Physics of Active Matter: Hydrodynamics and Energetics

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Thanks!

John Toner

Hugues Chate

What is active matter?

"**Active matter** is matter composed of large numbers of active "agents", each of which consumes **energy** in order to move or to exert mechanical forces. Such systems are intrinsically **out of thermal equilibrium**. Unlike thermal systems relaxing towards equilibrium and systems with boundary conditions imposing steady currents, active matter systems **break time reversal symmetry** because energy is being continually dissipated by the individual constituents. Most examples of active matter are biological in origin and span all the scales of the living, from bacteria and self-organising bio-polymers such as microtubules and actin (both of which are part of the cytoskeleton of living cells), to schools of fish and flocks of birds. However, a great deal of current experimental work is devoted to synthetic systems such as artificial **self-propelled particles**. Active matter is a relatively new material classification in soft matter: the most extensively studied model, the **Vicsek model**, dates from 1995.

Research in active matter combines analytical techniques, numerical simulations and experiments. Notable analytical approaches include **hydrodynamics,** kinetic theory, and **non-equilibrium statistical physics.** ….."

--- Wikipedia

Outline

- Lecture 1: Introduction to active matter
  - Motivation and set-up of the problem
  - The discrete models: Vicsek model, active Ising model (AIM)
  - The hydrodynamic approach: The Toner-Tu (TT) equation
  - Symmetry and spontaneous symmetry-breaking
  - Linear analysis: The Mermin-Wagner (MW) theorem

- Lecture 2: Nonlinear analysis of the hydrodynamic model (TT equation)
  - The breakdown of linear hydrodynamics in $d < 4$
  - The idea of scaling and renormalization group (RG) theory
  - The RG analysis for the TT equation
  - Long-range order in 2D flocking: The break-down of the MW theorem
  - The hydrodynamic modes of fluctuations in flocking

- Lecture 3: The energetics of flocking
  - Nonequilibrium system and the breakdown of detailed balance
  - The cost of maintaining a nonequilibrium steady state (NESS)
  - The energy cost of flocking in AIM
  - The energy-performance tradeoff in flocking

Lecture 1: Introduction to active matter

Motivation: collective motion of agents are ubiquitous in nature

Flocking behaviors at the macroscopic scales

Fish School

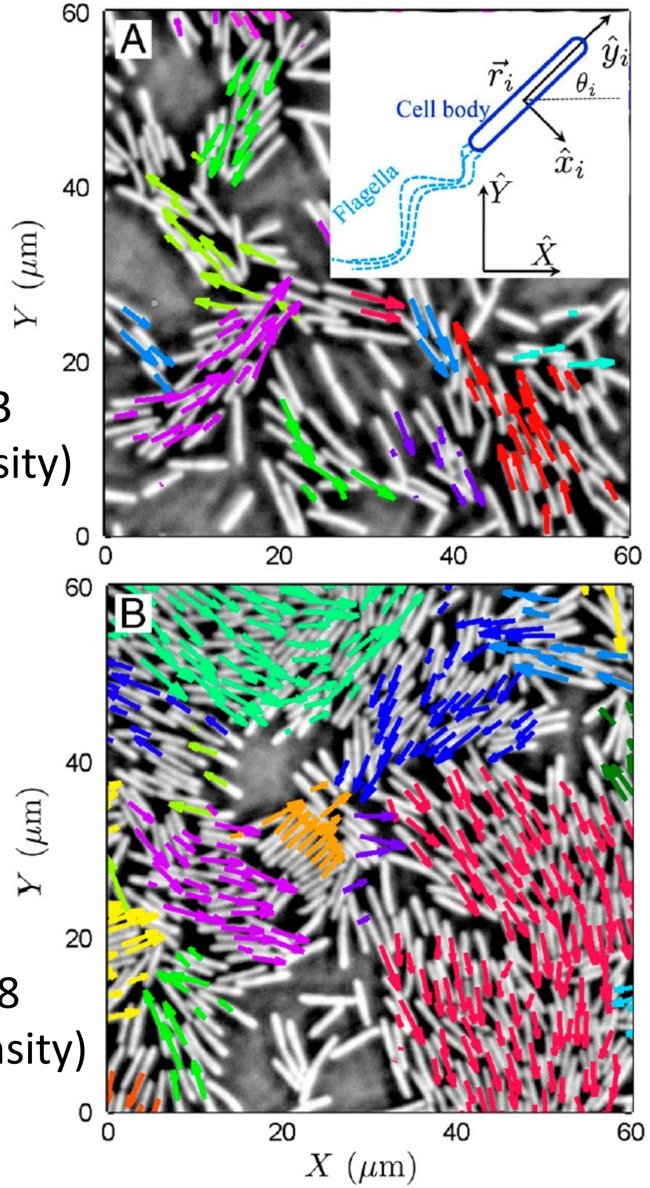
Bird Flock

Grazing Wildebeests

You can easily find movies on youtube, e.g., https://www.youtube.com/watch?v=V4f_1_r80RY

Flocking behaviors at the microscopic scales

N$_{cell}$=343
(lower density)

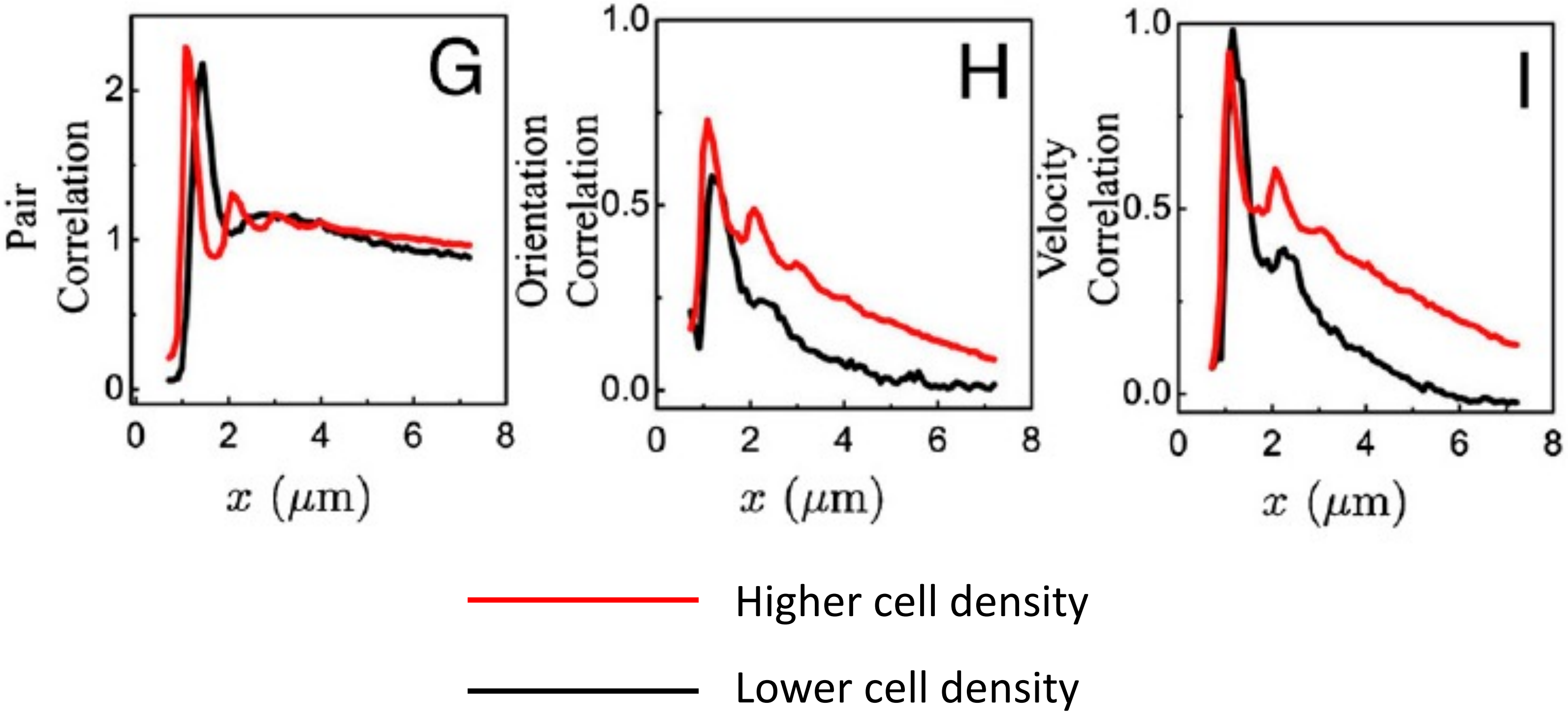


N$_{cell}$=718
(higher density)

Collective motion and density fluctuations in bacterial colonies

H. P. Zhang[1], Avraham Be'er, E.-L. Florin, and Harry L. Swinney[1]

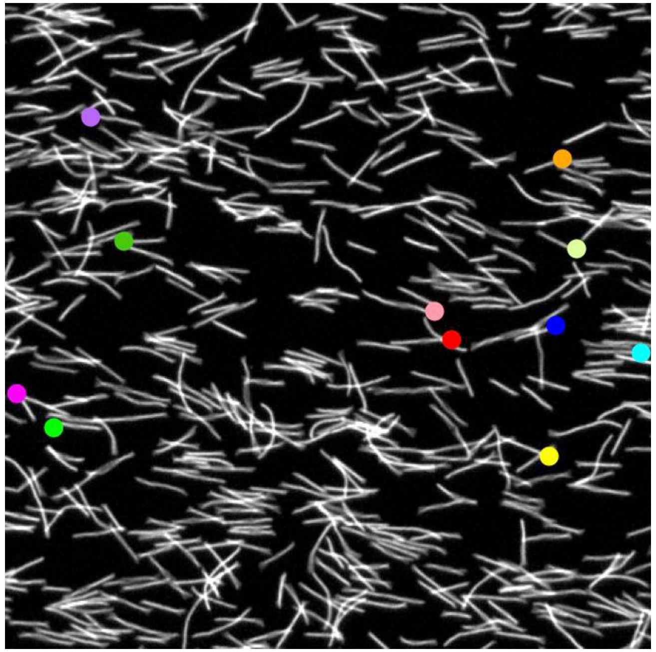
(PNAS, 107 (31), 2010)



Other examples of swimming bacterial cells

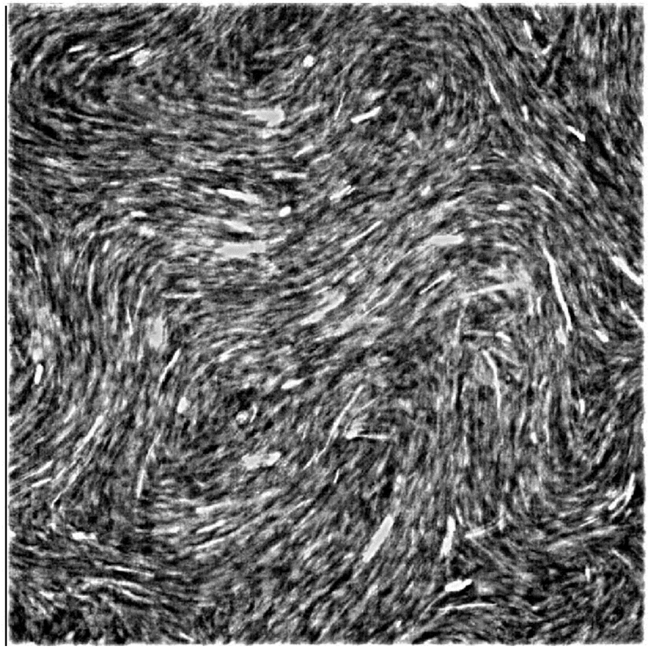
1) *E. coli* strongly confined in 2D exhibit dry Vicsek-rods behavior

Nishiguchi et al, PRE , 95, 020601(R), 2017



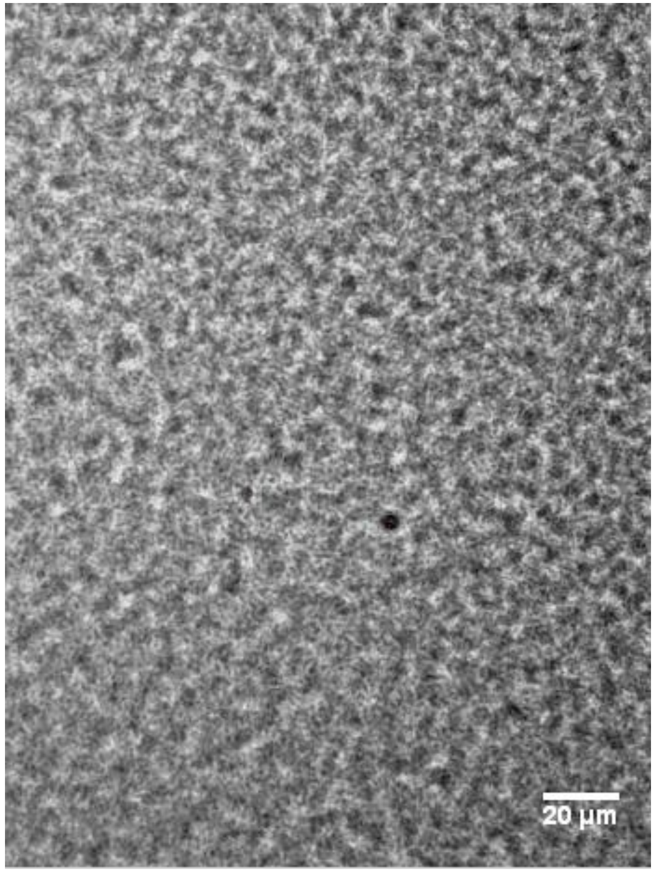
2) 2D wet active nematics at the edge of growing *Serratia* colony

Li et al, PNAS, 116(3), 777-785, 2019



3) Weak synchronization in quasi-2D swarming *E. coli*

Chen et al, Nature, 542, 210–214, *2017*

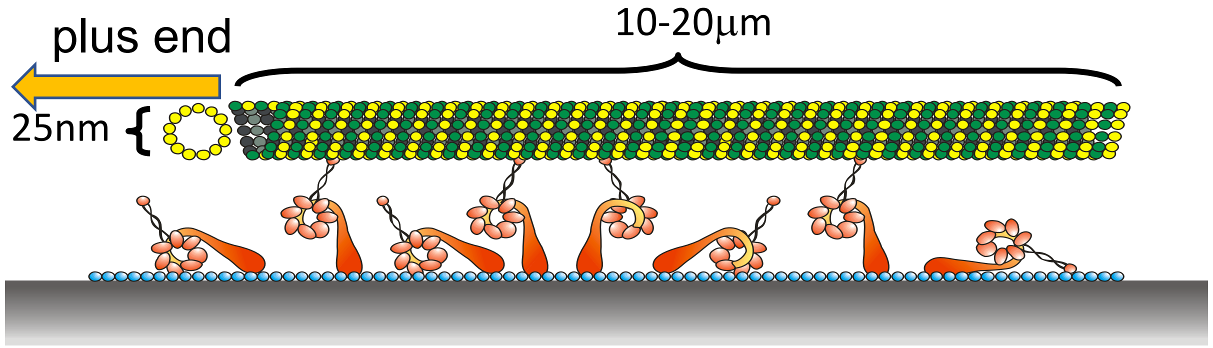


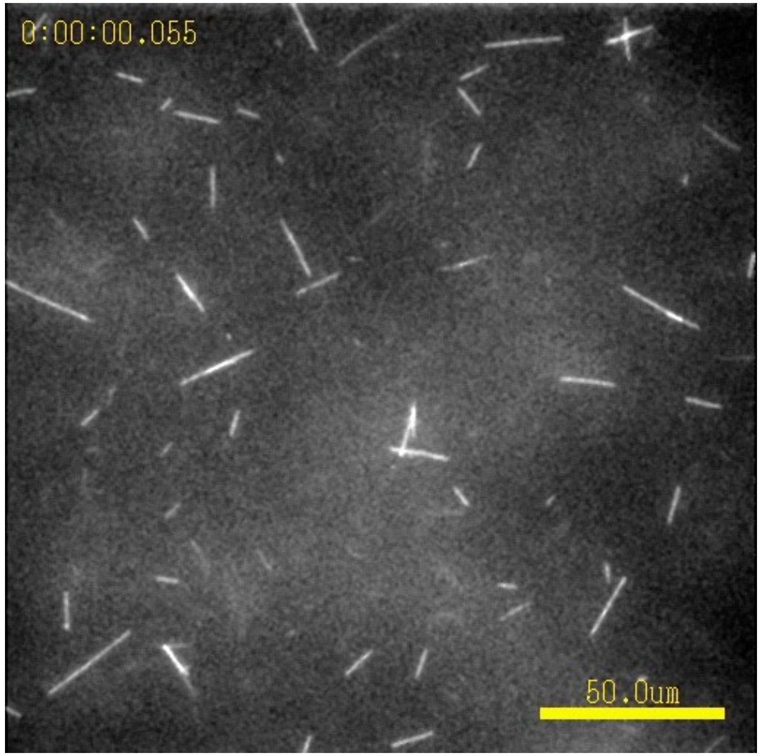
Another class of microscopic active matter: High-density motility assays

Motility assays: motor proteins, grafted on a substrate, consume ATP to displace track filaments such as microtubules (MT)

For example: dynein motors and microtubules

- with high density of motors (1000/um^2), smooth, constant-speed motion of single MT
- Alignment upon collision





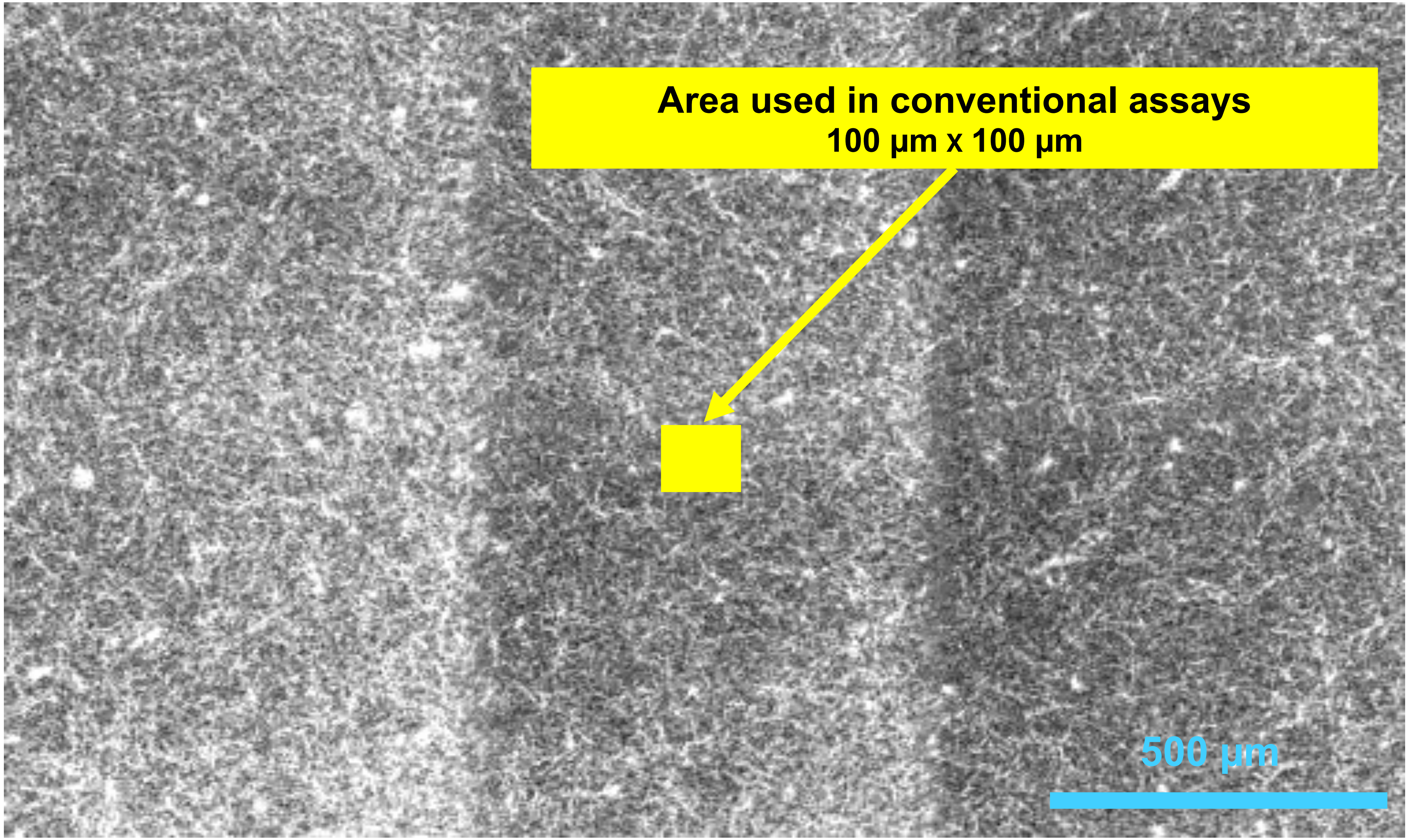
Large-scale vortex lattice emerging from collectively moving microtubules

Yutaka Sumino[1*], Ken H. Nagai[2*], Yuji Shitaka[3], Dan Tanaka[4‡], Kenichi Yoshikawa[5], Hugues Chaté[6] & Kazuhiro Oiwa[3,7]

(Nature, 483, 2012)

Quasi-2D active flow (thin layer)

High-density motility assays



150x speed: 2 sec of this movie corresponds to 5 min

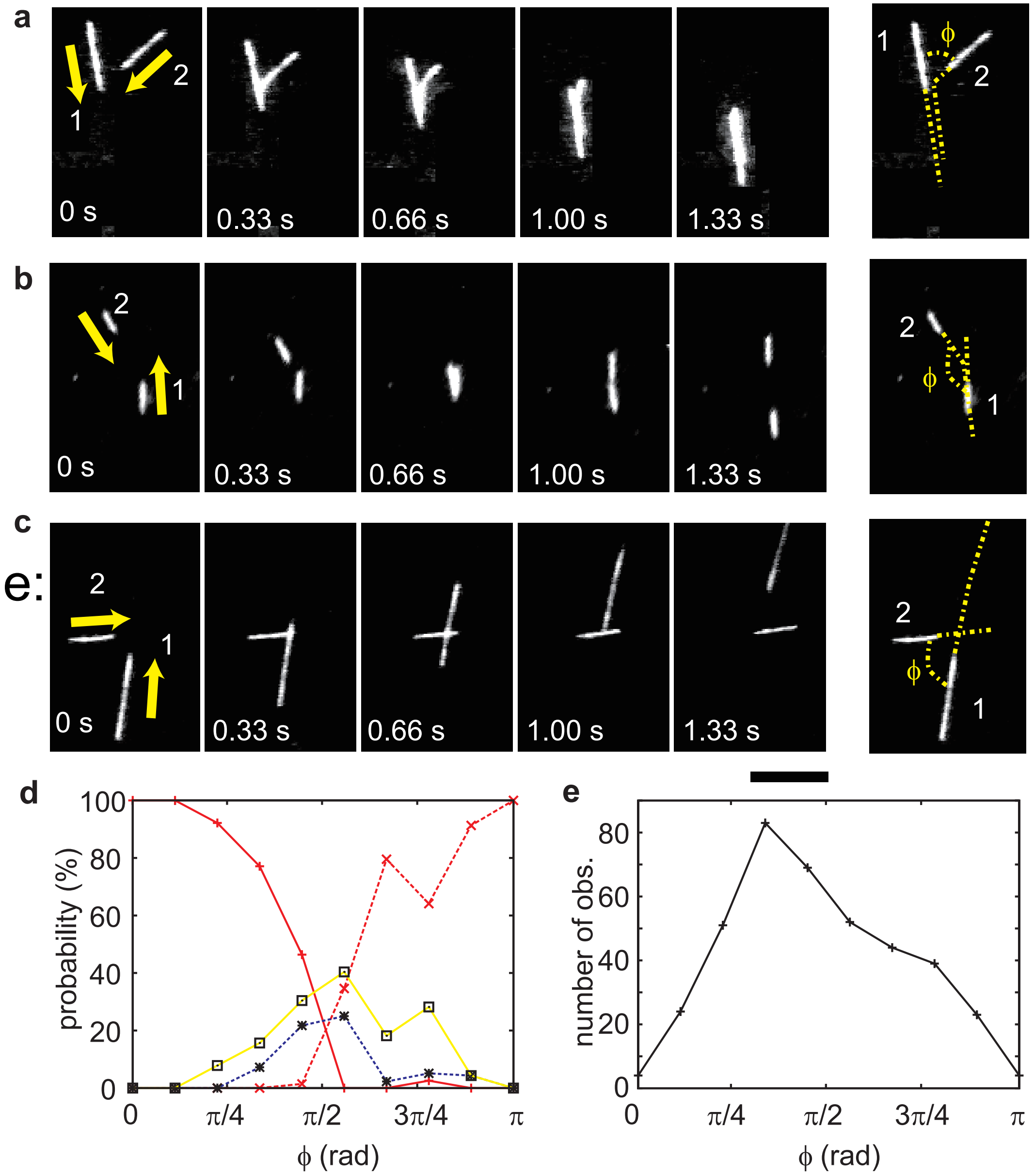
Near-perfect nematic alignment via collisions

Acute incoming angle:
Complete alignment

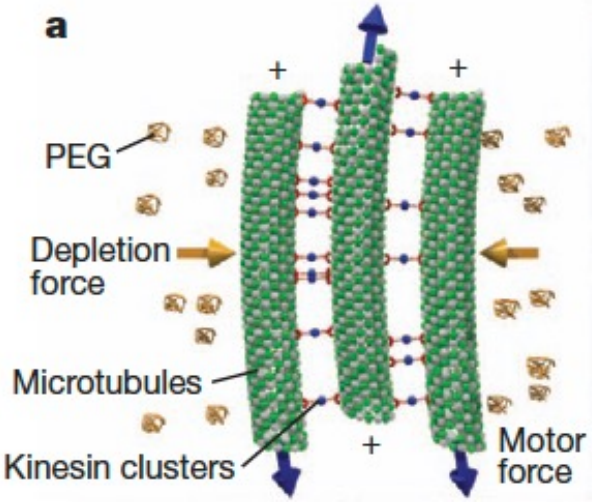
Obtuse incoming angle:
Complete anti-alignment

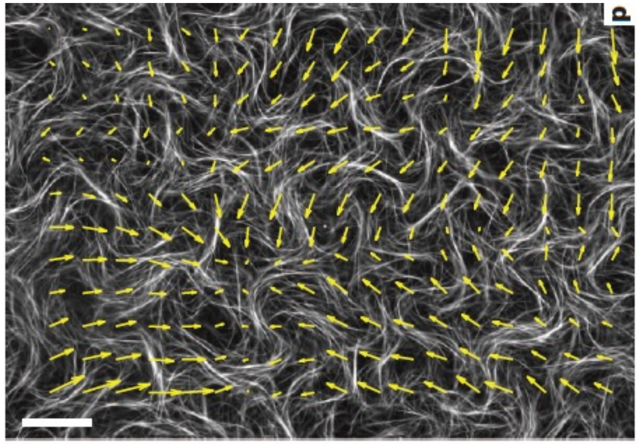
(Near-) right incoming angle:
Crossing (or stopping)

Statistics over some 400 binary collisions



The active microtubule (MT)--kinesin (or dynein) flow





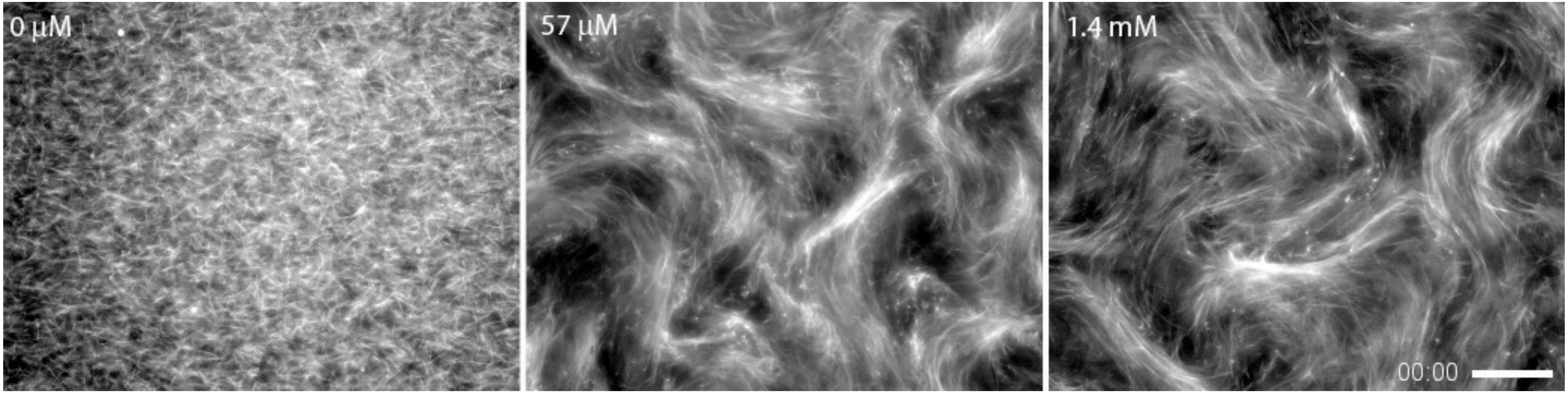
Spontaneous motion in hierarchically assembled active matter

Tim Sanchez[1]*, Daniel T. N. Chen[1]*, Stephen J. DeCamp[1]*, Michael Heymann[1,2] & Zvonimir Dogic[1]

(Nature,491,2012)

(3D active flow)

Active flow with different ATP concentration



The three key properties of individual boids in flocking systems

- The “flockers” (boids) always **move.**

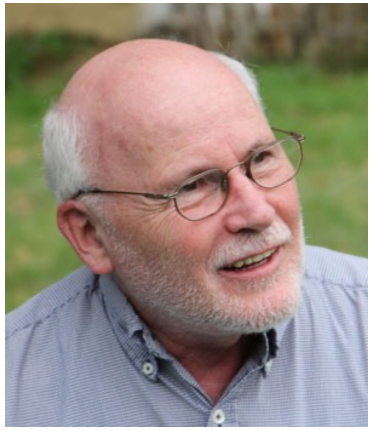
The directed motion is driven internally by ”activity” of the agent, which **consumes energy**.
Boids are often called “**self-propelle**d particles”.

- The boids **align** their directions of motion.

The alignment **interactions are purely local** in space

- The boids make mistakes: the alignment is not perfect, there are **noise in the system.**

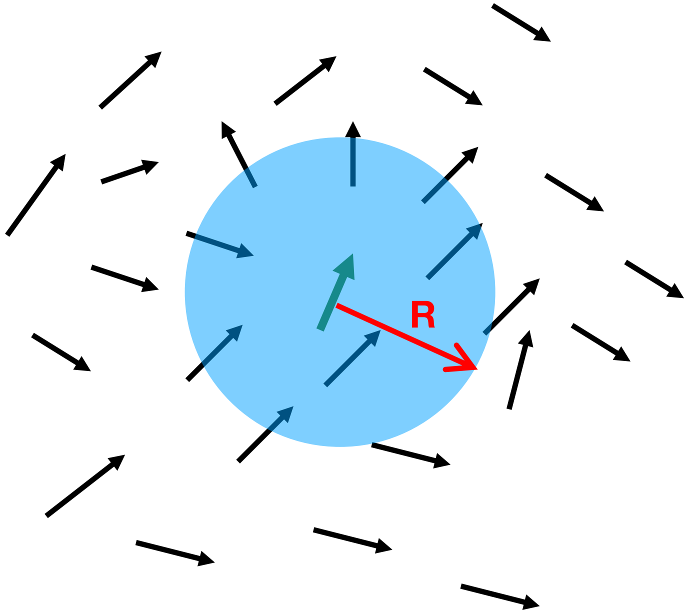
What is the hydrodynamic theory of flocking? where does it come from?



(Tamas Vicsek)

It started from a visit by Tamas Vicsek to IBM T. J. Watson Research Center at YKT in late 1994 (~28 years ago).

The Vicsek model: the minimal model for flocking



Motion: $\vec{x_i}(t+1) = \vec{x_i}(t) + \vec{v_i}(t)\Delta t$

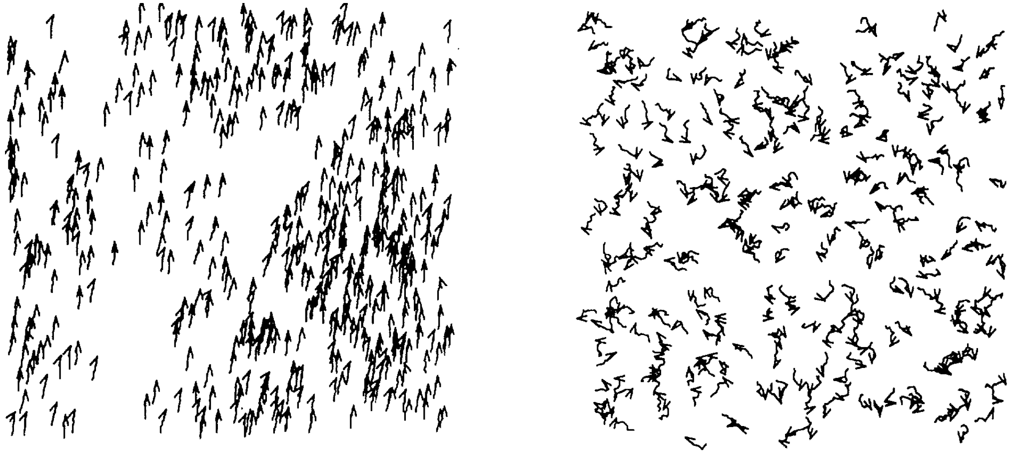
Local Alignment: $\theta_i(t+1) = \langle \theta_j(t) \rangle_{d_{ij}<R} + \delta\theta$

Noise: $\delta\theta \in [-\frac{\eta}{2}, \frac{\eta}{2}]$

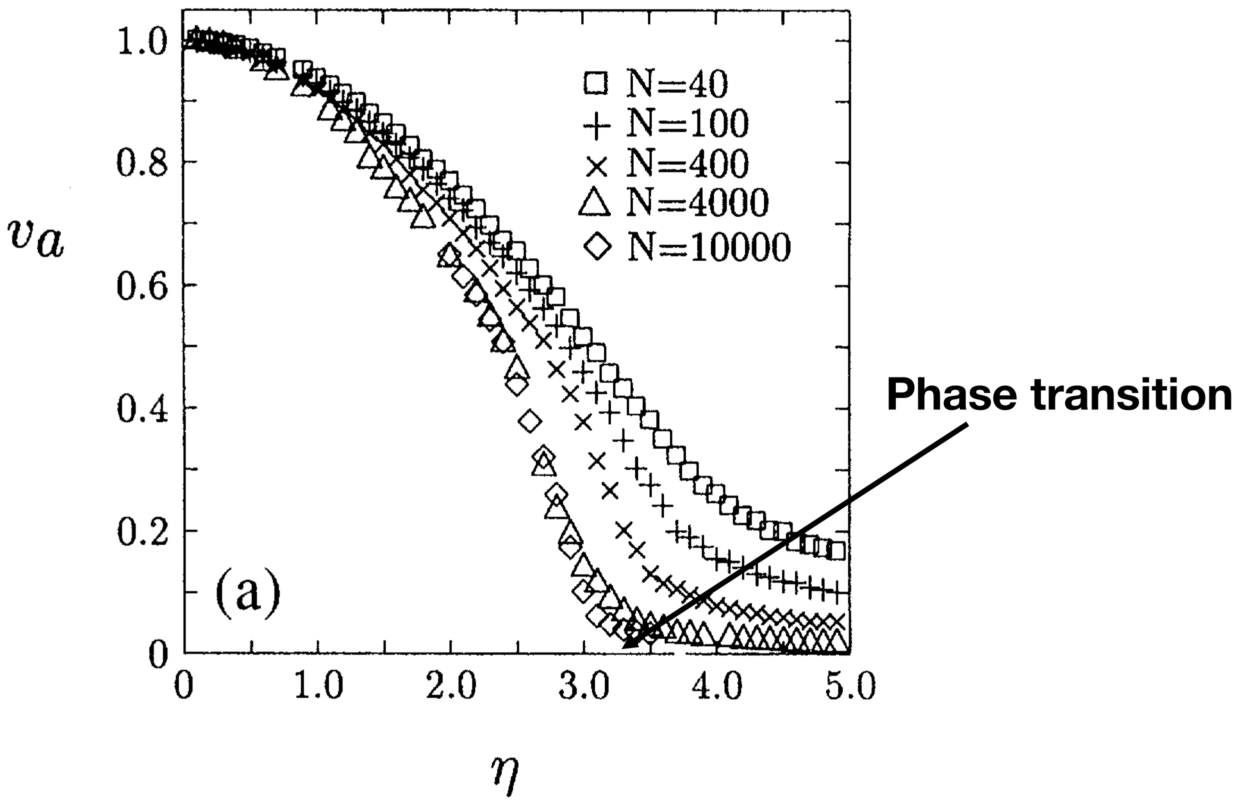
$|\vec{v_i}(t)| = v$

The flocking transition in the Vicsek model

Increasing noise η
(or by decreasing density)



(ordered) (disordered)

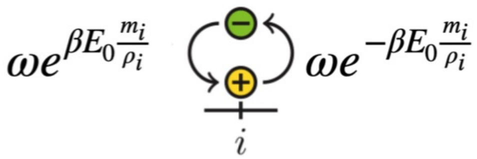


Order parameter: $v_a = \frac{1}{Nv}\left|\sum_{i=1}^{N} \vec{v_i}\right|$

The Active Ising Model (AIM): a lattice flocking model

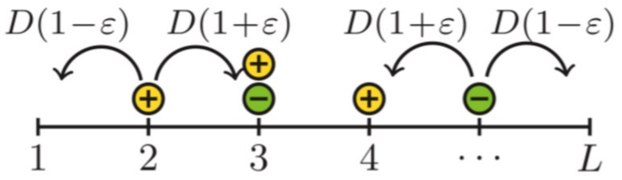
- N particles (Ising spins), $L_x \times L_y$ lattice, no volume exclusion, continuous-time Markov process.
- State variables: local occupation number $(n_{i,j}^{+}, n_{i,j}^{-}), i = 1,2,\ldots,L_x, j = 1,2,\ldots,L_y$.
- Local density and magnetization: $\rho_{i,j} = n_{i,j}^{+} + n_{i,j}^{-}, m_{i,j} = n_{i,j}^{+} - n_{i,j}^{-}$.
- Dynamics (reactions): local alignment + active transport

Flipping



$$k_{s\to(-s)} = \omega \exp\left(-s\beta E_0 \frac{m_{\mathrm{r}}}{\rho_{\mathrm{r}}}\right) = \omega e^{-s\beta E_0 \lambda_{\mathrm{r}}}.$$

Hopping



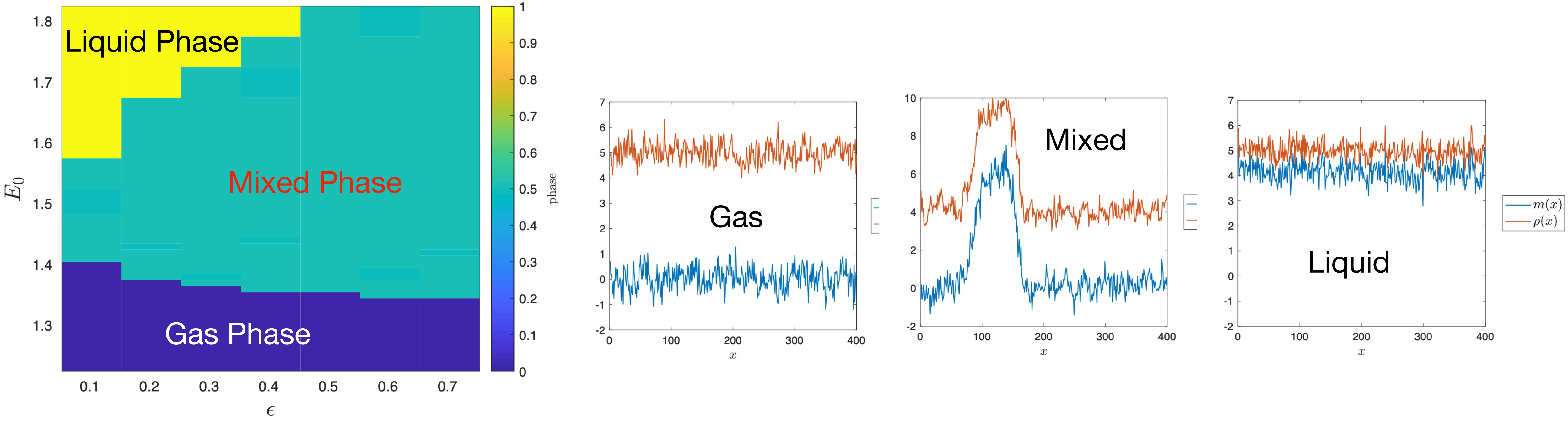
$$k_{(x,y)\to(x+1,y)} = D(1+s\epsilon)$$
$$k_{(x,y)\to(x-1,y)} = D(1-s\epsilon)$$
$$k_{(x,y)\to(x,y+1)} = D$$
$$k_{(x,y)\to(x,y-1)} = D,$$

Key control parameters: $\left(\frac{\omega}{D}, E_0, \epsilon\right)$

time scale — coupling energy scale — bias

A. P. Solon and J. Tailleur, PRL 2013; PRE 2015

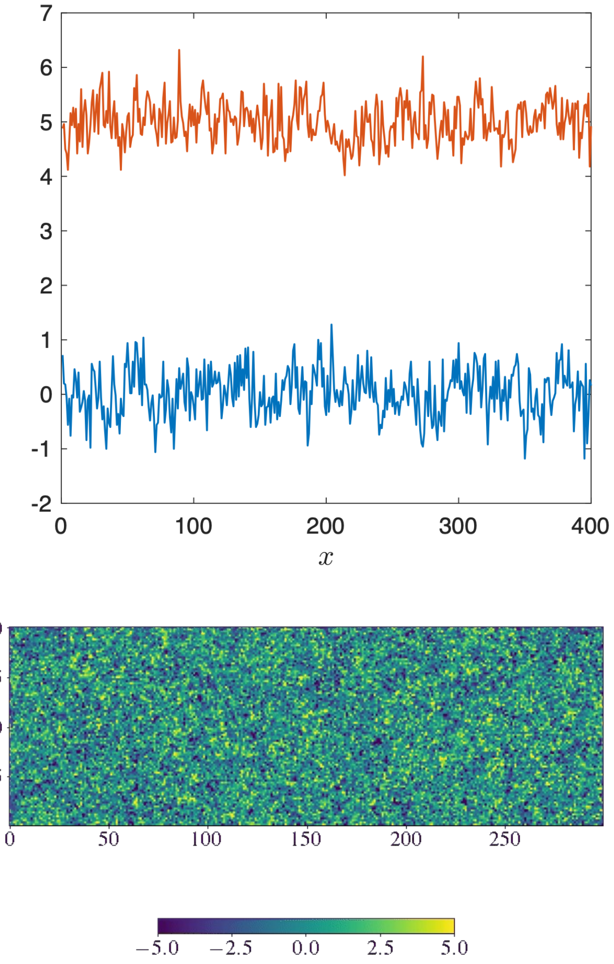
Phase diagram in parameter space (E_0, ϵ)



The three phases in AIM: Simulation results:

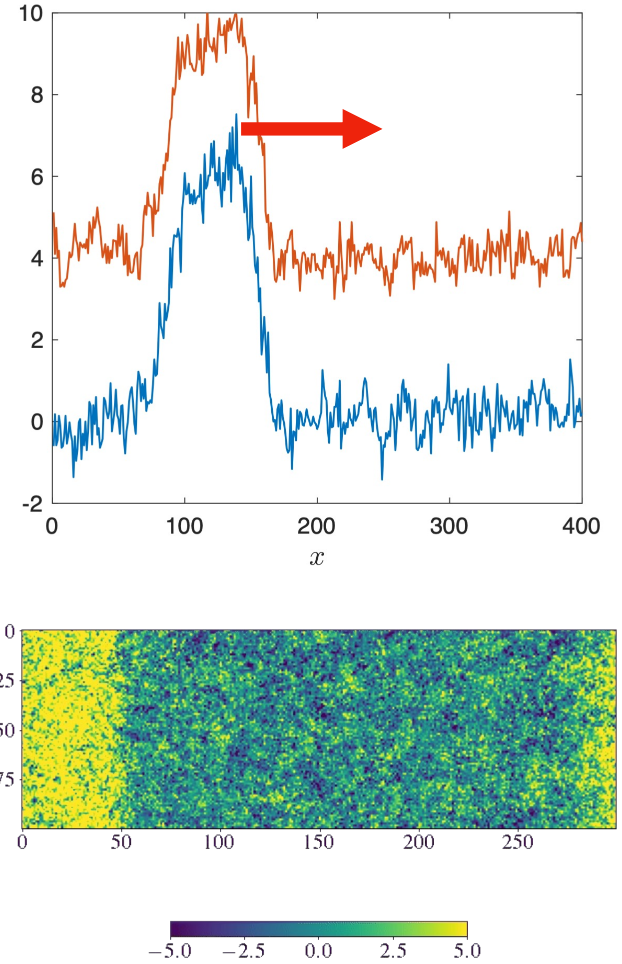
Gas Phase

(No flocking)



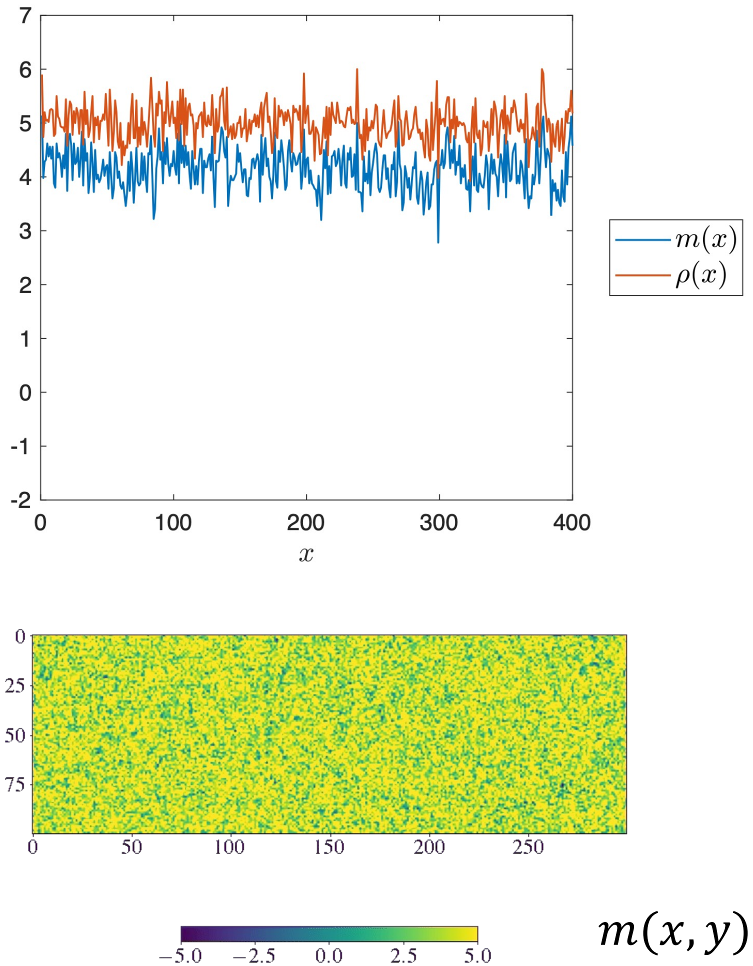
Mixed Phase

(flocking)



Liquid Phase

(flocking)

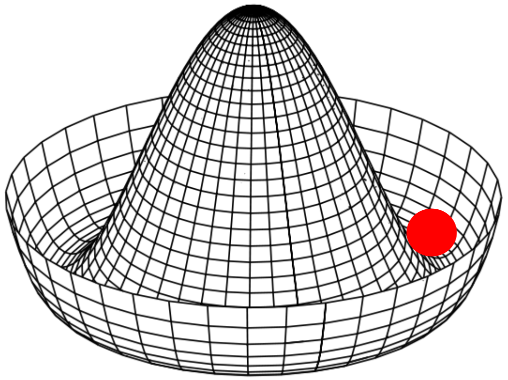


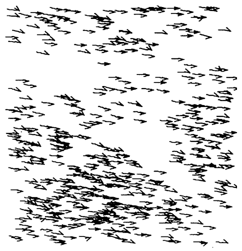
But wait, there is a big problem!

The Mermin-Wagner theorem

In quantum field theory and statistical mechanics, the **Mermin–Wagner theorem** states that continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$.

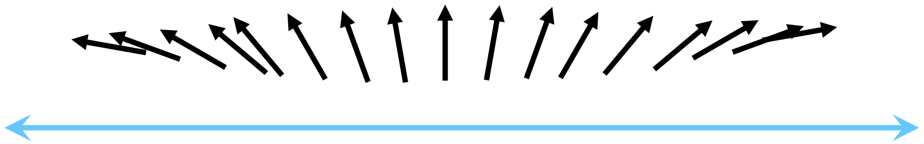
Spontaneous symmetry breaking





The Goldstone modes

Excited state with low energy $\propto k^2$
for long wavelength mode



wavelength $\lambda = 2\pi/k$

Variance due to the Goldstone modes: $\langle (\delta v)^2 \rangle \sim T \int \frac{d^d\vec{k}}{k^2} \sim T ln(\frac{L}{R}) \rightarrow \infty$ **in 2D**

The ordered state is unstable with finite T → No Long-range order (LRO) possible ☹

The Vicsek model manuscript ran into trouble in PRL because of the M-W theorem !

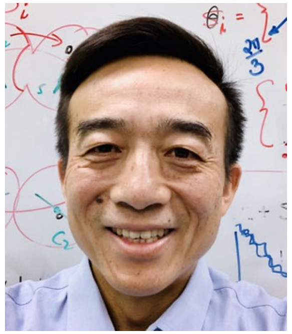
The Toner-Tu theory/equation comes to the rescue

John and I were at Tamas's seminar (probably in room 20-043), and intrigued…

We went to work immediately! and by the next day, we have written down the hydrodynamic equation for flocking, now known as the Toner-Tu equation

$$\frac{\partial \vec{v}}{\partial t} + \underbrace{\lambda_1 (\vec{v} \cdot \nabla)\vec{v}}_{\text{motion (advection term)}} + \cdots = \underbrace{\alpha \vec{v} - \beta |\vec{v}|^2 \vec{v}}_{\text{alignment}} + D\nabla^2 \vec{v} + \cdots + \vec{\eta}$$

motion (advection term) **alignment**



By mid-1995, we were able to show:

- **The critical dimension is $d_c = 4$**
- **The nonlinear convective term becomes relevant in $d < 4$**
- **Using renormalization group theory, we find $E_k \sim k^{2-\zeta}$ with $\zeta > 0 \; for \; d < 4$.**

$$\langle (\delta v)^2 \rangle \sim \int \frac{d^d \vec{k}}{E_k} = finite \text{ in d=2}$$

LRO is stable in 2D at low noise.
Mermin-Wagner theorem is broken in nonequilibrium systems.

A happy ending – flocking theory

VOLUME 75, NUMBER 6 PHYSICAL REVIEW LETTERS 7 AUGUST 1995

Novel Type of Phase Transition in a System of Self-Driven Particles

Tamás Vicsek,[1,2] András Czirók,[1] Eshel Ben-Jacob,[3] Inon Cohen,[3] and Ofer Shochet[3]
[1]*Department of Atomic Physics, Eötvös University, Budapest, Puskin u 5-7, 1088 Hungary*
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[3]*School of Physics, Tel-Aviv University, 69978 Tel-Aviv, Israel*
(Received 25 April 1994)

VOLUME 75, NUMBER 23 PHYSICAL REVIEW LETTERS 4 DECEMBER 1995

Long-Range Order in a Two-Dimensional Dynamical *XY* Model: How Birds Fly Together

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(Received 9 June 1995)

PHYSICAL REVIEW E VOLUME 58, NUMBER 4 OCTOBER 1998

Flocks, herds, and schools: A quantitative theory of flocking

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(Received 16 April 1998)

and new beginnings…..

What is hydrodynamic theory (hydrodynamics)?

Hydrodynamics is an effective (coarse-grained) continuum theory that describes the long-time, long-distance (small frequency and wave-number) dynamics of most interacting many-body systems.

$$l \gg R, d_0 \left(= \frac{L}{N^{\frac{1}{d}}}\right) \qquad t \gg R/v_0, d_0/v_0$$

How do you construct a hydrodynamic theory?

Write down all **relevant** terms allowed by the **symmetries** and **conservation laws** of the problem.

E.g., in the case of hydrodynamics for fluids, the relevant hydrodynamics variables are the velocity field $\vec{v}(\vec{x})$ and the density field $\rho(\vec{x})$.

Symmetries: rotational invariance, space and time translation invariance, and Galilean invariance
Conservation laws: Conservation of particle number, momentum and energy.

How do we know which are relevant terms?

In hydrodynamics limit, keep only the lowest order derivatives for both space and time.

E.g., for hydrodynamics of fluid, keep $\frac{d\vec{v}}{dt}$ term but not $\frac{d^2\vec{v}}{dt^2}$ term; keep $\nabla^2\vec{v}$ term but not $\nabla^4\vec{v}$ term

Incompressible Navier-Stokes equation

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} = D\nabla^2\vec{v} + \nabla P$$

$$\nabla \cdot \vec{v} = 0$$

The hydrodynamic theory of flocking: the Toner-Tu equation

In the case of flocking systems, the relevant hydrodynamics variables are again the velocity field $\vec{v}(\vec{x})$ and the density field $\rho(\vec{x})$.

Symmetries: rotational invariance, space and time translation invariance, ~~and Galilean invariance~~
Conservation laws: Conservation of particle number, ~~momentum and energy~~.

The Toner-Tu equation

$$\frac{\partial \vec{v}}{\partial t} + \underline{\lambda_1 (\vec{v} \cdot \nabla)\vec{v}} + \cdots = \underline{\alpha \vec{v} - \beta |\vec{v}|^2 \vec{v}} - \underline{\nabla} P + \nabla^2 \vec{v} + \cdots + \underline{\vec{\eta}}$$

IV. Pressure in the system

I. They **move** and transport (advection)

II. They **align** with their neighbors

III. There is noise in the system

The flocks are compressible: density can fluctuate

Conservation of the total number of active particles (boids)

$$\frac{\partial \rho}{\partial t} + (\vec{v} \cdot \nabla)\rho = 0$$

Pressure depends on the local boid-density

$$P(\rho) = \sum_{n=0} \sigma_n (\rho - \rho_0)^n$$

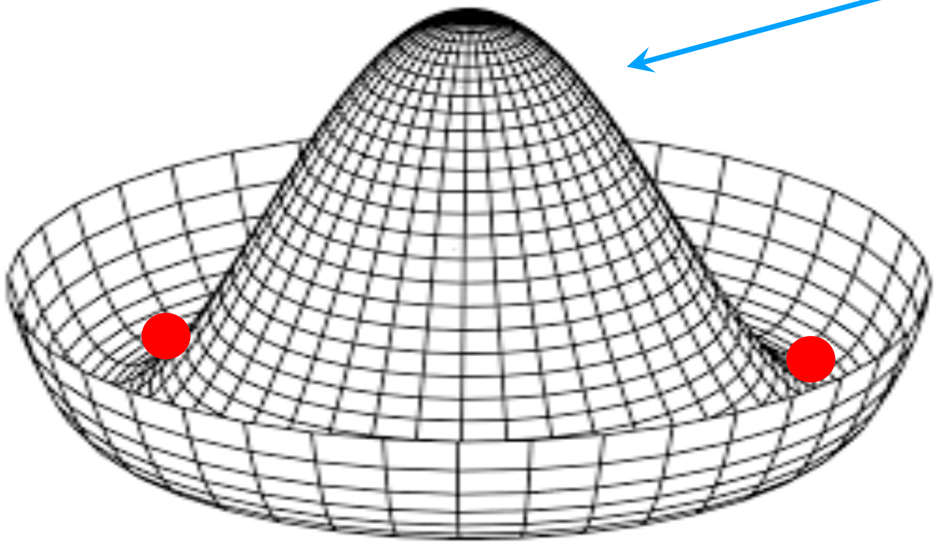
$\rho_0 =< \rho >$ **---- mean density**

Mean Field Theory: Looking for spatially homogeneous solutions

$$\frac{\partial \vec{v}}{\partial t} = \alpha \vec{v} - \beta |\vec{v}|^2 \vec{v} = -\frac{\partial U_m(\vec{v})}{\partial \vec{v}} = 0 \qquad (\boldsymbol{\beta} > \mathbf{0})$$

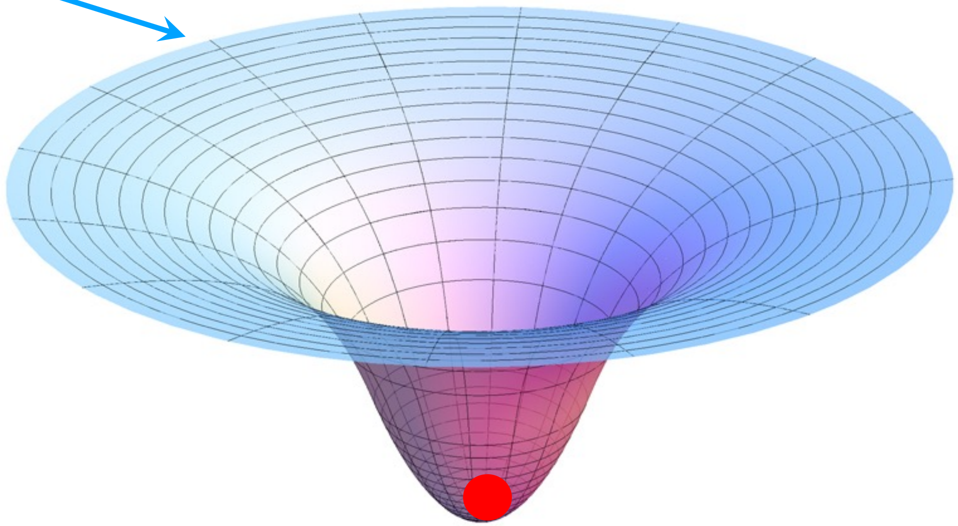
$$U_m(\vec{v}) = -\frac{\alpha}{2} |\vec{v}|^2 + \frac{\beta}{4} |\vec{v}|^4$$

$\boldsymbol{\alpha} > \mathbf{0}$



Ordered state: $|<\vec{v}>| = \sqrt{\frac{\alpha}{\beta}}$

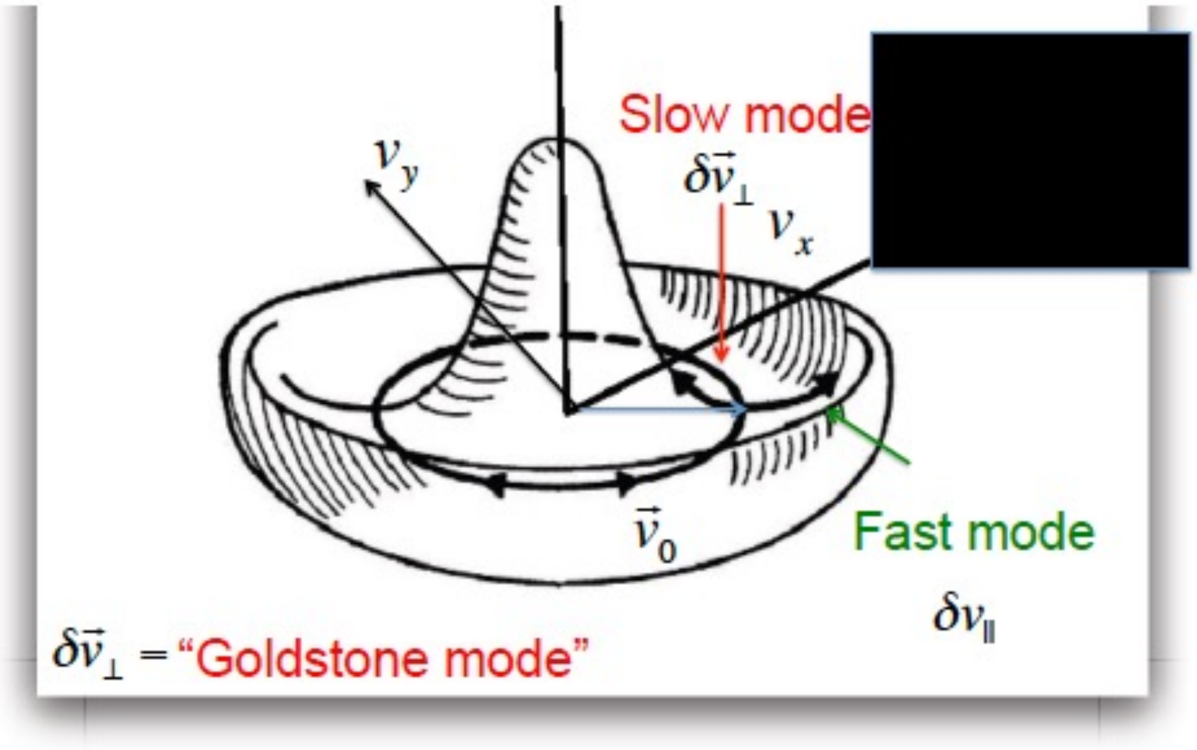
$\boldsymbol{\alpha} < \mathbf{0}$

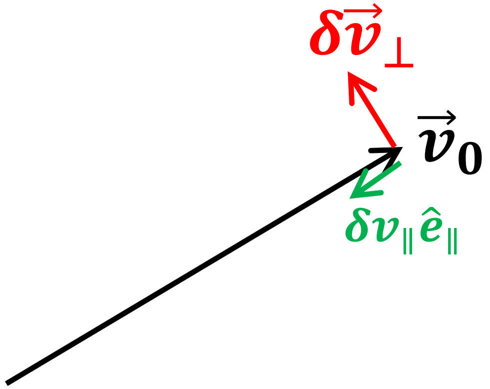


Disordered state: $|<\vec{v}>| = 0$

Spontaneous Symmetry Breaking and Goldtston Mode

$$U_m(\vec{v}) = -\frac{\alpha}{2}|\vec{v}|^2 + \frac{\beta}{4}|\vec{v}|^4$$





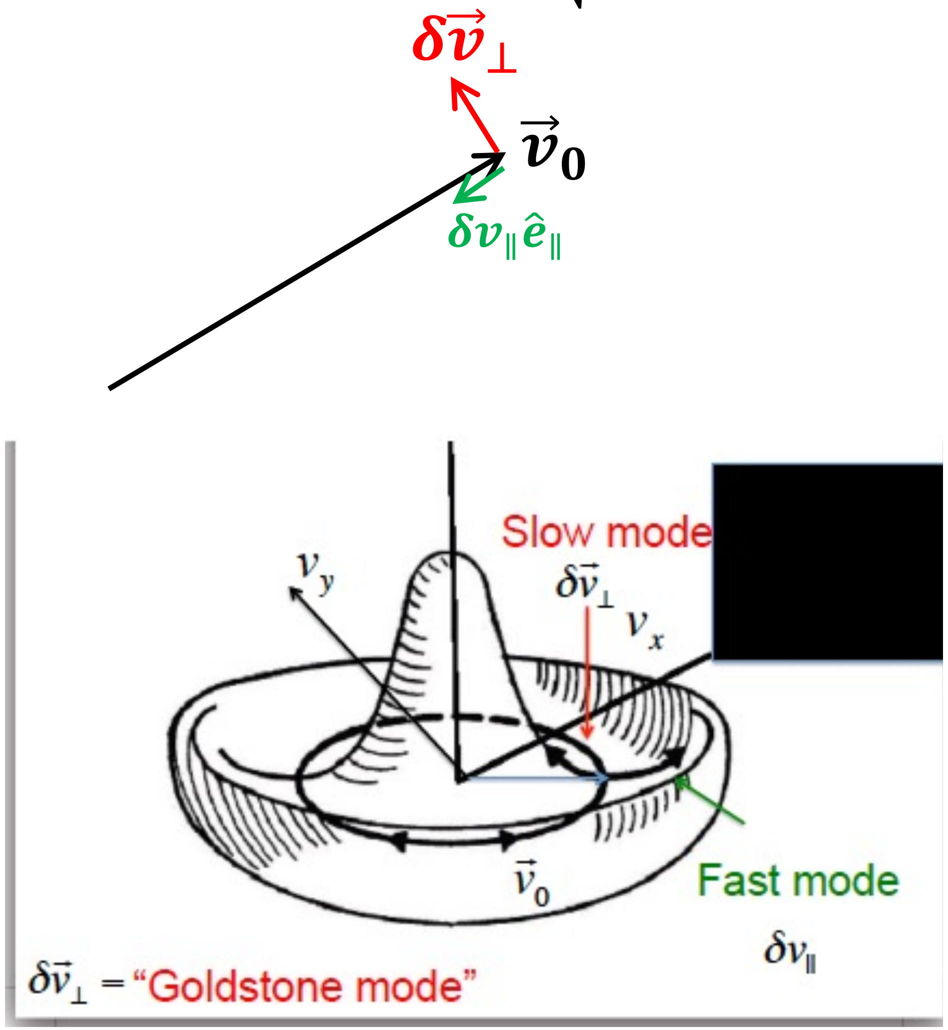
Spontaneous Symmetry Breaking: Among all the solutions, the system selects one of them, which breaks the O(2) symmetry.

Goldston mode: Perturbation around the selected solution along the symmetry direction $(\delta\vec{v}_\perp)$ is called the Goldstone mode, which decays slowly – also called the soft-mode

Dynamics near the symmetry-broken solution: the fast mode

$\vec{v} = \vec{v}_0 + \delta\vec{v}_\perp + \delta v_\parallel \hat{e}_\parallel \qquad \hat{e}_\parallel = \vec{v}_0 / |\vec{v}_0| \qquad \delta\vec{v}_\perp \cdot \hat{e}_\parallel = 0 \qquad |\vec{v}_0| = \sqrt{\frac{\alpha}{\beta}} = 1$

1) Fast mode $v_\parallel$



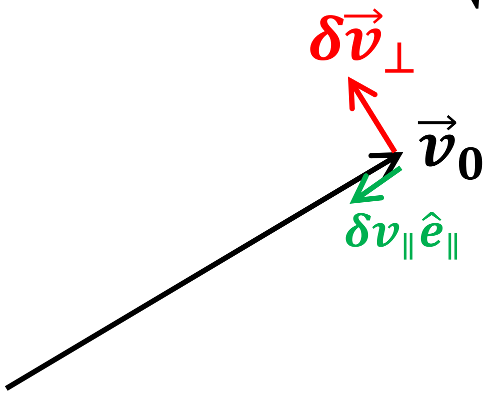
$$\frac{\partial v_\parallel}{\partial t} = [v_0^2 - (|\vec{v}_\perp|^2 + (v_0 + v_\parallel)^2)](v_0 + v_\parallel)$$
$$\approx -2\,(v_\parallel + |\vec{v}_\perp|^2/2)$$

Decay time: $\tau_\parallel = \frac{1}{2}$ (fast); $\quad v_\parallel = -\frac{|\vec{v}_\perp|^2}{2}$ (higher order)

Dynamics near the symmetry-broken solution: the slow mode

$\vec{v} = \vec{v}_0 + \delta\vec{v}_\perp + \delta v_\parallel \hat{e}_\parallel \qquad \hat{e}_\parallel = \vec{v}_0 / |\vec{v}_0| \qquad \delta\vec{v}_\perp \cdot \hat{e}_\parallel = 0 \qquad |\vec{v}_0| = \sqrt{\frac{\alpha}{\beta}} = 1$

2) The slow Goldston mode $\vec{v}_\perp$

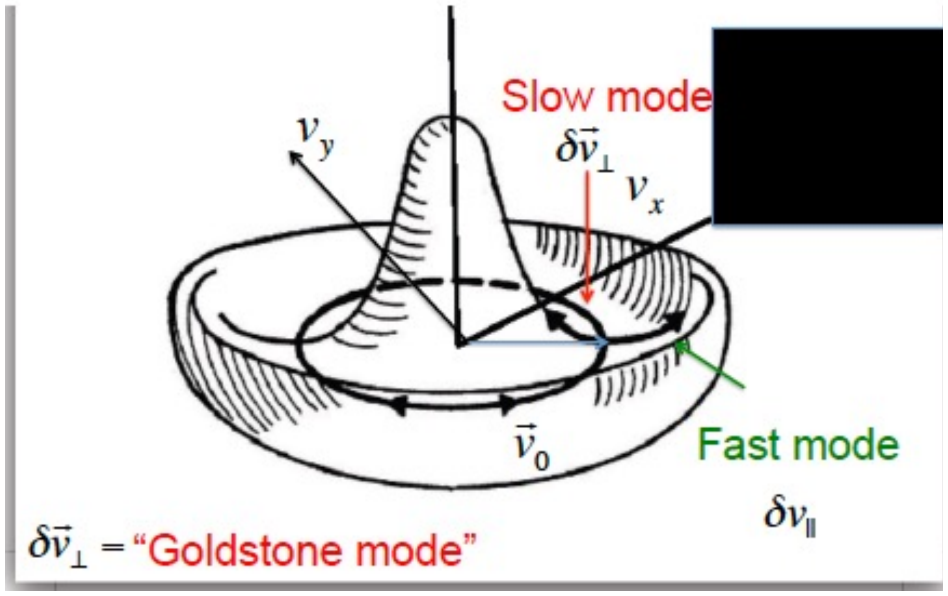


In the co-moving frame

$$\frac{\partial \vec{v}_\perp}{\partial t} + \lambda_1 (\vec{v}_\perp \cdot \nabla_\perp)\vec{v}_\perp = -\nabla_\perp P + D_\perp \nabla_\perp^2 \vec{v}_\perp + D_\parallel \nabla_\parallel^2 \vec{v}_\perp + \vec{\eta}_\parallel$$

$$\frac{\partial \delta\rho}{\partial t} + \lambda_1 \rho_0 (\nabla_\perp \cdot \vec{v}_\perp) + \lambda_1 \nabla_\perp \cdot (\vec{v}_\perp \delta\rho) = 0$$

$$P = \sigma_1 \delta\rho + \sigma_2 \delta\rho^2$$



Second order (nonlinear) terms

The linear analysis

$$\frac{\partial \vec{v}_\perp}{\partial t} + \lambda_1(\vec{v}_\perp \cdot \nabla_\perp)\vec{v}_\perp = -\nabla_\perp P + D_\perp \nabla_\perp^2 \vec{v}_\perp + D_\parallel \nabla_\parallel^2 \vec{v}_\perp + \vec{\eta}_\perp$$

$$\frac{\partial \delta\rho}{\partial t} + \lambda_1 \rho_0 (\nabla_\perp \cdot \vec{v}_\perp) + \lambda_1 \nabla_\perp \cdot (\vec{v}_\perp \delta\rho) = 0$$

$$P = \sigma_1 \delta\rho + \sigma_2 \delta\rho^2$$

The linearized equation can be solved easily in Fourier space $(\omega, \vec{k})$

$$\vec{v}_\perp(\vec{k}, \omega) = \frac{\vec{\eta}_\perp(\vec{k}, \omega)}{i\left(\omega - \frac{c^2 k_\perp^2}{\omega}\right) + D|\vec{k}|^2}$$

$$c^2 = \rho_0 \sigma_1 \quad D_\perp = D_\parallel = D$$

White-noise

$$< \eta_{\perp,i}(x,t)\, \eta_{\perp,i}(x',t') > = \Delta \delta_{ij} \delta(x - x') \delta(t - t')$$

The Velocity Fluctuations and the Mermin-Wagner theorem

$$\vec{v}_\perp(\vec{k},\omega) = \frac{\vec{\eta}_\perp(\vec{k},\omega)}{i\left(\omega - \frac{c^2 k_\perp^2}{\omega}\right) + D|\vec{k}|^2}$$

$$< \eta_{\perp,i}(x,t)\ \eta_{\perp,i}(x',t') >= \Delta\delta_{ij}\delta(x-x')\delta(t-t')$$

For 2D system (d=2)

$$\langle \vec{v}_\perp(\vec{x},t)\cdot\vec{v}_\perp(\vec{x},t)\rangle_{\vec{x}} = \Delta \iint \frac{d\omega d\vec{k}}{\left(\omega - \frac{c^2 k_\perp^2}{\omega}\right)^2 + D|\vec{k}|^4} = \frac{\Delta}{D}\int_{L^{-1}<|\vec{k}|<R^{-1}} \frac{d^d\vec{k}}{|\vec{k}|^2} \approx \frac{\Delta}{D} ln(\frac{L}{R})$$

$$\left\langle |\vec{v}_\perp(\vec{x},t) - \vec{v}_\perp(\vec{x},0)|^2 \right\rangle \approx \frac{\Delta}{D} ln(t)$$

Both spatial and temporal velocity fluctuations diverge in the hydrodynamic limit for any finite noise strength $(\Delta \neq 0)$

The (symmetry-broken) ordered state is unstable against noise in 2D

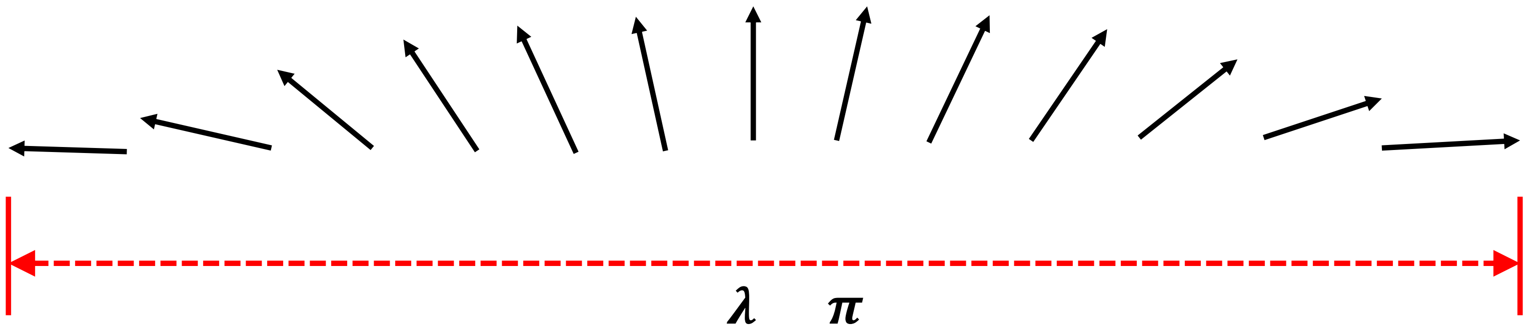
Mermin-Wagner theorem

The Mermin-Wagner theorem and a possible way out

$$\langle \vec{v}_\perp(\vec{x},t)\cdot\vec{v}_\perp(\vec{x},t)\rangle_{\vec{x}} = \int_{L^{-1}<|\vec{k}|<R^{-1}} \frac{\Delta d^d\vec{k}}{D|\vec{k}|^2} \approx \frac{\Delta}{D} ln(\frac{L}{R})$$

Energy cost: $D|\vec{k}|^2$

Entropy gain: $\Delta d^d\vec{k}$



$$\frac{\lambda}{2} = \frac{\pi}{k}$$

For $d \leq 2$, Entropy wins!
The system becomes disordered

Long wavelength (small k) fluctuation – the slow Goldston mode

$D|\vec{k}|^2$ -- diffusive term

If the effective diffusive term is $D|\vec{k}|^z$ with an exponent $z < 2$
Then the velocity variance decays as $L^{z-2} \to 0$ as $L \to \infty$
Long range order (LRO) will survive!

Next: Nonlinear effects, Renormalization group theory, and scaling