Collective Effects

in

Equilibrium and Nonequilibrium Physics

Website: http://cncs.bnu.edu.cn/mccross/Course/

Caltech Mirror: http://haides.caltech.edu/BNU/

Today's Lecture: Instability in Systems far from Equilibrium

Outline

- Closed and open systems
- Bénard's experiment and Rayleigh's theory
- Taylor-Couette instability
- Turing's paper on morphogenesis
- General remarks on pattern forming instabilities

Heat Death of the Universe (from Wikepedia)

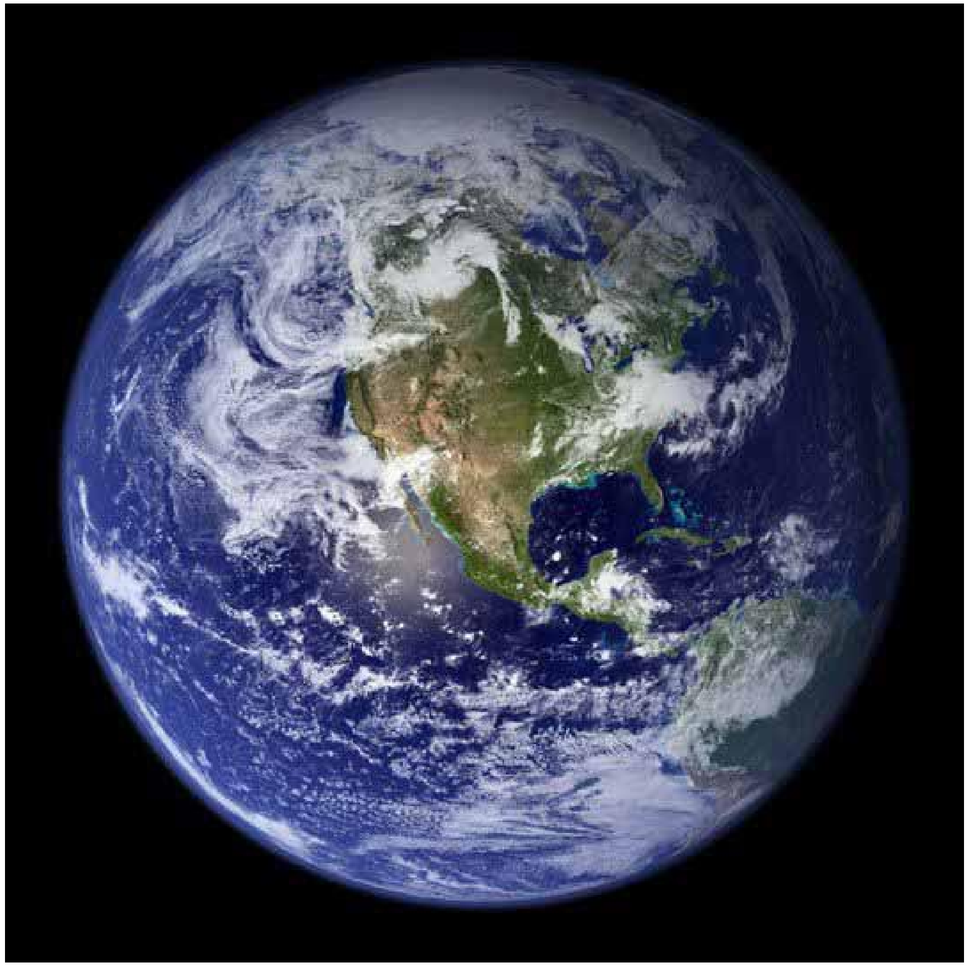
Heat death is a possible final state of the universe, in which it has “run down” to a state of no free energy to sustain motion or life. In physical terms, it has reached maximum entropy.

Origins of the idea

The idea of heat death stems from the second law of thermodynamics, which claims that entropy tends to increase in an isolated system.

If the universe lasts for a sufficient time, it will asymptotically approach a state where all energy is evenly distributed. Hermann von Helmholtz is thought to be the first to propose the idea of heat death in 1854, 11 years before Clausius’s definitive formulation of the Second law of thermodynamics in terms of entropy (1865).

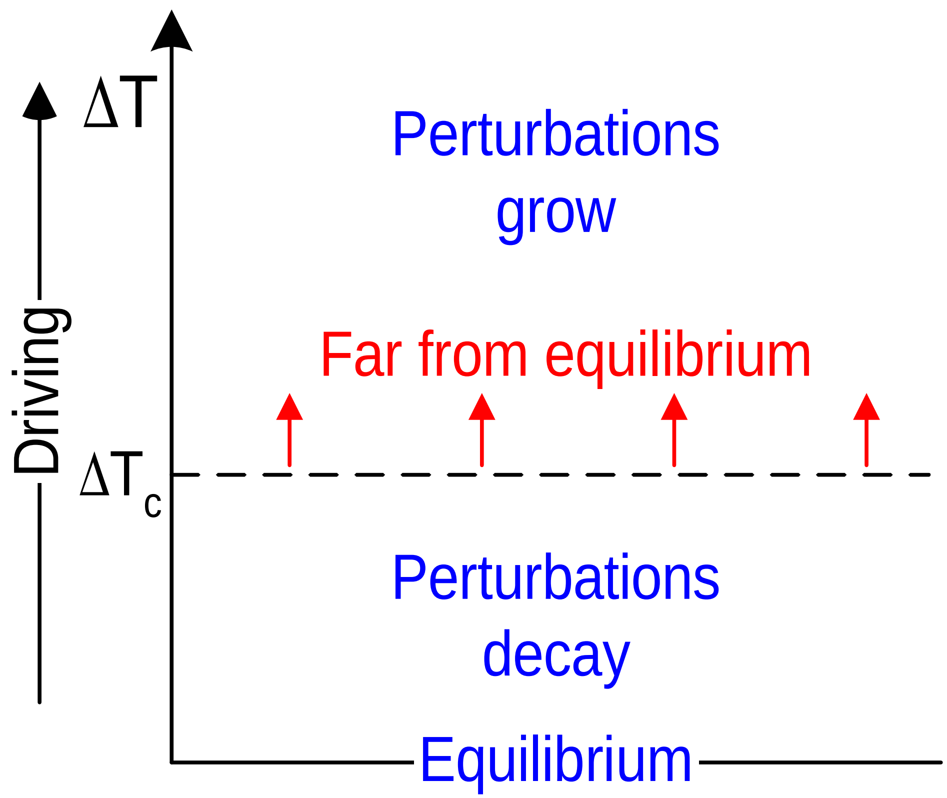
An Open System



Pattern Formation

The spontaneous formation of spatial structure in open systems driven far from equilibrium

Equilibrium - Far From Equilibrium



Origins

1900 Bénard's experiments on convection in a dish of fluid heated from below and with a free surface

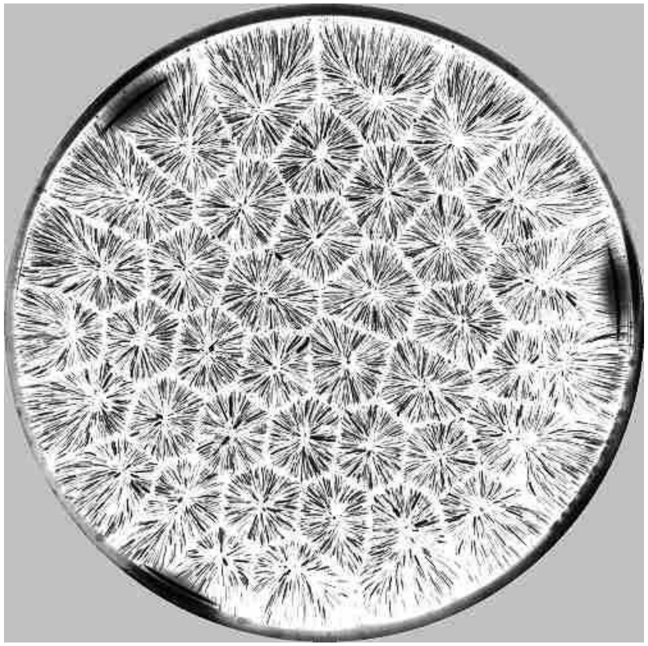
1916 Rayleigh's theory explaining the formation of convection rolls and cells in a layer of fluid with rigid top and bottom plates and heated from below

1923 Taylor's experiment and theory on the instability of a fluid between an inner rotating cylinder and a fixed outer one

1952 Turing's suggestion that instabilities in chemical reaction and diffusion equations might explain morphogenesis

1950s-60s Belousov and Zhabotinskii work on chemical reactions showing oscillations and waves

Bénard's Experiments



(Reproduced by Carsten Jäger)

Movie

Rayleigh's Description of Bénard's Experiments

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- Two phases are distinguished, of unequal duration, the first being relatively short. The limit of the first phase is described as the "semi-regular cellular regime"; in this state all the cells have already acquired surfaces *nearly* identical, their forms being nearly regular convex polygons of, in general, 4 to 7 sides. The boundaries are vertical….

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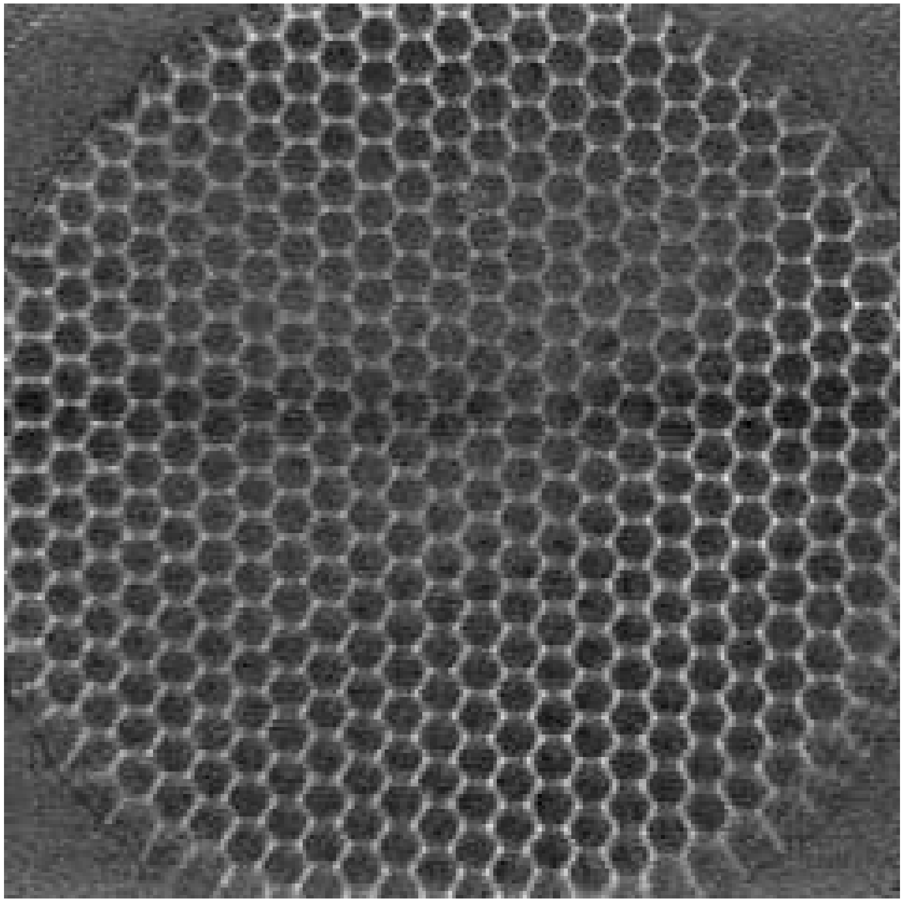
- The second phase has for its limit a permanent regime of regular hexagons…. It is extremely protracted, if the limit is regarded as the complete attainment of regular hexagons. The tendency, however, seems sufficiently established.

Ideal Hexagonal Pattern



From the website of Michael Schatz

Rayleigh's Simplifications

- The calculations which follow are based upon equations given by Boussinesq, who has applied them to one or two particular problems. The special limitation which characterizes them is the neglect of variations of density, *except in so far as they modify the actions of gravity*.

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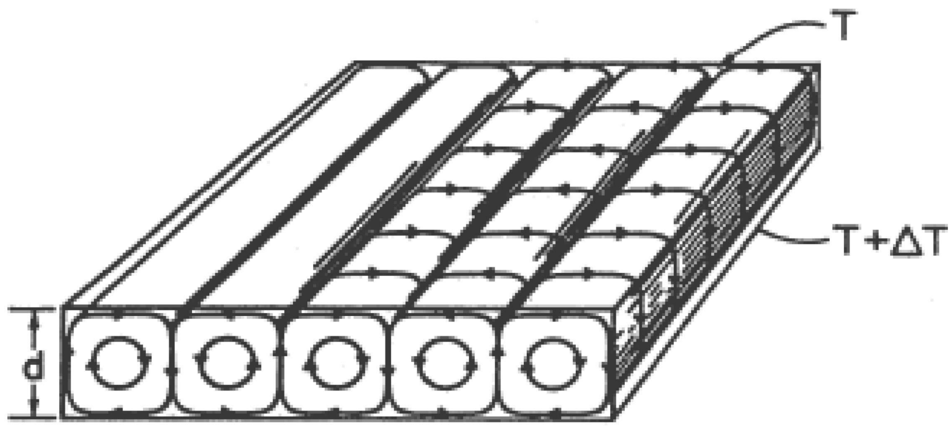
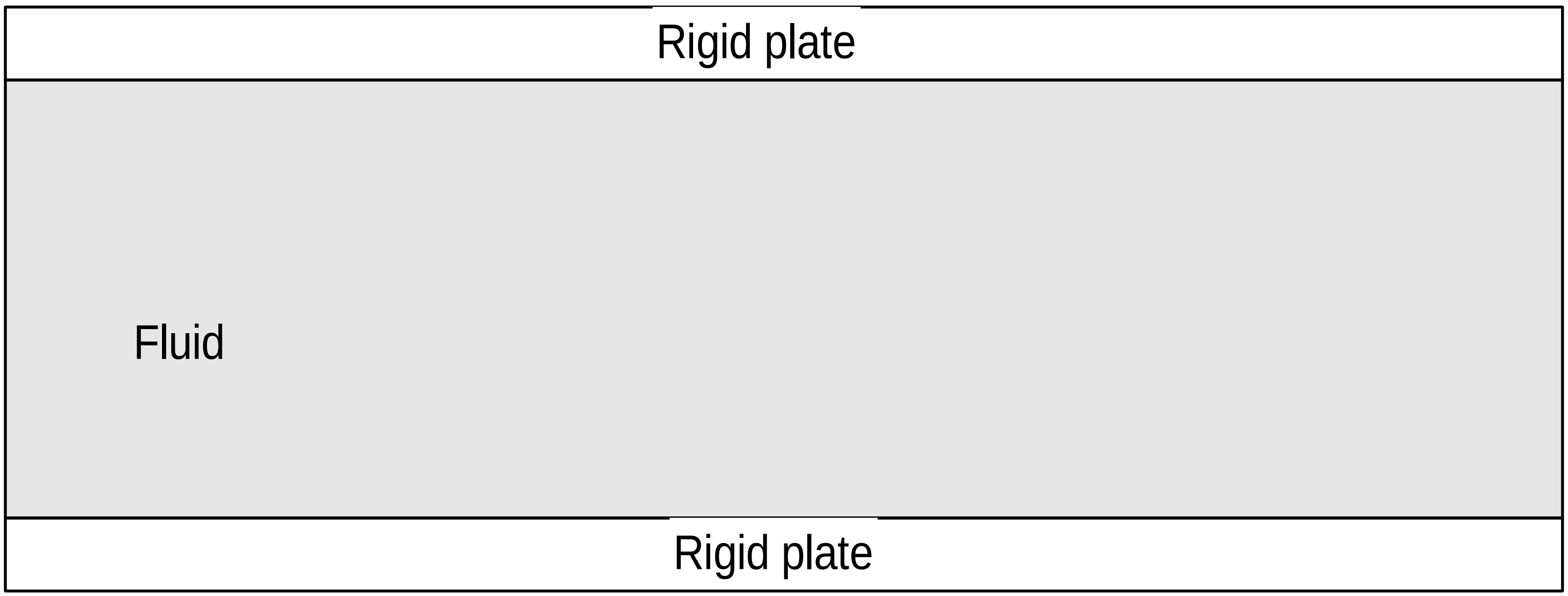
Rayleigh and his Solution



Schematic of Instability



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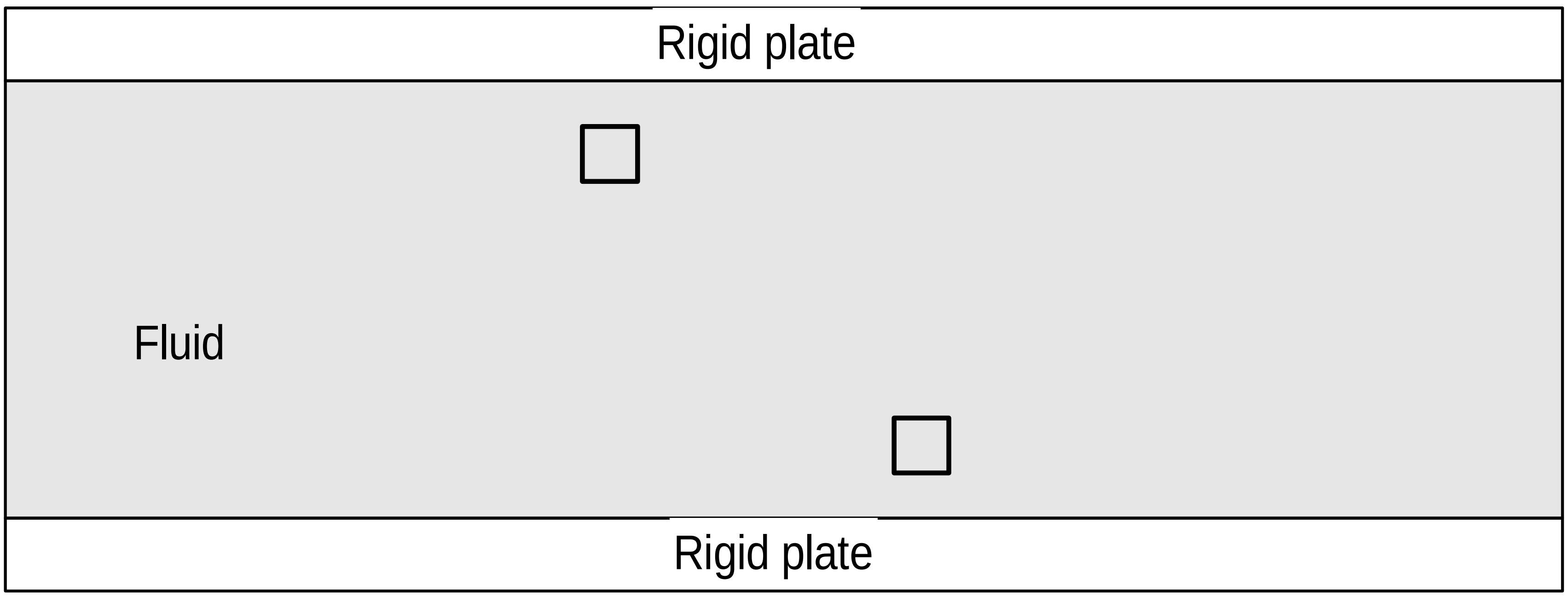

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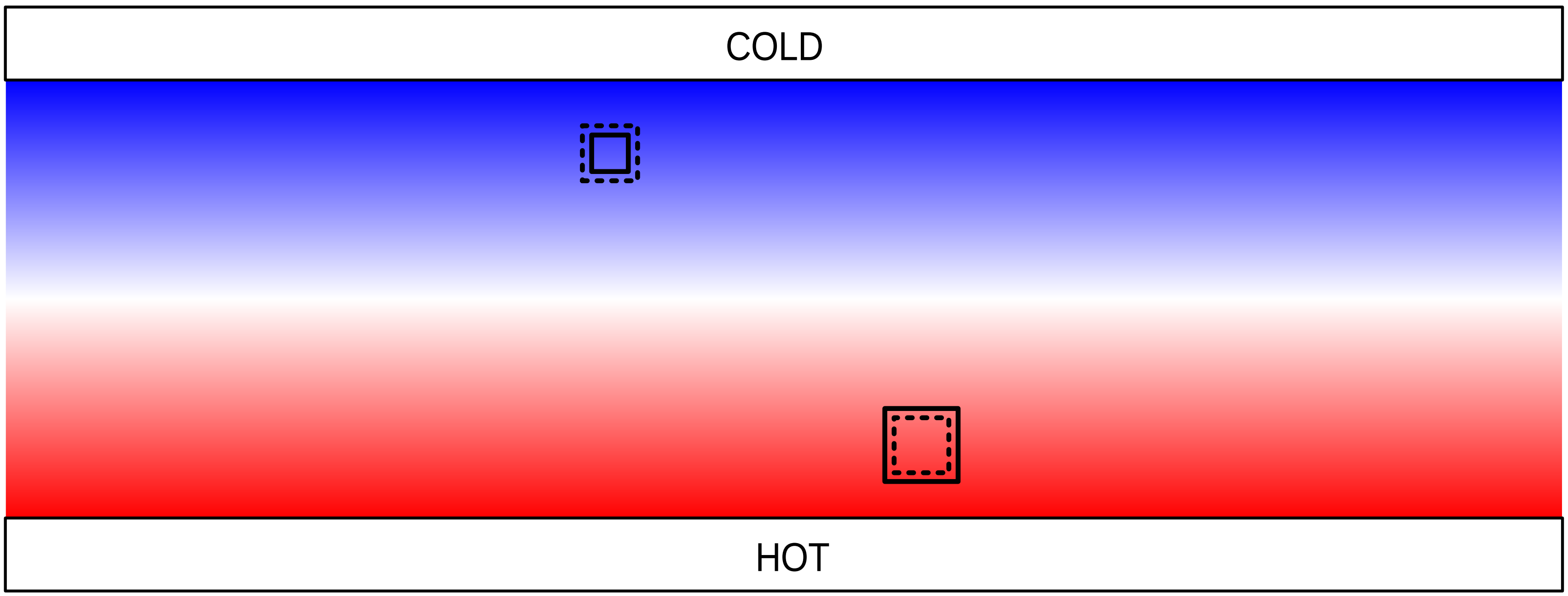

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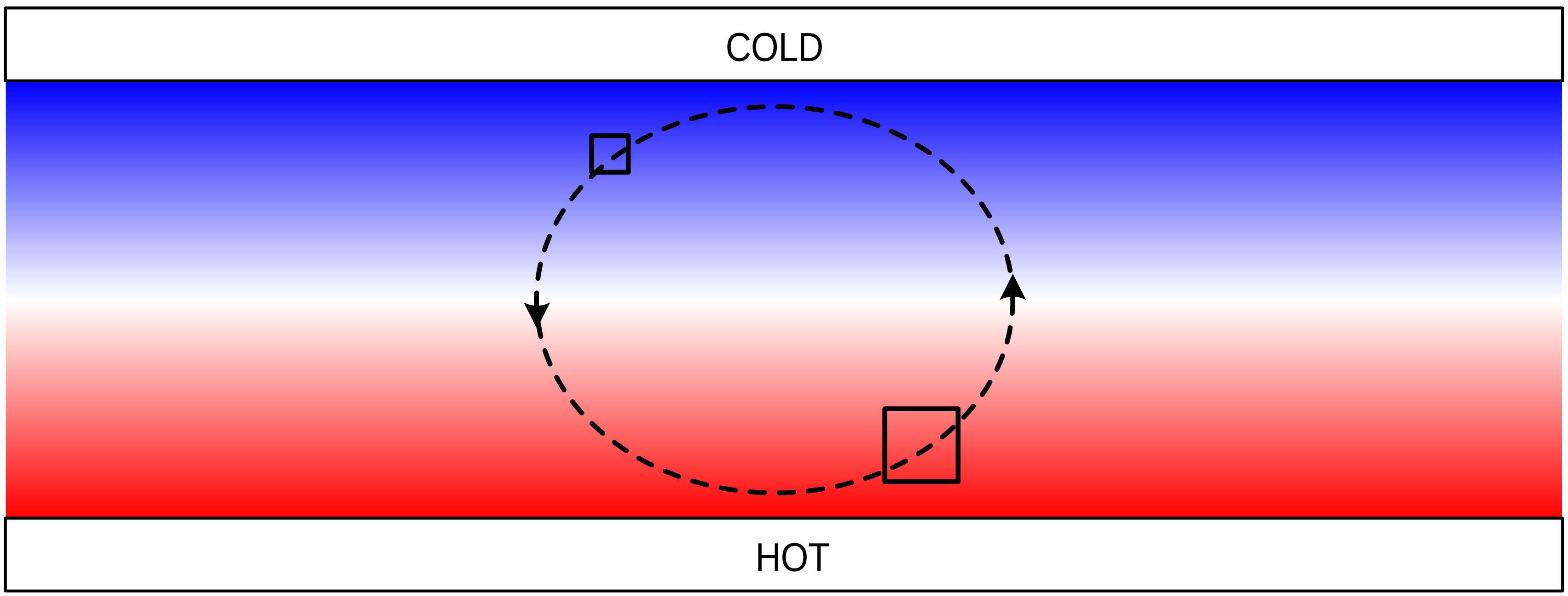

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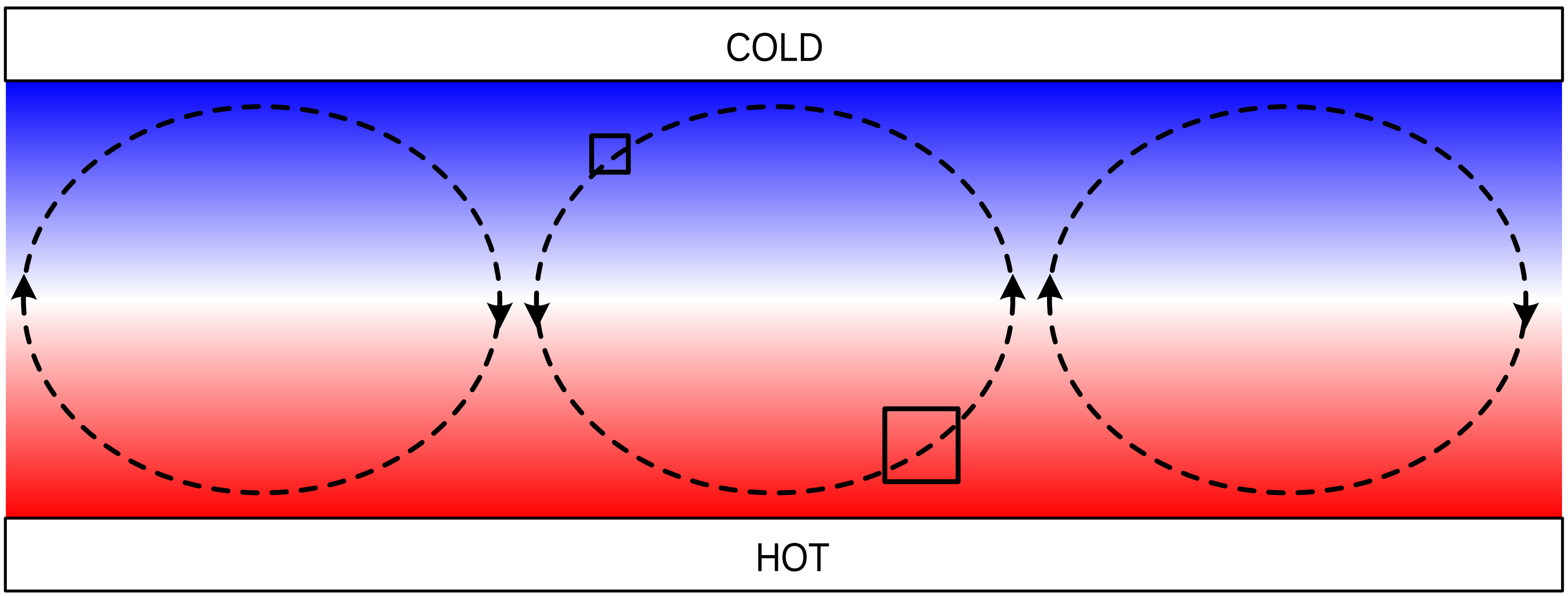

Equations for Fluid and Heat Flow

Mass conservation (LL1.2)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{g} = 0 \qquad \text{with} \qquad \mathbf{g} = \rho \mathbf{v}$$

Momentum conservation (LL15.1)

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{\Pi} + \rho g \hat{\mathbf{z}} = 0 \qquad \text{or} \qquad \frac{\partial (\rho v_i)}{\partial t} + \nabla_j \Pi_{ij} - \rho g \delta_{iz} = 0$$

with (LL15.3)

$$\Pi_{ij} = p\delta_{ij} + \rho v_i v_j - \eta \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial v_i}{\partial x_i} \right) - \zeta \delta_{ij} \frac{\partial v_i}{\partial x_i}$$

Entropy production (LL49.5-6)

$$\frac{\partial (\rho s)}{\partial t} + \nabla \cdot (\rho s \mathbf{v} - \frac{K}{T} \boldsymbol{\nabla} T) = \frac{K (\nabla T)^2}{T^2} + \frac{\eta}{2T} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial v_i}{\partial x_i} \right)^2 + \frac{\zeta}{T} \left(\frac{\partial v_i}{\partial x_i} \right)^2$$

Buoyancy Force

- Assume density is just a function of the temperature, and expand about reference temperature T_0

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with $\bar{\mathbf{\Pi}}$ as before except for a redefined pressure $\bar{p} = p + \rho_0 g z$

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- Also approximate specific heat, viscosity, thermal conductivity as constants (independent of temperature)

Boussinesq Equations

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$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} \mathbf{v} = -\boldsymbol{\nabla} (\bar{p}/\rho_0) + \rho_0 \alpha g (T - T_0) \hat{\mathbf{z}} + \nu \nabla^2 \mathbf{v} \qquad \text{with} \qquad \nu = \eta / \rho_0$$

Entropy production

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$$\frac{\partial T}{\partial t} + \mathbf{v}\cdot\boldsymbol{\nabla} T = \kappa\nabla^2 T \qquad \text{with} \qquad ds \to C dT \text{ and } \kappa = K/C$$

Boussinesq Equations

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Conducting solution ($\mathbf{v} = 0$)

$$T_{\text{cond}} = T_0 - \Delta T z/d$$

$$\bar{p}_{\text{cond}} = p_0 - \alpha g \rho_0 \Delta T z^2/2d$$

Lesson from Fluid Mechanics: Dedimensionalize

$$\mathbf{x}' = \mathbf{x}/d$$

$$t' = t/(d^2/\kappa)$$

$$\mathbf{v}' = \mathbf{v}/(\kappa/d)$$

$$\theta' = (T - T_{\text{cond}})/(\kappa\nu/\alpha g d^3)$$

$$p' = (\bar{p} - \bar{p}_{\text{cond}})/(\rho_0 \kappa\nu/d^2)$$

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Note that

$$\mathbf{v} \cdot \nabla T \Rightarrow \text{const} \times \left(\mathbf{v}' \cdot \nabla'\theta' - R w'\right) \qquad \text{with} \qquad R = \frac{\alpha g d^3 \Delta T}{\kappa\nu}$$

(writing $\mathbf{v} = (u, v, w)$)

Scaled Equations for Fluid and Heat Flow

Go to primed variables (and then drop the primes)

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Entropy production/heat flow

$$\frac{\partial \theta}{\partial t} + \mathbf{v} \cdot \nabla \theta = R w + \nabla^2 \theta$$

Dimensionless ratios: Prandtl number $\mathcal{P} = \nu/\kappa$; Rayleigh number $R = \alpha g d^3 \Delta T/\kappa\nu$

Boundary conditions at top and bottom plates $z = \pm\frac{1}{2}$

Fixed temperature	$\theta = 0$
Zero velocity (no slip)	$\mathbf{v} = 0$

Rayleigh's Calculation

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$$\frac{\partial \theta}{\partial t} = Rw + \nabla^2 \theta$$

Boundary conditions at top and bottom plates $z = \pm\frac{1}{2}$

Fixed temperature	$\theta = 0$
Free slip for $\mathbf{v} = (u, v, w)$	$w = \partial u/\partial z = \partial v/\partial z = 0$

Two dimensional mode, exponential time dependence

$$w = w_0 e^{\sigma t} \cos(qx)\cos(\pi z)$$

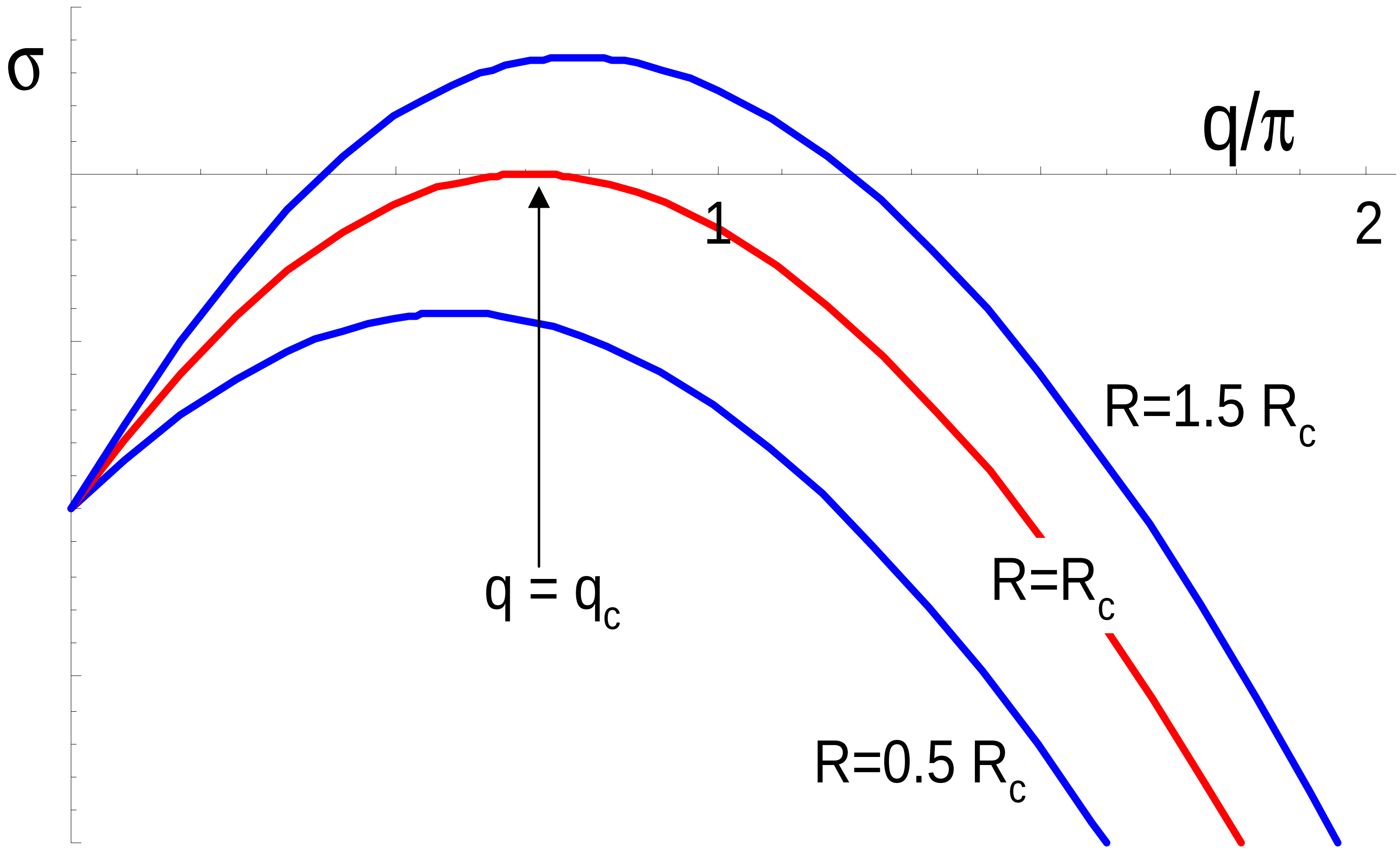
$$u = w_0 e^{\sigma t} (\pi/q)\sin(qx)\sin(\pi z)$$

$$\theta = \theta_0 e^{\sigma t} \cos(qx)\cos(\pi z)$$

gives

$$(\pi^2 + q^2)(\mathcal{P}^{-1}\sigma + \pi^2 + q^2)(\sigma + \pi^2 + q^2) - Rq^2 = 0$$

Rayleigh's Growth Rate (for $\mathcal{P} = 1$)



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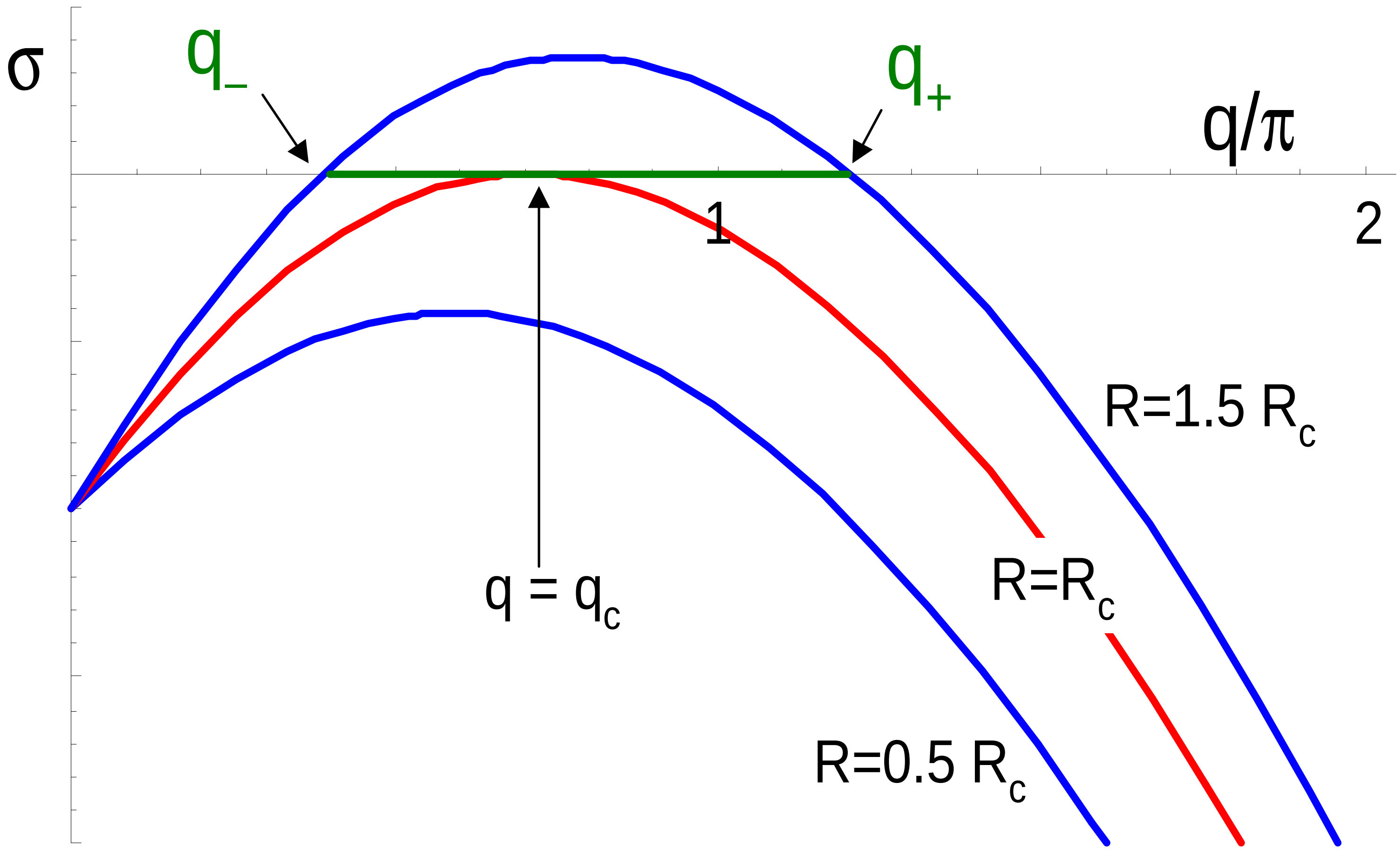

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Comments

- Rayleigh seems to have been unaware that a hexagonal state is easily produced as a sum of three stripe states with wave vectors $q(1,0)$, $q(-1/2,\sqrt{3}/2)$, $q(-1/2,-\sqrt{3}/2)$. Since the calculation is *linear* the *principle of superposition* applies, and the growth rate and R_c, q_c are the same for hexagons as for stripes.

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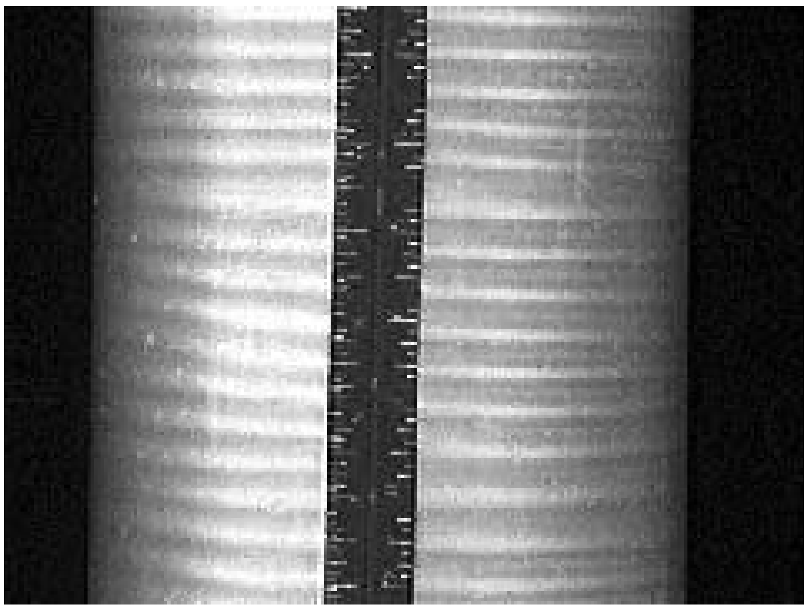
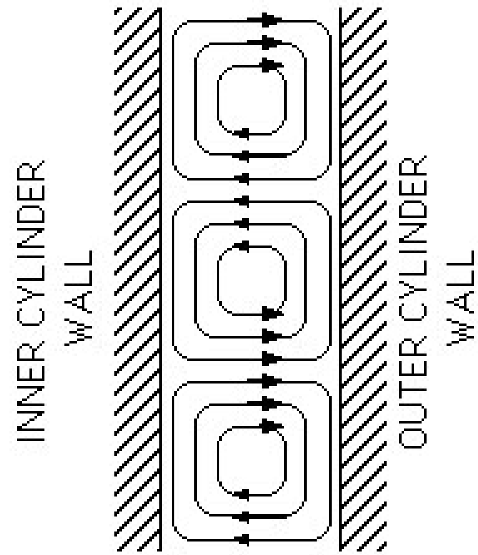
- The linear instability with rigid plates with physical (no-slip) boundaries is harder because the equations are not separable. A handout on the website works through the calculation. The qualitative results are similar, but now $R_c \simeq 1707$ and $q_c \simeq 3.114$ ($q_c = \pi$ would give rolls with diameter equal the depth).

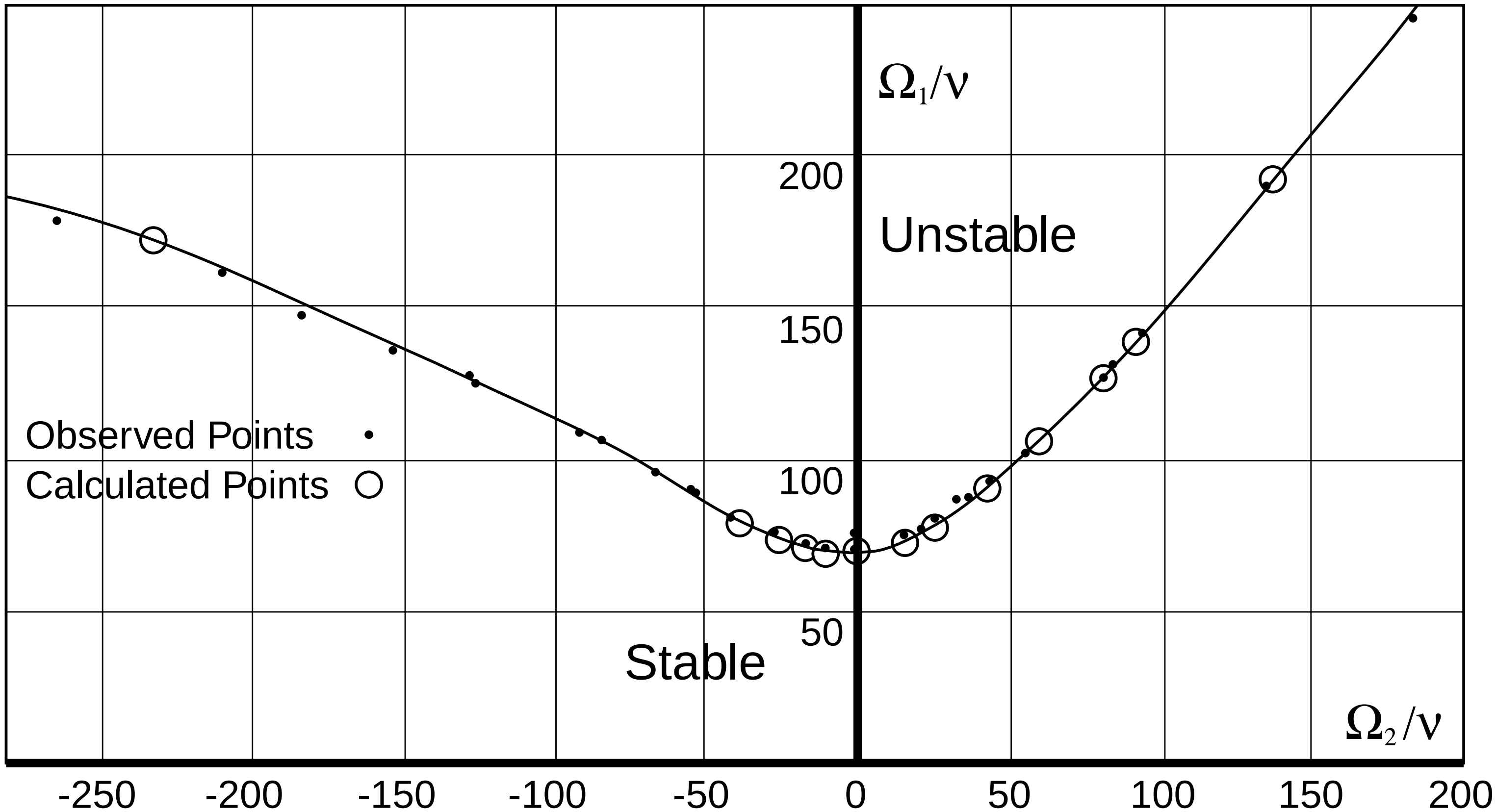
Taylor-Couette Instability





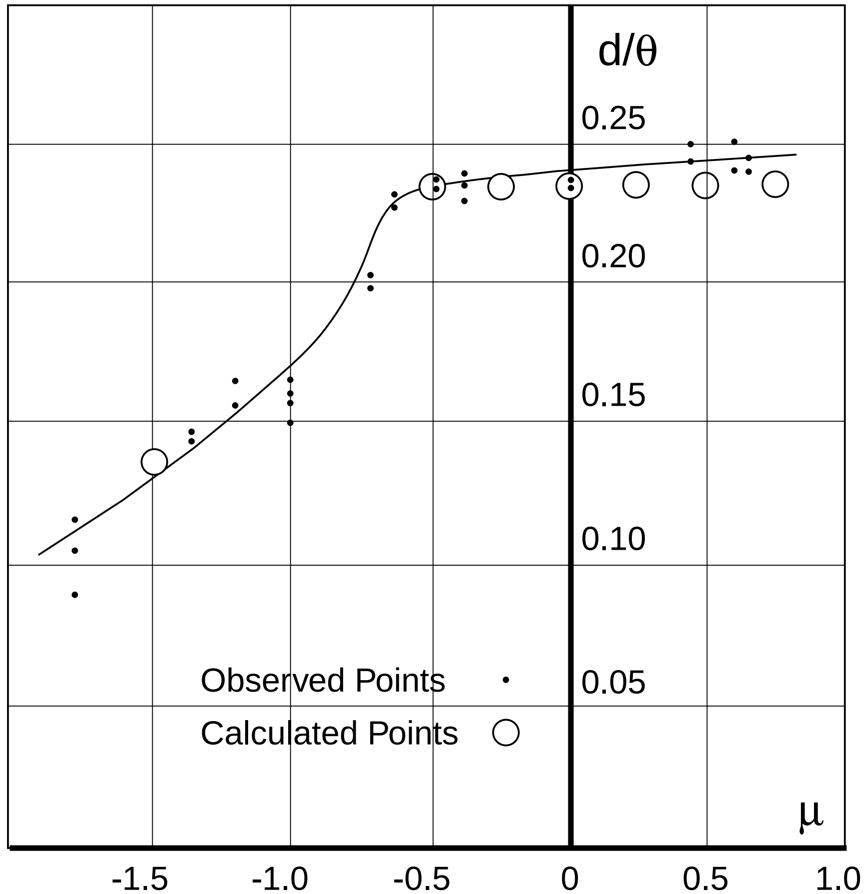
From the website of Arel Weisberg

Taylor's 1923 Results: Onset



G. I. Taylor, *Stability of a Viscous Liquid Contained Between Two Rotating Cylinders*, Phil. Tran. Roy. Soc. A**223,** 289 (1923)

Taylor's 1923 Results: Wavenumber



The outer and inner radii were $r_o = 4.04\,\text{cm}$, and $r_i = 3.80\,\text{cm}$. μ is the ratio of outer to inner rotation rates Ω_2/Ω_1. The vertical label d/θ is the average width of a vortex in centimeters.

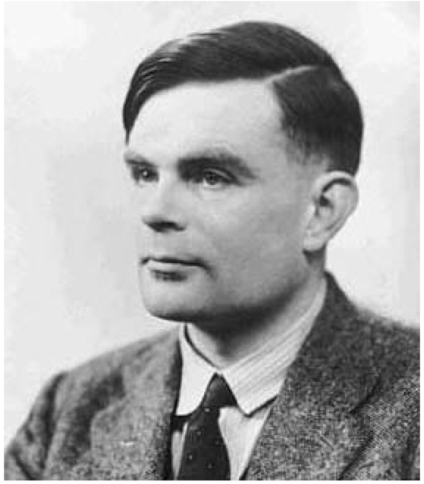
Turing: The Chemical Basis of Morphogenesis

Wikipedia: Morphogenesis (from the Greek morphê shape and genesis creation) is one of three fundamental aspects of developmental biology…. The study of morphogenesis involves an attempt to understand the processes that control the organized spatial distribution of cells that arises during the embryonic development of an organism and which give rise to the characteristic forms of tissues, organs and overall body anatomy.

Turing (Phil. Tran. R. Soc. Lon. **B237**, 37 (1952)): It is suggested that a system of chemical substances, called morphogens, reacting together and diffusing through a tissue, is adequate to account for the main phenomena of morphogenesis. Such a system, although it may originally be quite homogeneous, may later develop a pattern or structure due to an instability of the homogeneous equilibrium, which is triggered off by random disturbances.

Quotes from Turing's Paper

This model will be a simplification and an idealization, and consequently a falsification. It is to be hoped that the features retained for discussion are those of greatest importance in the present state of knowledge.



One would like to be able to follow this more general [nonlinear] process mathematically also. The difficulties are, however, such that one cannot hope to have any very embracing *theory* of such processes, beyond the statement of the equations. It might be possible, however, to treat a few particular cases in detail with the aid of a digital computer.

Turing on Broken Symmetry

There appears superficially to be a difficulty confronting this theory of morphogenesis, or, indeed, almost any other theory of it. An embryo in its spherical blastula stage has spherical symmetry.... But a system which has spherical symmetry, and whose state is changing because of chemical reactions and diffusion, will remain spherically symmetrical for ever..... It certainly cannot result in an organism such as a horse, which is not spherically symmetrical.

There is a fallacy in this argument. It was assumed that the deviations from spherical symmetry in the blastula could be ignored because it makes no particular difference what form of asymmetry there is. It is, however, important that there are *some* deviations, for the system may reach a state of instability in which these irregularities, or certain components of them, tend to grow.....In practice, however, the presence of irregularities, including statistical fluctuations in the numbers of molecules undergoing the various reaction, will, if the system has an appropriate kind of instability, result in this homogeneity disappearing.

Mathematical Content of Turing's Paper

- Linear stability analysis of:
  - ◇ Ring of discrete cells
  - ◇ Ring of continuous medium
  - ◇ Surface of sphere
- Discussion of types of instabilities:
  - ◇ uniform instabilities (wave number $q_c = 0$)
  - ◇ instabilities leading to spatial structure ($q_c \neq 0$)
  - ◇ oscillatory instabilities (2 chemicals) ($q_c = 0$, $\mathrm{Im}\,\sigma \neq 0$)
  - ◇ wave instabilities ($q_c \neq 0$, $\mathrm{Im}\,\sigma \neq 0$) (3 or more chemicals)
- Evolution from random initial condition in 1 and 2 dimensions
- Manual computation of nonlinear state in small discrete rings

Reaction-Diffusion

Two chemical species with concentrations u_1, u_2 that react and diffuse

$$\partial_t u_1 = f_1(u_1, u_2) + D_1 \partial_x^2 u_1$$
$$\partial_t u_2 = f_2(u_1, u_2) + D_2 \partial_x^2 u_2$$

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- Reaction:

$$a\,\mathrm{A} + b\,\mathrm{B} \to c\,\mathrm{C} + d\,\mathrm{D}$$

gives the reaction rate (law of mass action)

$$\nu(t) = -\frac{1}{a}\frac{d[\mathrm{A}]}{dt} = \cdots = k[A]^{m_\mathrm{A}}[B]^{m_\mathrm{B}}$$

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- Diffusion: conservation equation

  $$\partial_t u_i = -\nabla \cdot \mathbf{j}_i$$

  with

  $$\mathbf{j}_i = -D_i \nabla u_i$$

  (Skip to example)

Turing Instability

- Stationary uniform base solution $\mathbf{u}_b = (u_{1b}, u_{2b})$

$$f_1(u_{1b}, u_{2b}) = 0$$

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Stability Analysis

- Eigenvalue equation

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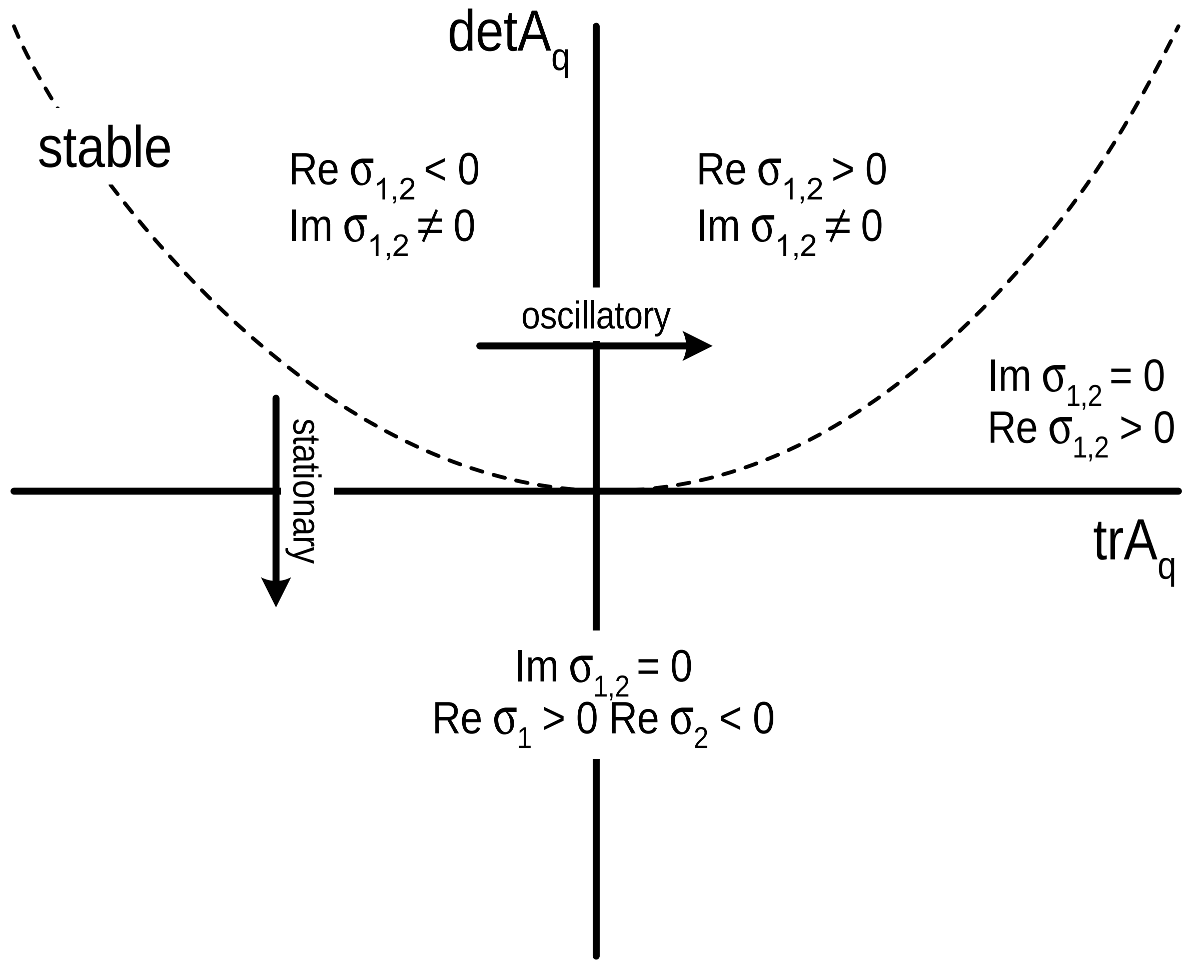
Stability Regions



Conditions for Turing Instability

- Uniform state is stable to a spatially uniform instability

$$
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- (Now we see $a_{11} > 0$ and a_{12}, a_{21} must have opposite signs)

Turing Length Scale

Turing condition can be expressed as

$$q_m^2 = \frac{1}{2}\left(\frac{1}{l_1^2} - \frac{1}{l_2^2}\right) > \sqrt{\frac{a_{11}a_{22} - a_{12}a_{21}}{D_1 D_2}}$$

with $l_i = \sqrt{D_i/a_{ii}}$ are diffusion lengths: “local activation with long range inhibition”

Example: the Brusselator

$$\partial_t u_1 = a - (b+1)u_1 + u_1^2 u_2 + D_1 \partial_x^2 u_1$$
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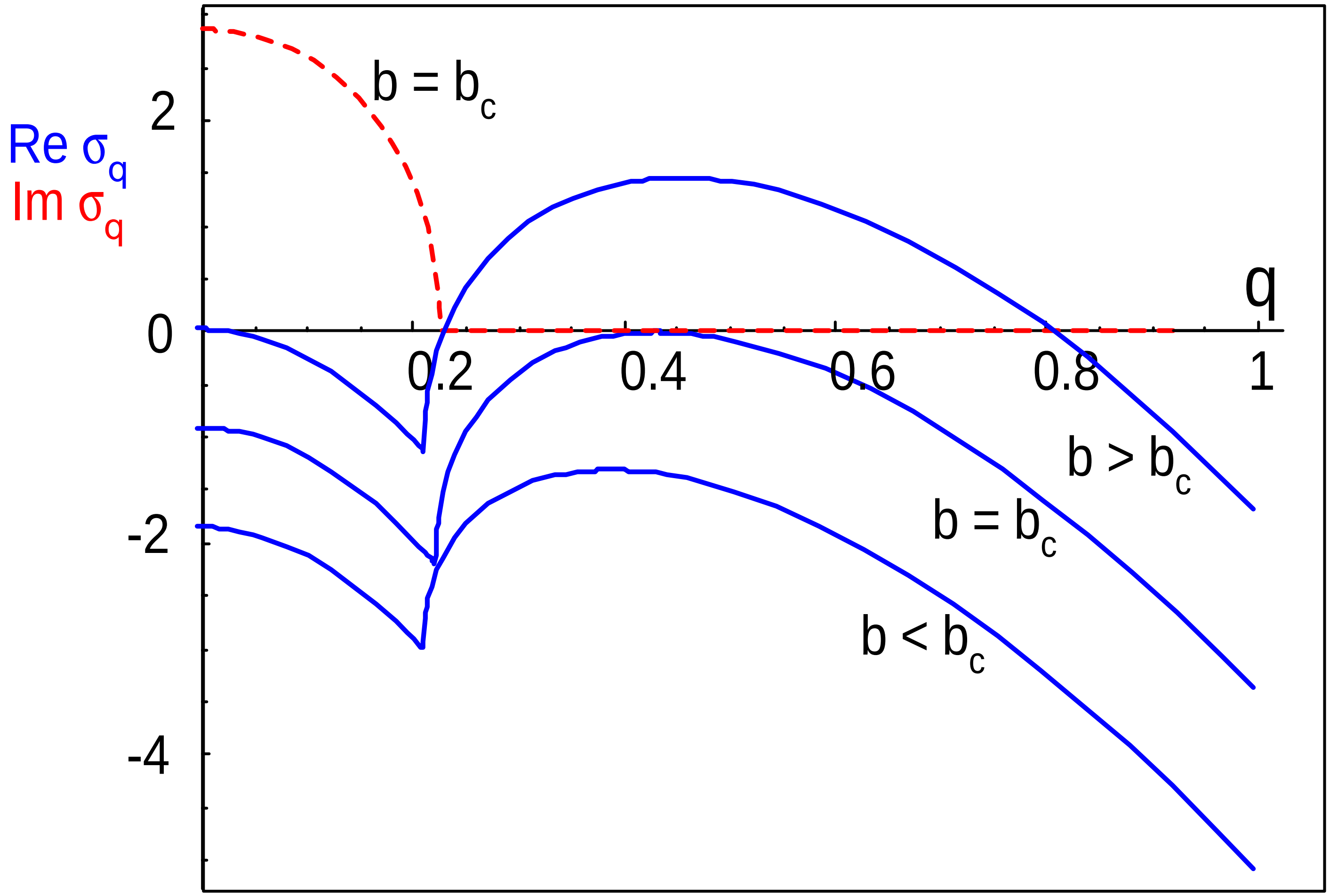
- Instability for $b \geq b_c$ at wave number q_c with

$$b_c = \left(1 + a\sqrt{\frac{D_1}{D_2}}\right)^2 \approx 2.34, \quad q_c = \sqrt{\frac{D_1 a_{22} + D_2 a_{11}}{2 D_1 D_2}} \approx 0.435$$

Brusselator: Results



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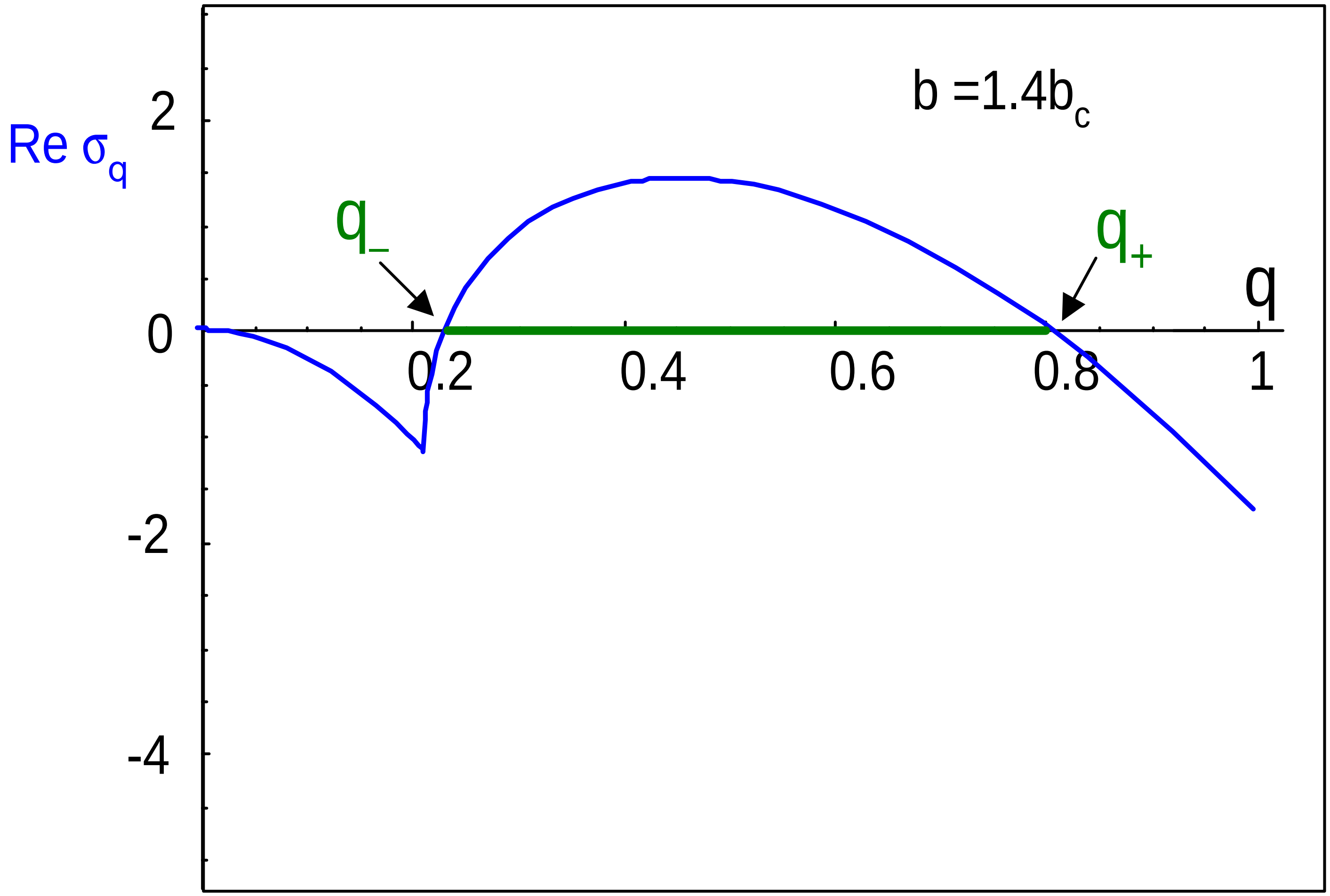
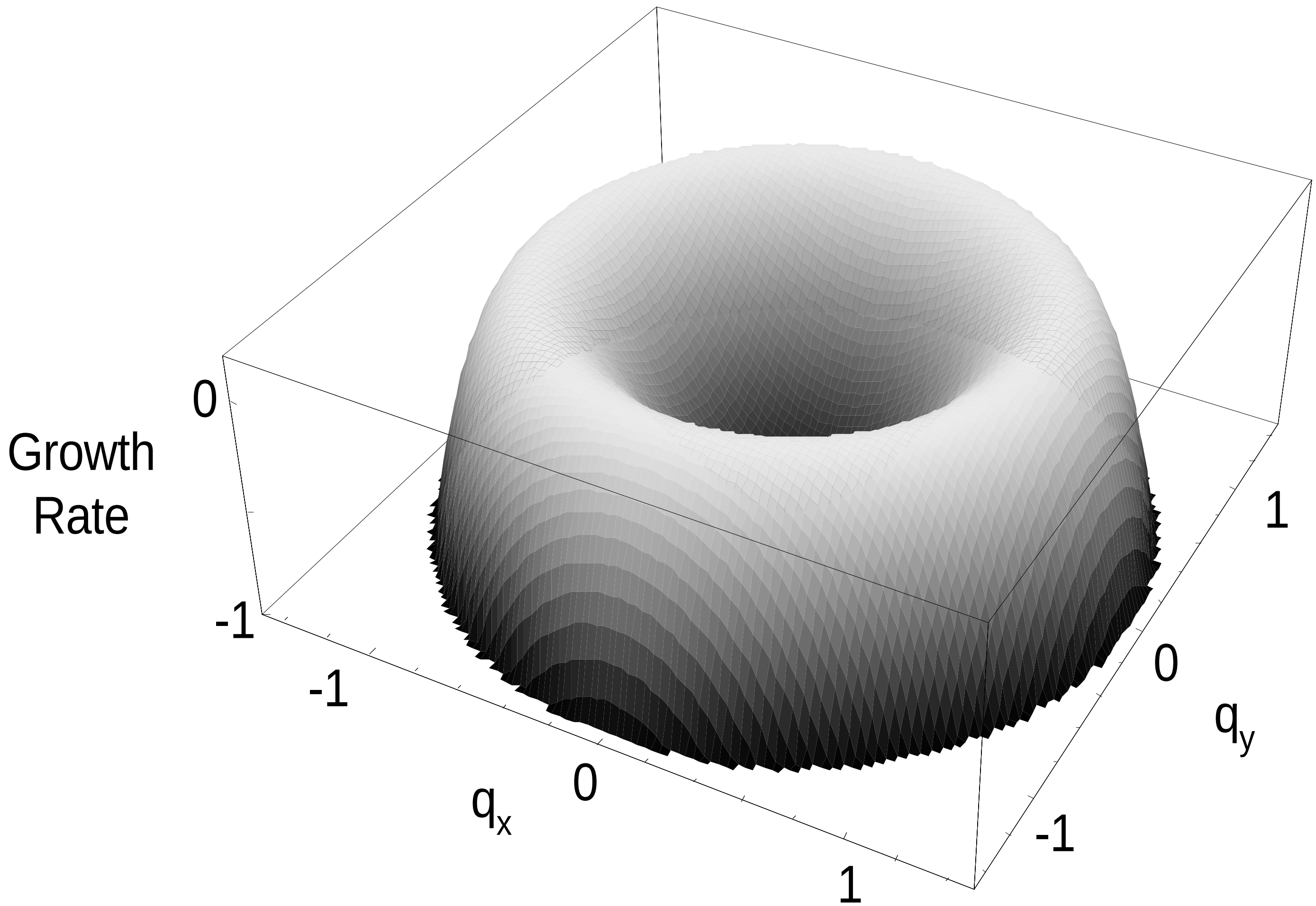
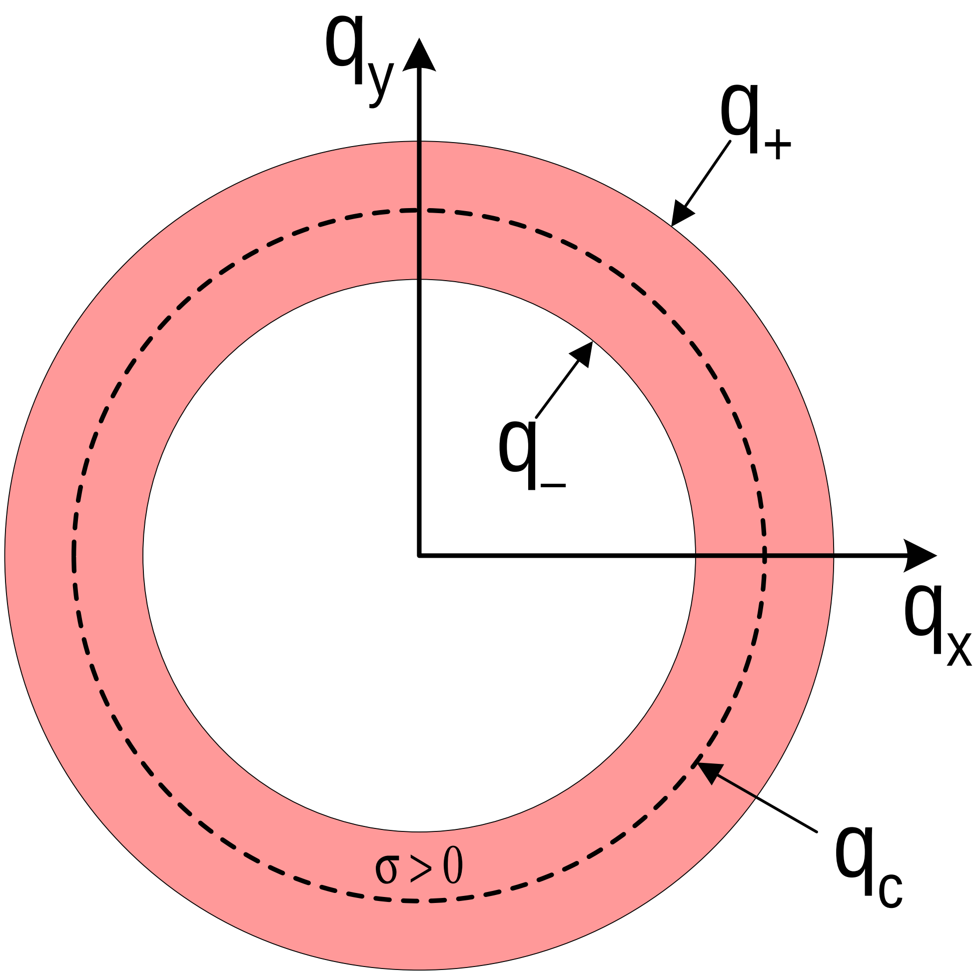


Onset in Systems with Rotational Symmetry



Pattern Formation



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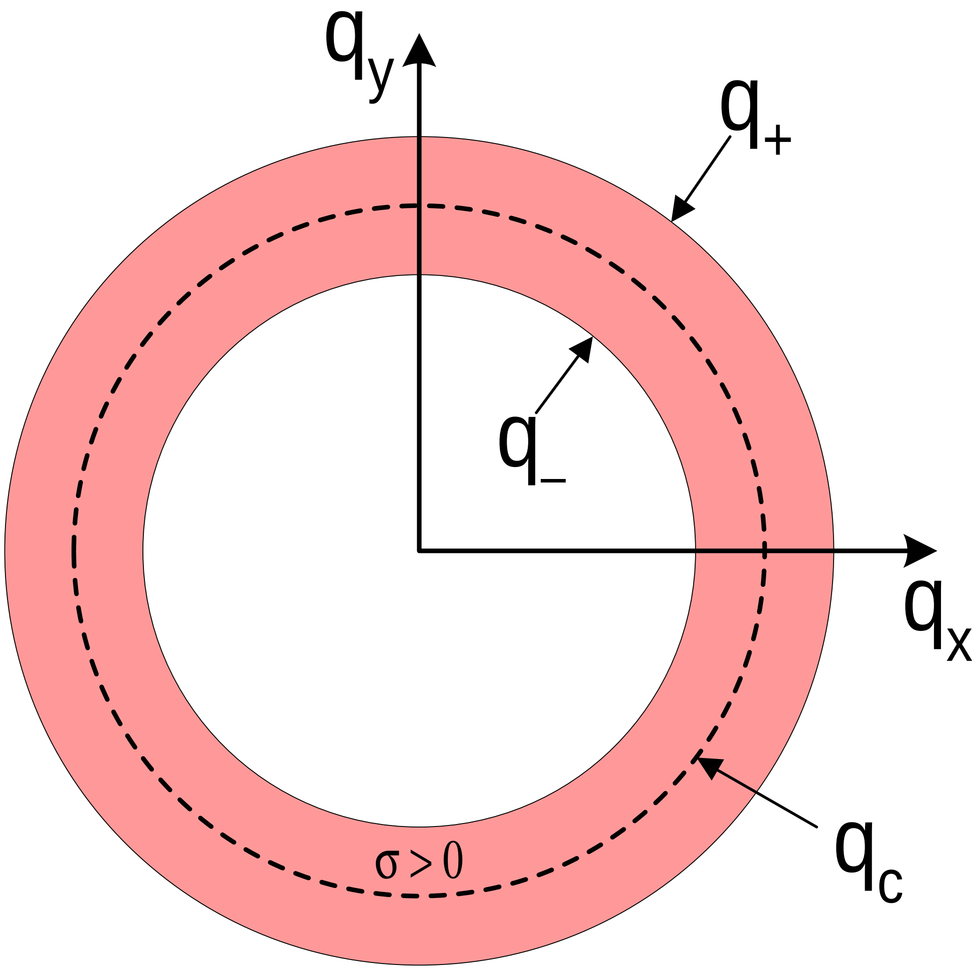
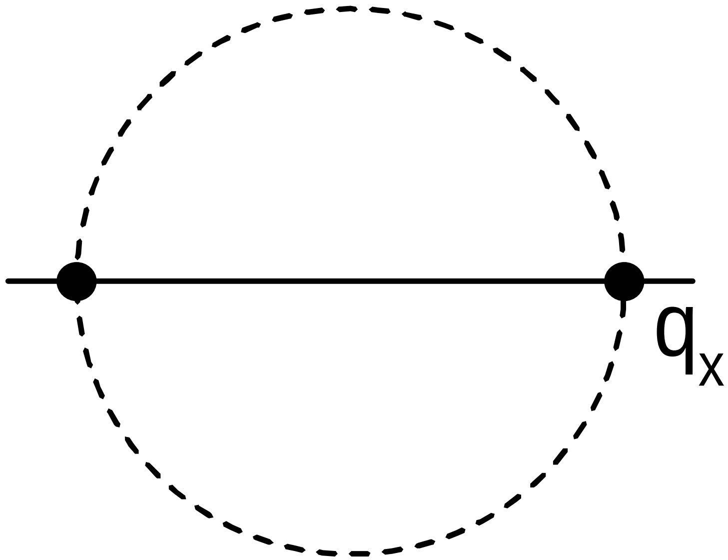
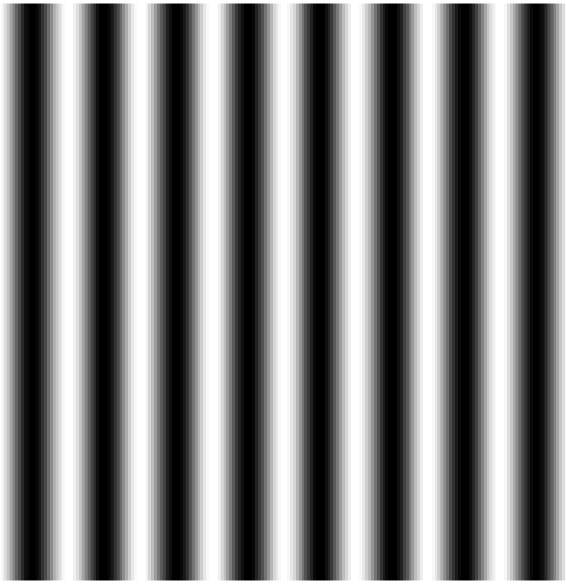


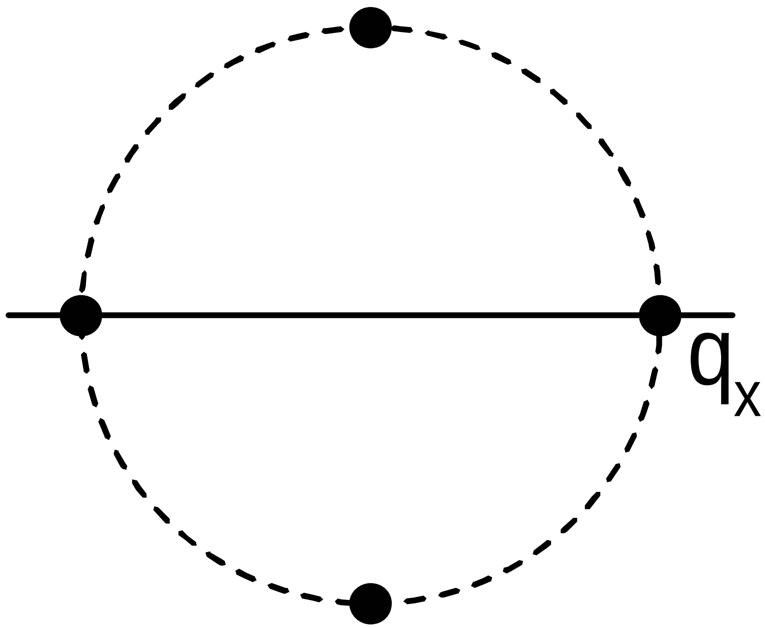
What states form from the nonlinear saturation of the unstable modes?

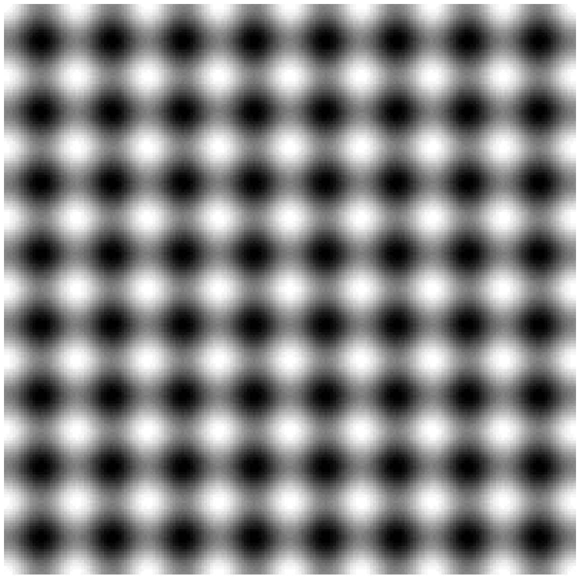
Stripe state



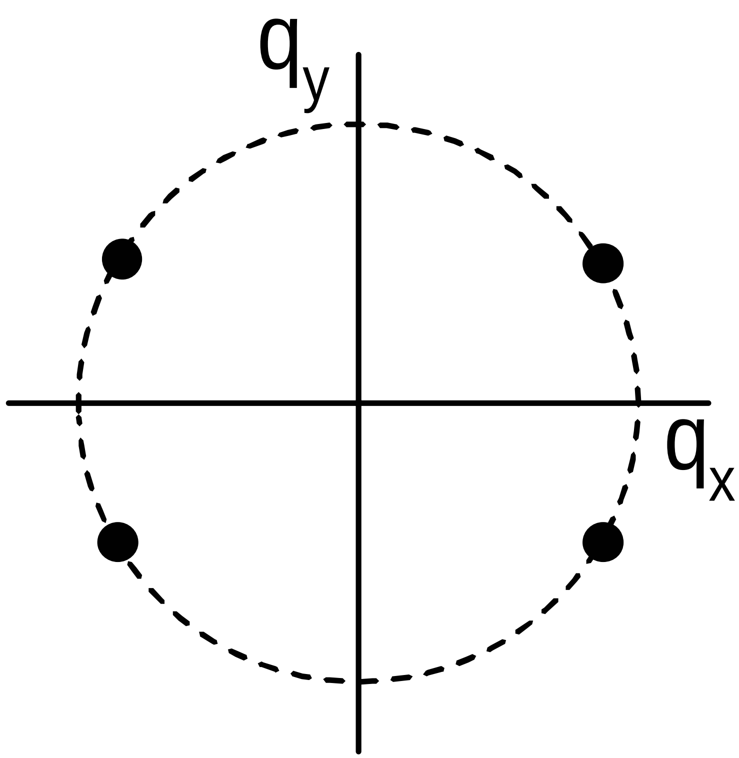


Square state

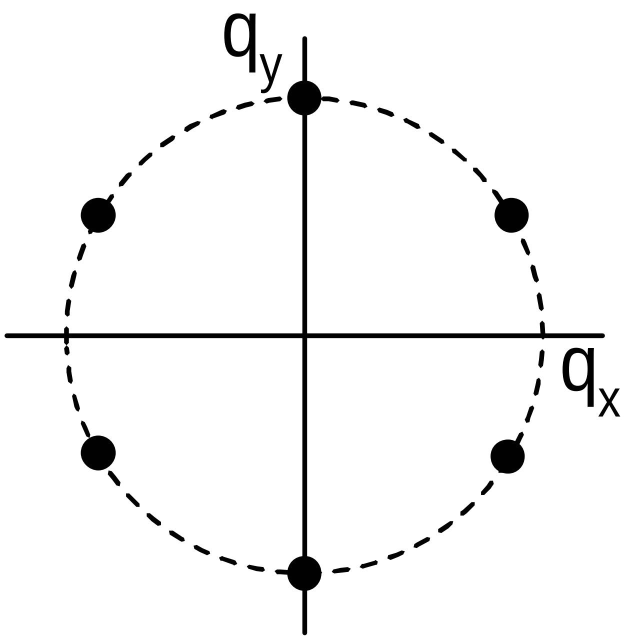


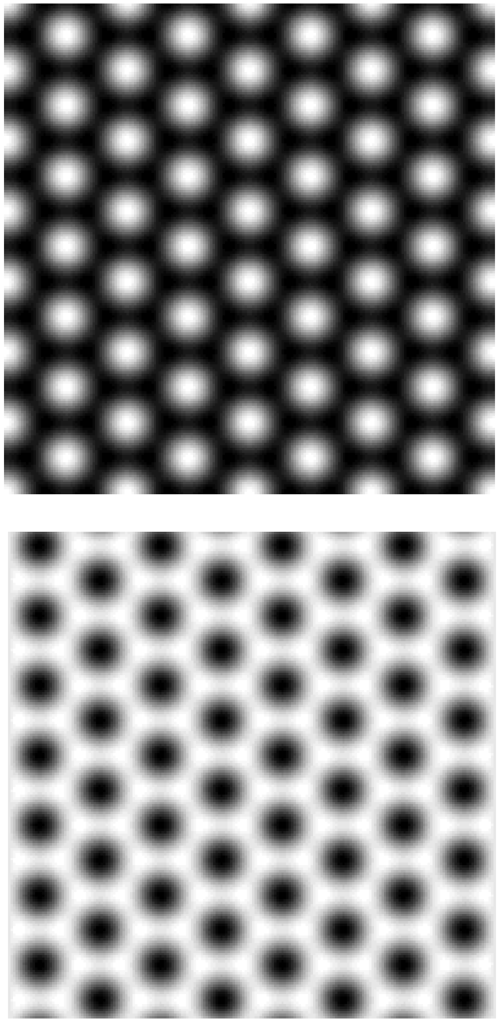


Rectangular (orthorhombic) state

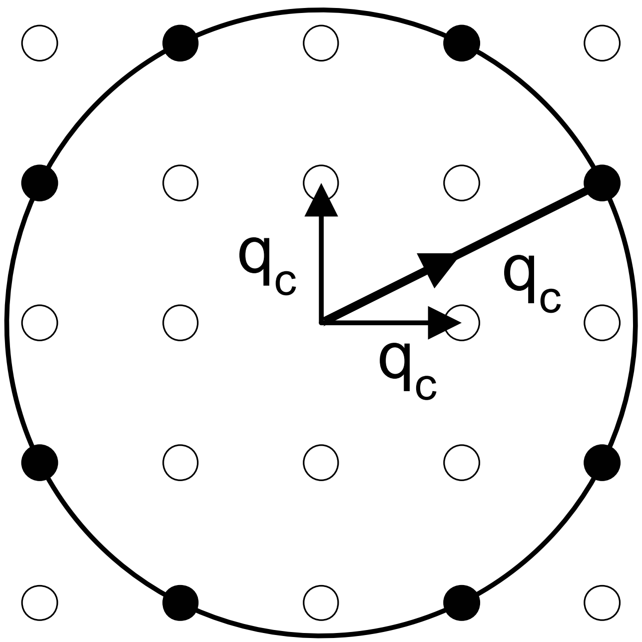


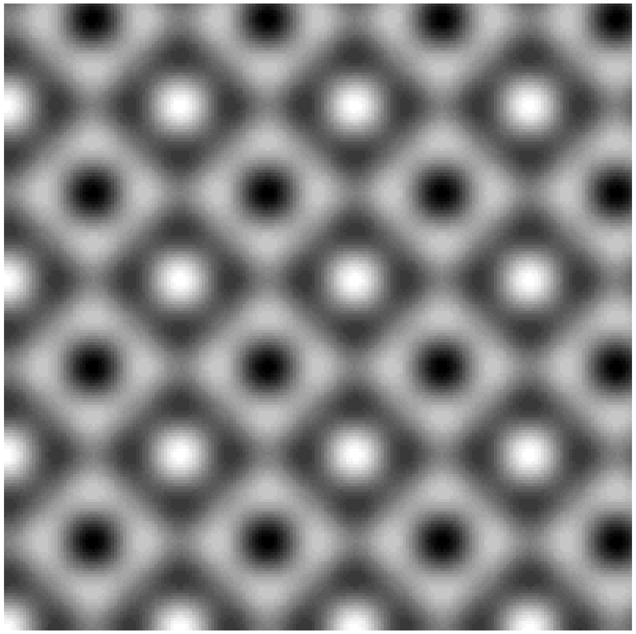
Hexagonal state



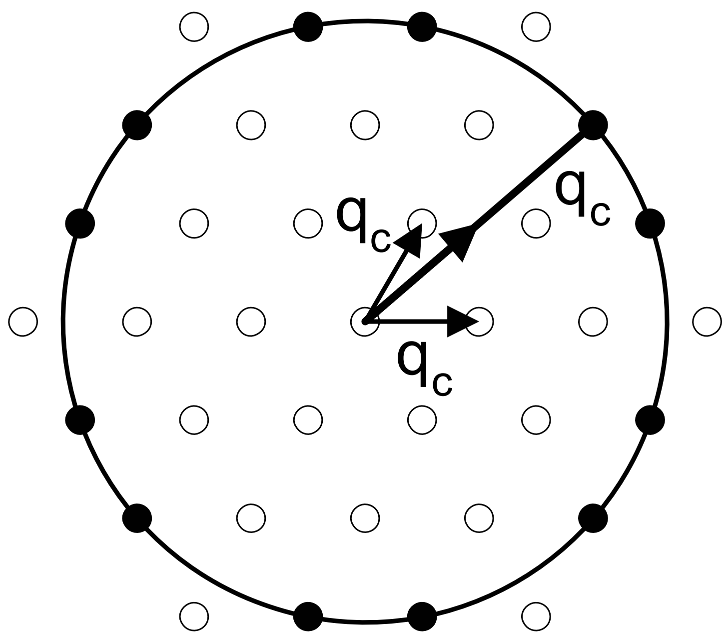


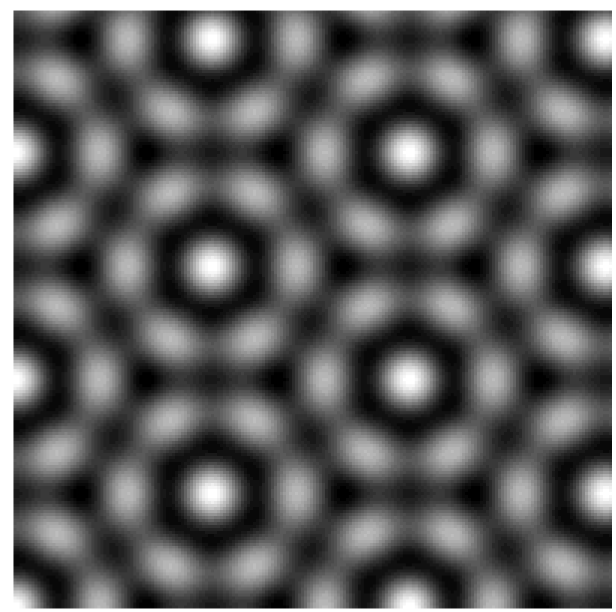
Supersquare state



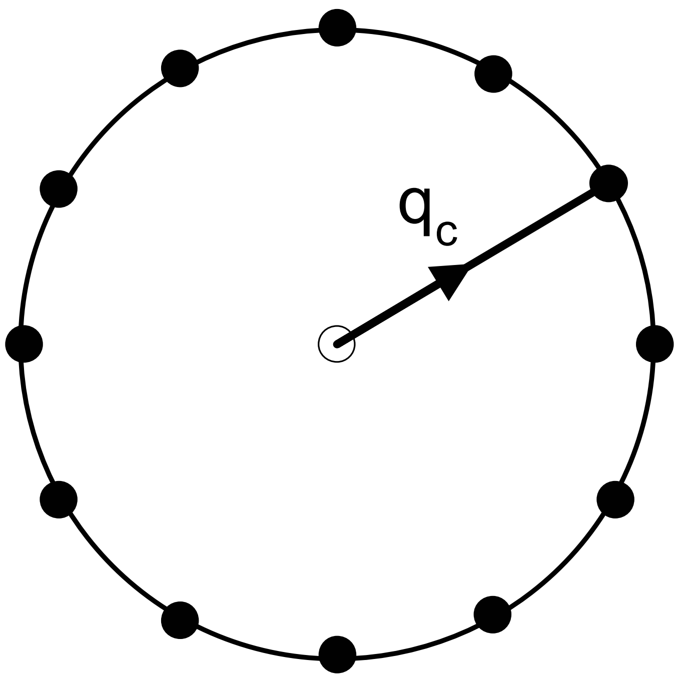


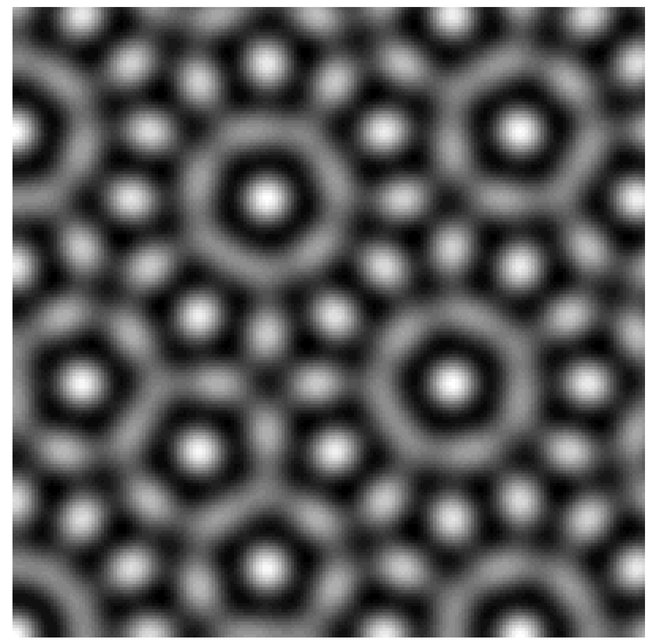
Superhexagon state





Quasicrystal state





Next Lecture

Pattern Formation: Nonlinearity and Symmetry

- Amplitude equations
- Symmetry, the phase variable and rigidity
- Topological defects