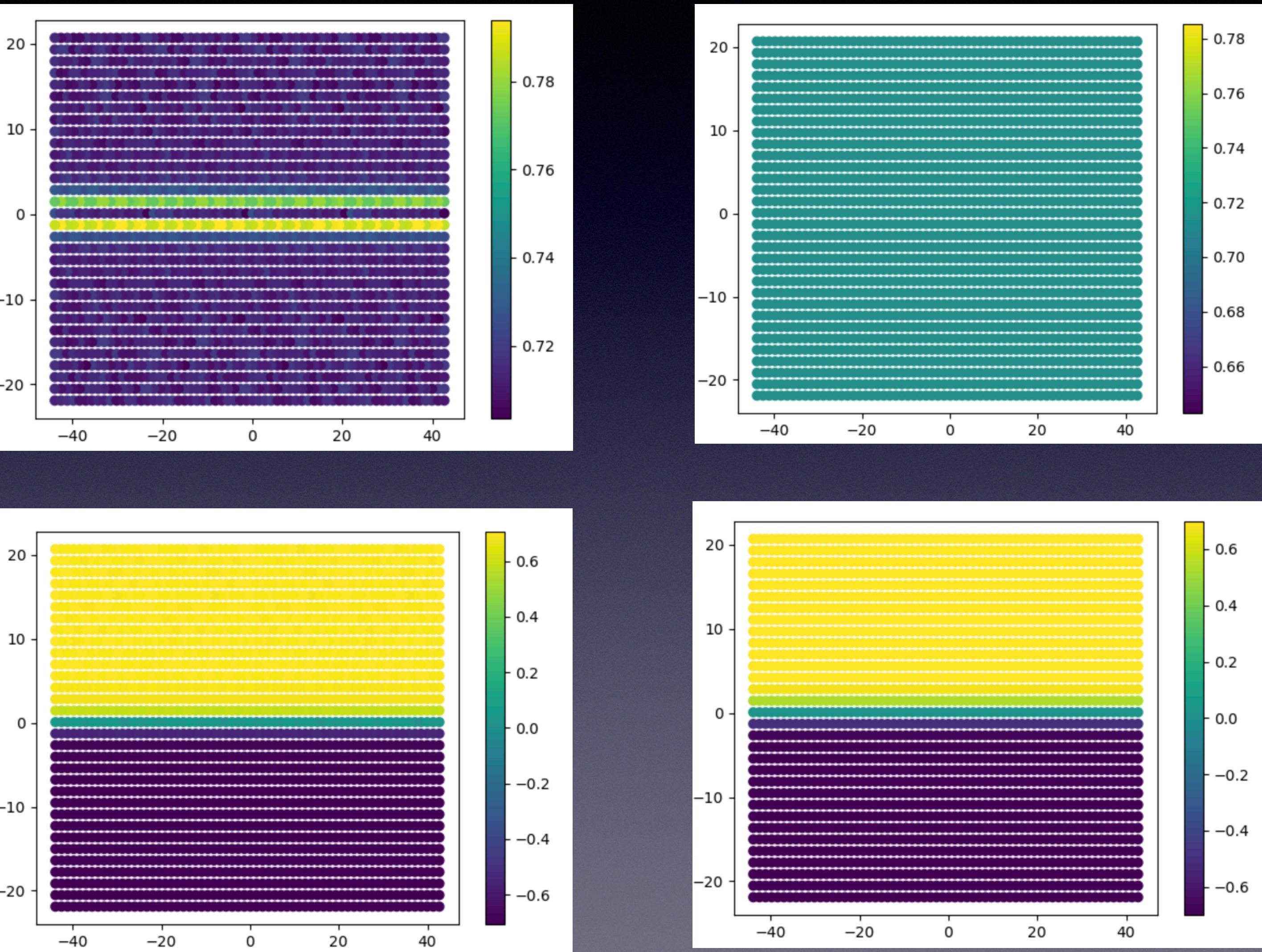
Wave Vector Estimation (1)

- At a point r_0 , the wave vector direction ϕ_0 should be parallel to the direction of greatest change in the field.
ie, $\phi_0 = \arctan \frac{r_y^*}{r_x^*}$, $r^* = \max_{r \in B_\gamma(r_0)} |u(r_0) - u(r)|$
- Given ϕ_0 , we can get the field profile in the ϕ_0 direction, and estimate the distances L_+ , L_- traveled to increase ϕ_0 by $\pm\pi$. The wave vector magnitude λ_0 is then estimated through the relation $\frac{2\pi}{\lambda_0} = L_- + L_+$.
- Heuristic is simple, but doesn't hold for all points.



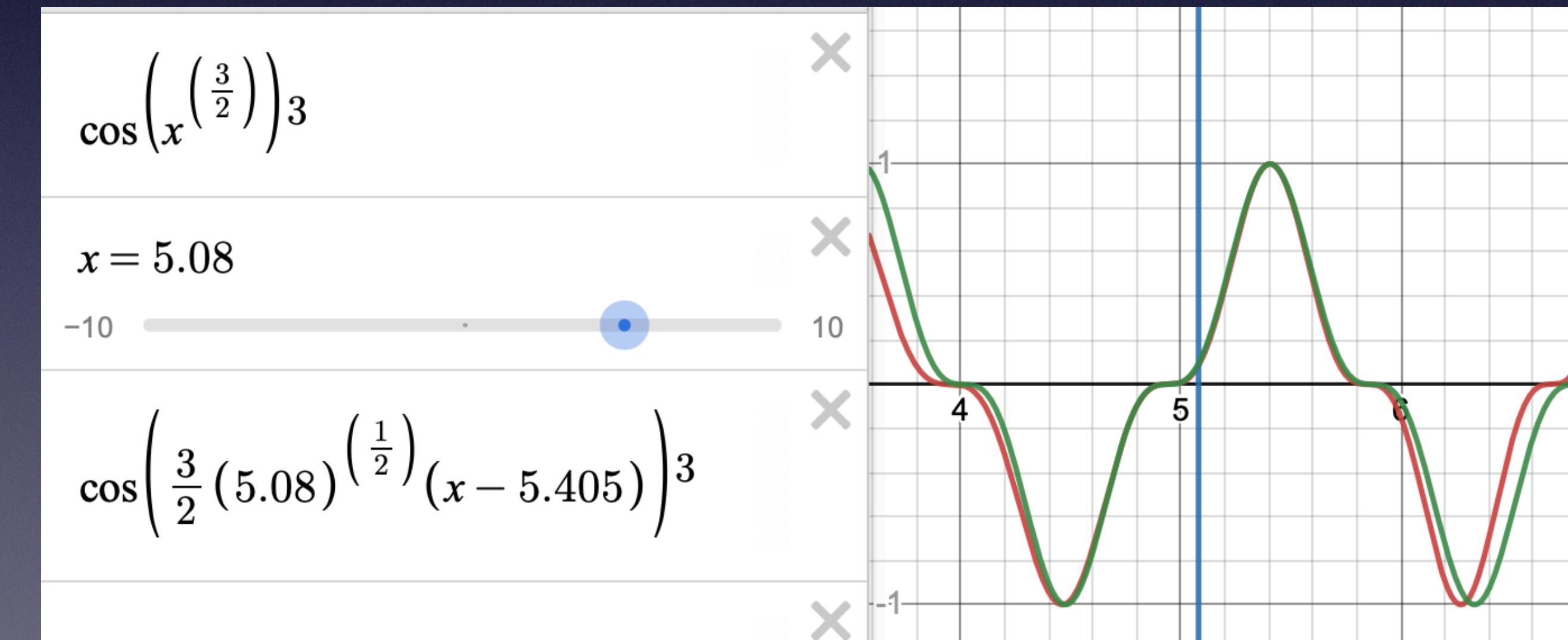
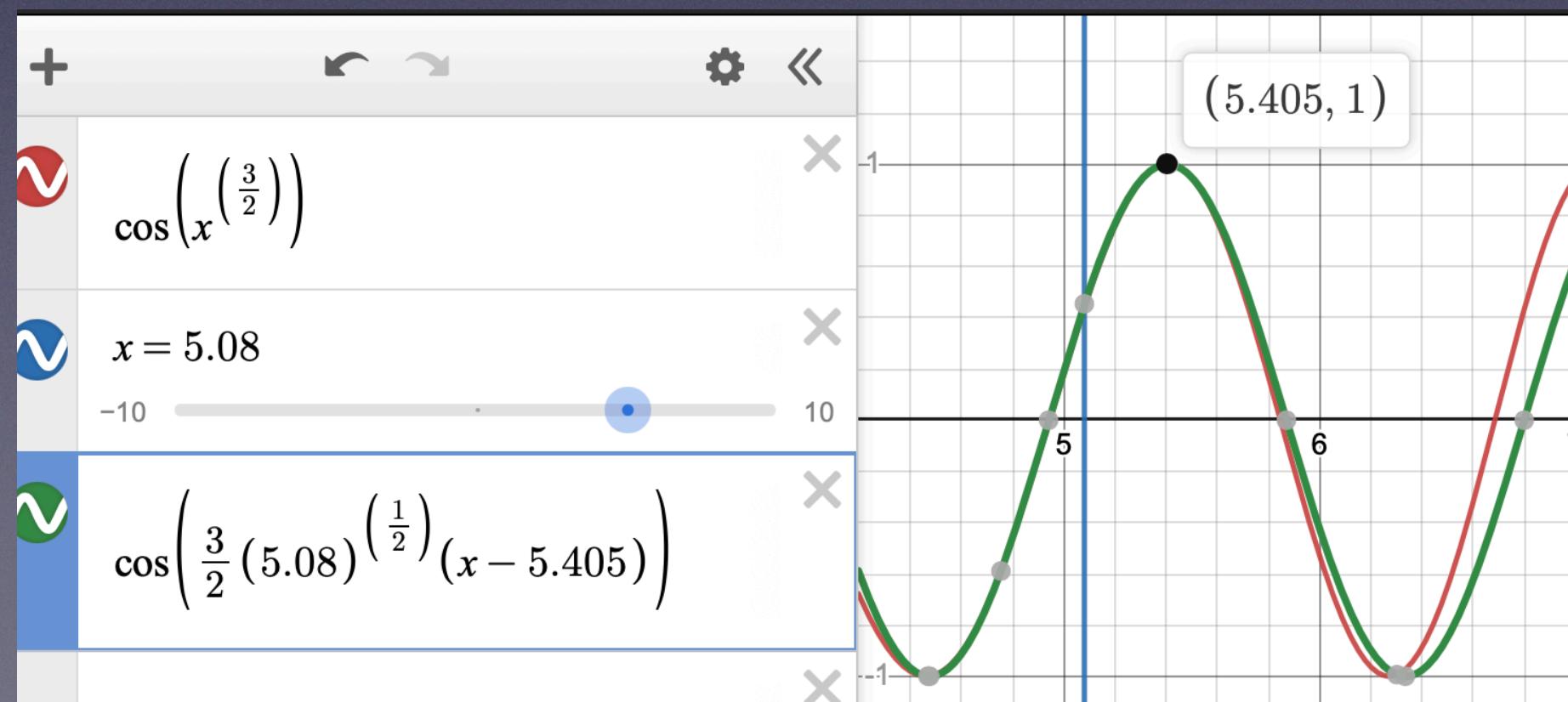
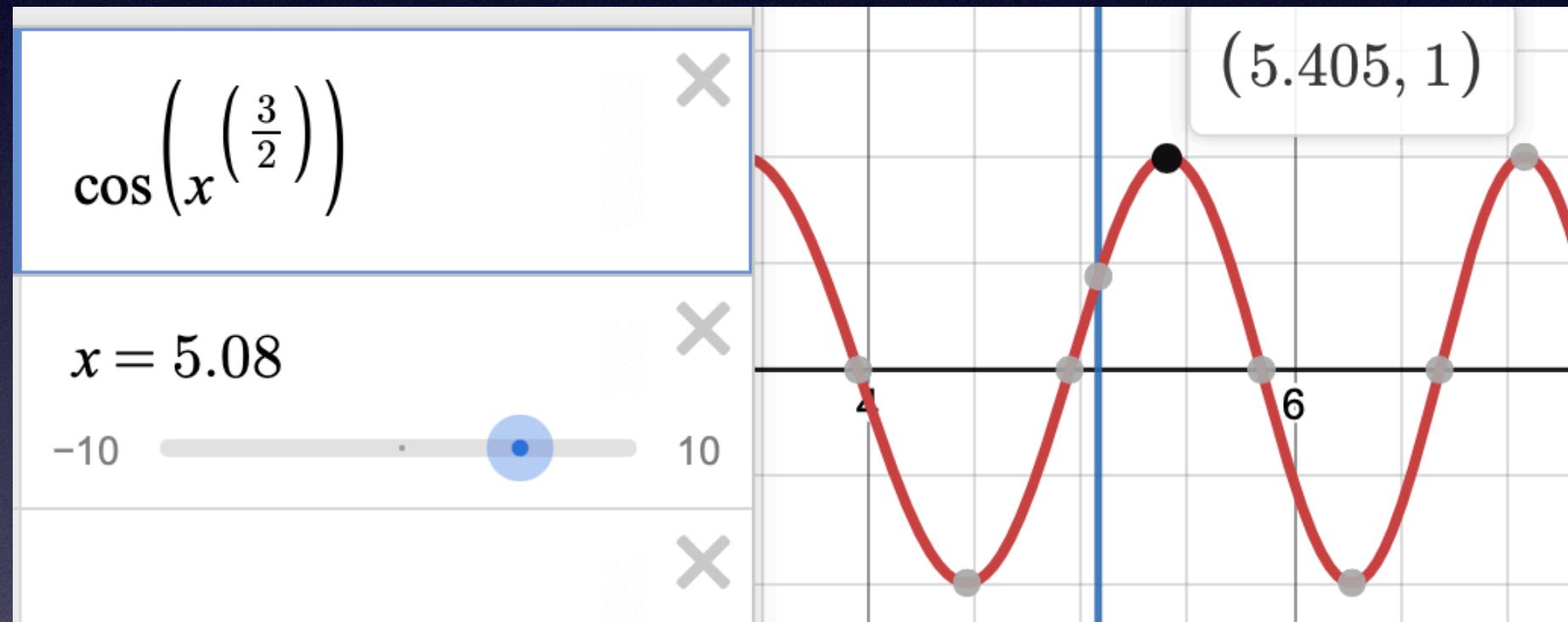
Wave Vector Estimation (2)

- Global relative errors are $\approx .025, .019$
- Main source of error is in the wave number estimate.
- For the patterns shown here, it seems there is a limit to the minimum observed error of $\approx .10$
- The instantaneous phase derivative needs a more localized estimate near defects.



Wave Vector Estimation (3)

- An idea to improve the accuracy relies on an assumption that a given profile is close to something of the form $A \sin(\theta), A \sin(\theta)^3, A \sin(\theta)^5, \dots$ for a small distance around r_0 in the wave vector direction.
- Fit the profile to a function of the form $A_0 \cos(a(x - \omega_0))^n$, where A_0, ω_0 are derived from the profile, and a, n are determined through optimization. The wavenumber would be $\lambda = \frac{2\pi}{a}$.



Research Directions: Analytical Work

- The current analysis uses the fields $|\vec{k}|$ and $\nabla \cdot \vec{k}$ to analyze patterns. What other order parameters could there be?
- How much information is lost in the averaging procedure?
- Should the higher order amplitude equation be analyzed?
- Can we derive expressions for inter-defect forces?
- Can we do a similar analysis for PDEs with different symmetries?
- What equations do we get by solving the coupled stationary RCN PDEs perturbatively?
- What does it mean to solve PDEs with multi-valued solutions?

Research Directions: Computational Work

- Algorithms to extract the \vec{k} field from microscopic data, and analyze the fields $\vec{k}, \theta, \nabla \cdot \vec{k}, \nabla \times \vec{k}, |\vec{k}|, \dots$
- Algorithms to identify order parameters from microscopic data.
- SINDy like methods to fit order parameter PDEs to data.
- Numerical solutions of the coupled stationary RCN PDEs.

Questions?