Giant density fluctuations and other out-of-equilibrium properties of active matter

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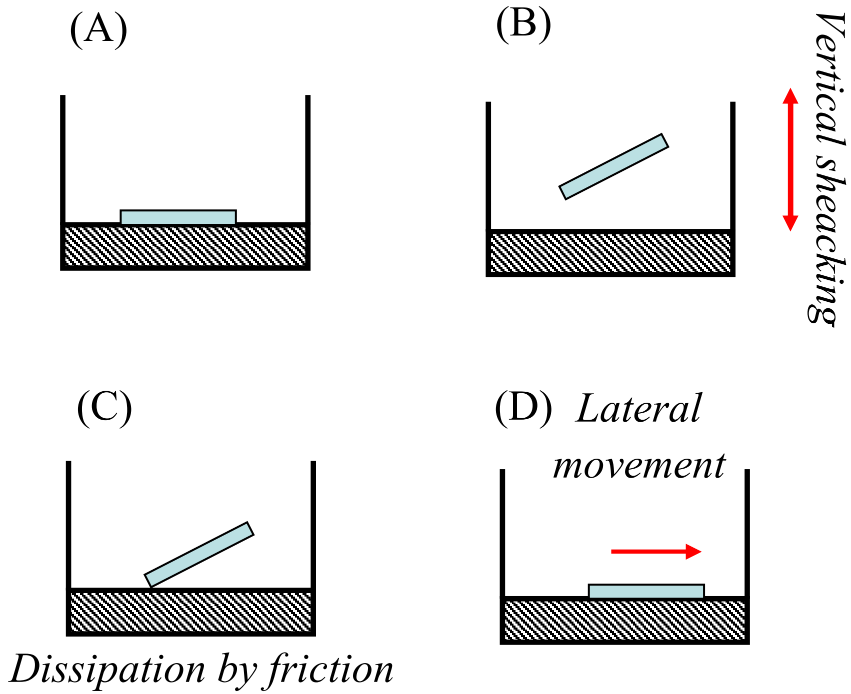
Active particles possess internal degrees of freedom which allow them to **self propel** themselves by extracting energy from their environment and dissipate it to move with a preferred direction.

Self propelled particles thus carry a preferred **direction of motion** which can be oriented by interactions with nearby particles.

European starling



Driven granular rods on a substrate

Ensembles of interacting active particles:
spontaneous symmetry breaking and collective motion

Starlings flock - Predation attempt in Rome

thanks to Claudio Carere
Istituto Superiore di Sanità - Roma - Italy
STARFLAG

Collective motion is characterized by a spontaneous symmetry breaking phenomenon.

Symmetry breaking may happen with local interactions only, no global ordering field(s) and without any obvious leader.

The symmetry broken ordered phase is characterized by remarkable out-of equilibrium properties

Simple microscopic models approach

- **Simple microscopic dynamics.**
- **Particles are described by their off-lattice position $\boldsymbol{r}_i$ and direction $\boldsymbol{n}_i$** $\quad i = 1, \ldots, N$
- **They have only local interactions.**
- **Driven-overdamped approximation: they evolve with a synchronous discrete time stochastic dynamics (**whose time step is of the order of the relaxation time**)** with constant modulo velocity v_0.
- **No external fields are present.**

Vicsek model ("moving spins")

Vicsek et al, PRL (1995)

- Strictly local interaction range:
- Alignment according to *local* order parameter in neighborhood (average direction of the neighbors)
- Displacement with constant modulo velocity v_0, broken Galileian invariance

$$\mathbf{n}_j^{t+1} = \mathbf{R}_j^t(\eta) \circ \frac{\sum_{i\sim j} \mathbf{n}_i^t}{\left\| \sum_{i\sim j} \mathbf{n}_i^t \right\|}$$

$$i \sim j \quad \text{if} \quad \left| \mathbf{r}_i^t - \mathbf{r}_j^t \right| < 1$$

$$\mathbf{r}_j^{t+1} = \mathbf{r}_j^t + v_0 \, \mathbf{n}_j^{t+1}$$

$\mathbf{R}_j^t(\eta)$ is a rotation by random, delta correlated angle(s)

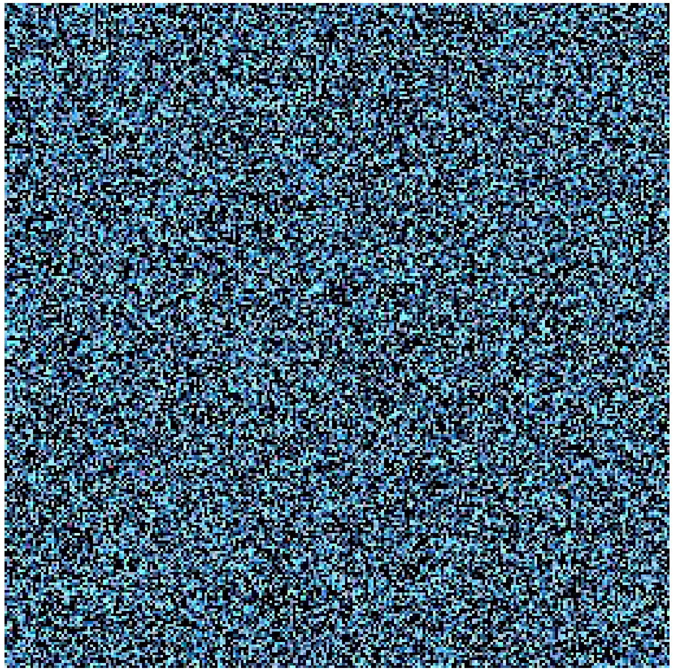
$\mathbf{R}_j^t(\eta) \circ \mathbf{v}$ uniformly distributed in a (solid) angle lying around $\mathbf{v}$ with amplitude η

Competition between density and noise leads to order

Strong noise: disordered state

Low noise: **long range order**

(Mermin-Wagner theorem does not hold)



Quench into ordered phase
(coarse-grained density field)
L=16384, ρ=1/8 (32M particles)

Low density critical line: $\eta_c \sim \rho^{1/d}$

$$\langle l \rangle \sim \rho^{-1/d} \quad \Leftrightarrow \quad l_{pers} \propto 1/\eta$$

Giant number fluctuations characterize the ordered phase in the low noise regime

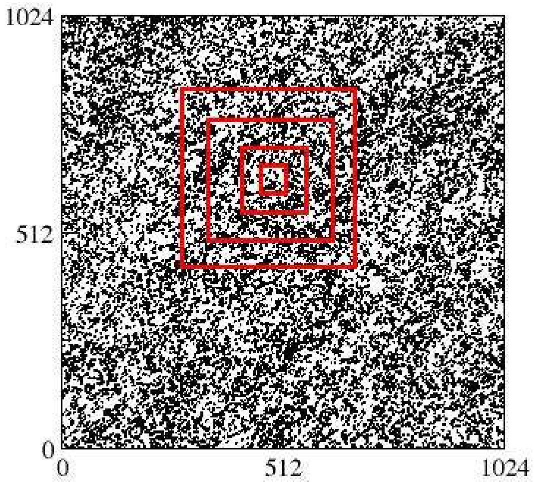
Define volumes of increasing linear size l

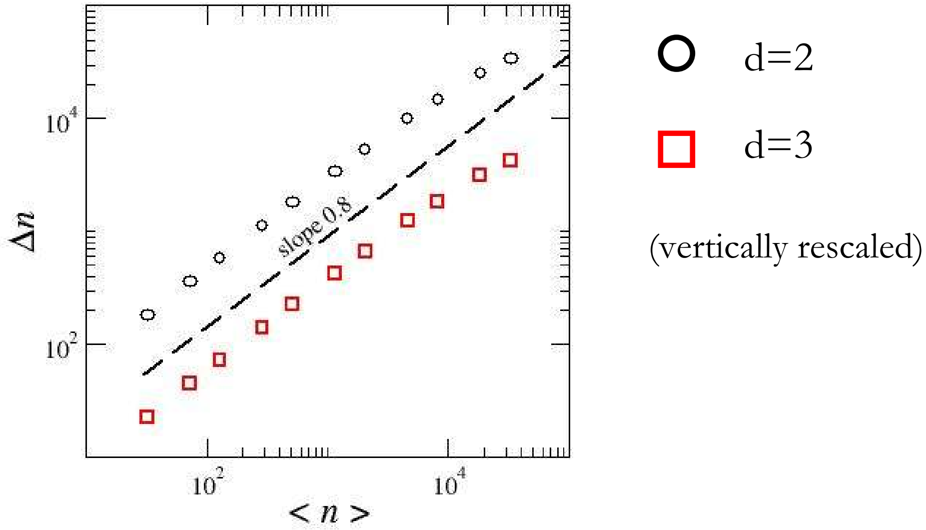
Measure the average (in time) number of particles n in the volume and its rms fluctuations Δn

$$n = \rho l^{d} \qquad \Delta n \sim n^{\alpha}$$

At equilibrium $\alpha = 1/2$

Vicsek model (d=2, d=3) $\alpha \approx 0.8$





A hydrodynamic approach

Toner & Tu, PRL (1995), PRE (1998)

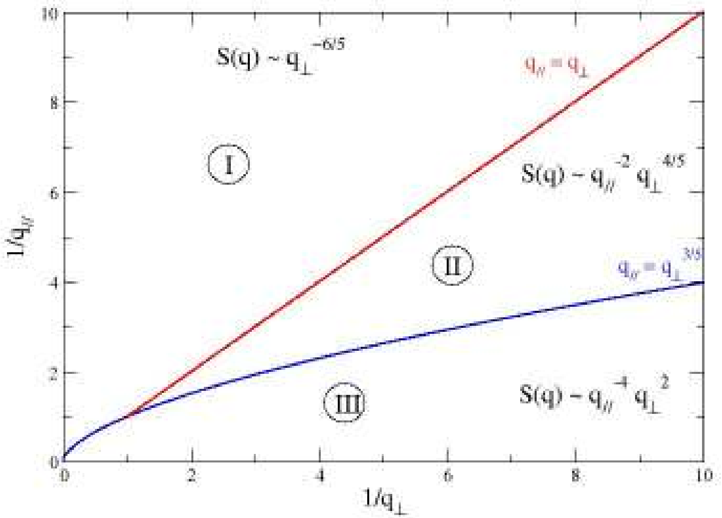
- Write "hydrodynamic-like" Langevin equations for density $c(\mathbf{r}, t)$ and $\mathbf{v}(\mathbf{r}, t)$ velocity fields (slow variables). Allow for violation of Galilean invariance
- Solve by linearization around a density homogeneous, ordered state

$$c(\mathbf{r},t) = c_0 + \delta c(\mathbf{r},t)$$
$$\mathbf{v}(\mathbf{r},t) = \mathbf{v}_0 + \delta \mathbf{v}(\mathbf{r},t)$$

- Check nonlinear terms by DRG analysis

- Compute number density structure factor (it diverges at large wavelength!!!)

$$S(q \to 0) = \frac{\Delta n^2}{n}$$



d=2 (DRG result) $\Delta n \sim n^{4/5}$

d=3 (conjecture) $\Delta n \sim n^{23/30 \approx 0.7666...}$

Active nematic on a substrate, d = 2

- Include nematic symmetry $\mathbf{n}_j^t \to -\mathbf{n}_j^t$
- Driven overdamped dynamics: synchronous algorithm
- Finite interaction range, no external fields

$$[\mathbf{Q}]_{\alpha\beta} = [\mathbf{n}]_\alpha [\mathbf{n}]_\beta - \frac{\delta_{\alpha\beta}}{2}$$

$$\begin{cases} \mathbf{Q}_j^{t+1} = \mathbf{R}_j^t(\eta) \dfrac{\langle \mathbf{Q}_i^t \rangle_{i\sim j}}{\sqrt{2}\left\| \langle \mathbf{Q}_i^t \rangle_{i\sim j} \right\|} \mathbf{R}_j^t(\eta)^T \\ \mathbf{r}_j^{t+1} = \mathbf{r}_j^t + \kappa_j^t \mathbf{n}_j^t \end{cases}$$

$$i \sim j \quad \text{if} \quad \left| \mathbf{r}_i^t - \mathbf{r}_j^t \right| < 1$$

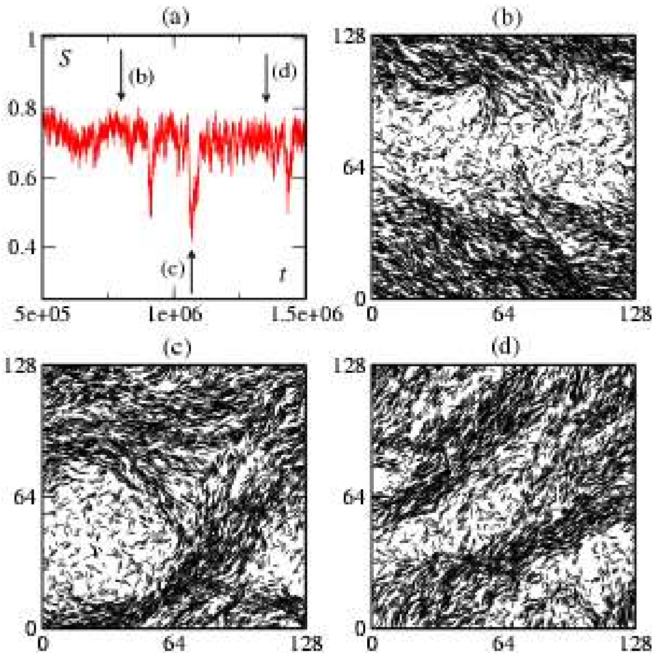
$$\kappa_j^t = \pm D_0$$

Scalar order parameter: largest eigenvalue of the global nematic tensor $\frac{1}{N}\sum_i \mathbf{Q}_i^t$

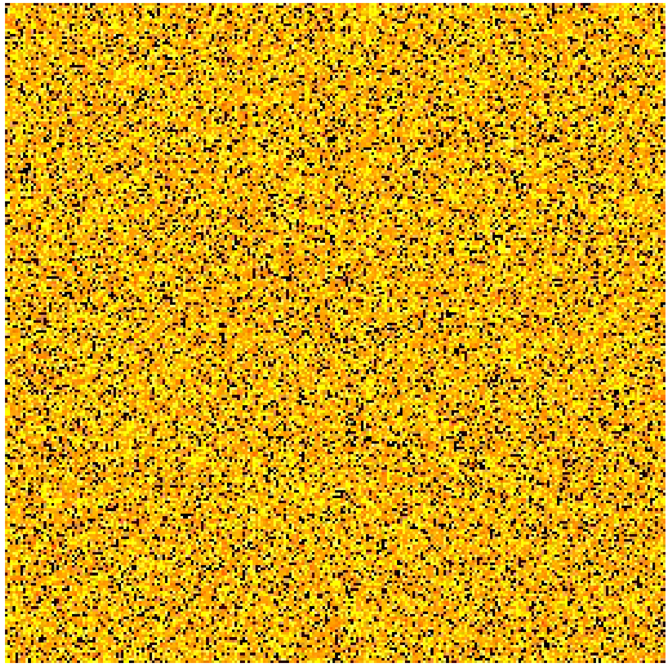
Some numerical results: d=2

Strong noise: disorder

Low noise: quasi **long range order**
(Mermin-Wagner theorem holds)

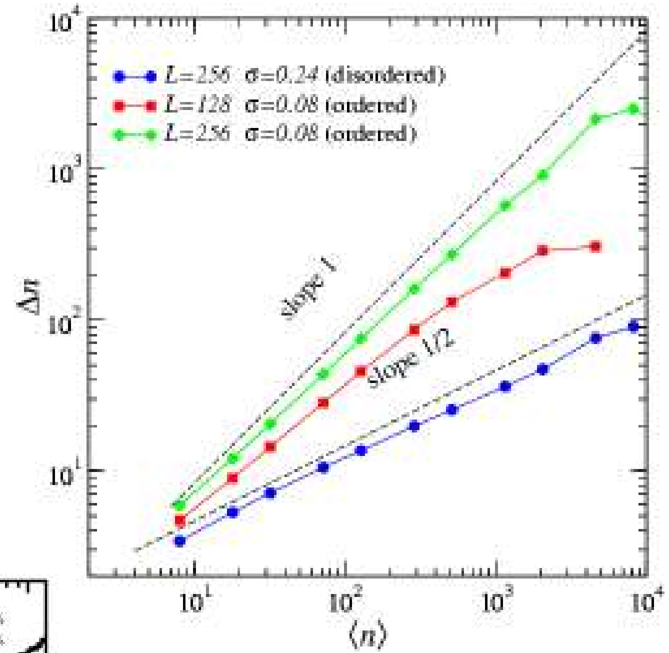


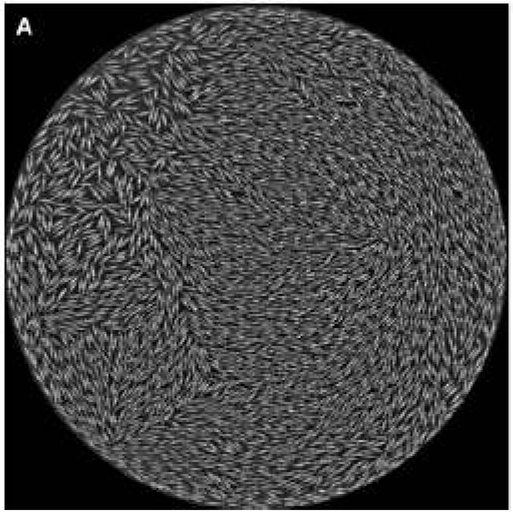
Quench into ordered phase

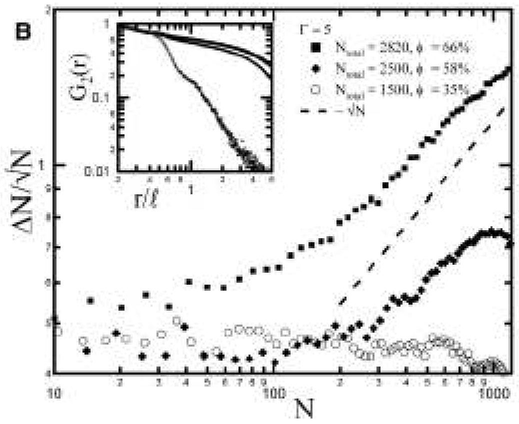


Even larger giant number fluctuations in the ordered phase

$$\Delta n \sim n$$



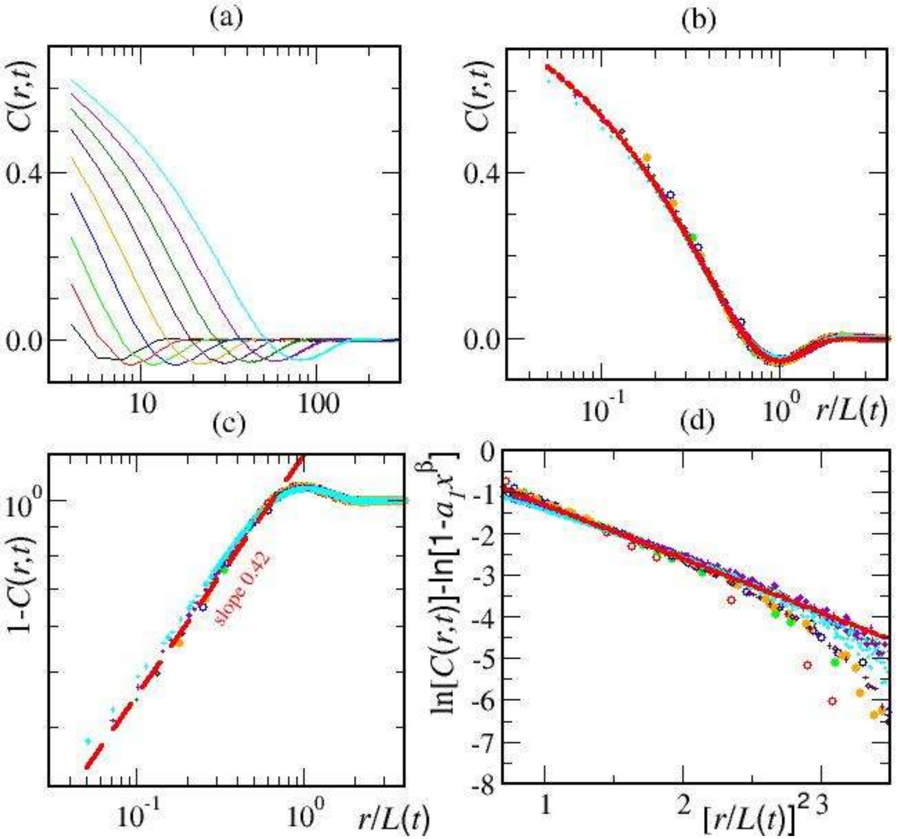




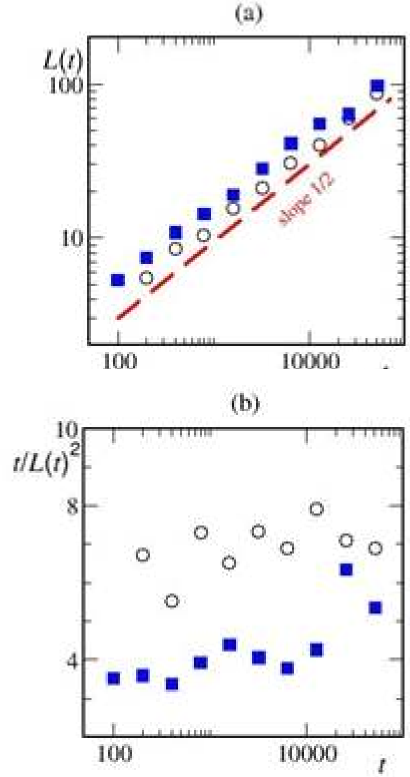
V. Narayan, S. Ramaswamy & N. Menon, Science (2007)

Nematic coarsening

Deviations from integer Porod's law: short distance cusp



$$L \sim t^{1/2}$$



$$C(r) \approx g_2(r) \approx \left[1 - c\left(\frac{r}{L(t)}\right)^b\right] \exp\left[-\left(\frac{r}{L(t)}\right)^2\right]$$

$$S(k) \approx (kL)^{-(1+b)} \qquad b \approx 0.4$$

Deriving a mesoscopic description by direct coarse graining

Density evolution

Define $$\rho(\mathbf{x},t)=\sum_{i=1}^{N} f_s\left(\mathbf{r}_i^t-\mathbf{x}\right) \qquad \mathbf{Q}(\mathbf{x},t)\rho(\mathbf{x},t)=\sum_{i=1}^{N} f_s\left(\mathbf{r}_i^t-\mathbf{x}\right)\mathbf{Q}_i^t$$

remembering $$\mathbf{r}_j^{t+\Delta t}=\mathbf{r}_j^t+\Delta t\ \kappa_j^t\ \mathbf{n}_j^t$$

$$\frac{\rho(\mathbf{x},t+\Delta t)-\rho(\mathbf{x},t)}{\Delta t}=\frac{1}{\Delta t}\sum_{i=1}^{N}\left[f_s\left(\mathbf{r}_i^{t+\Delta t}-\mathbf{x}\right)-f_s\left(\mathbf{r}_i^t-\mathbf{x}\right)\right]$$

(by Ito calculus) $$\xrightarrow{\Delta t\to 0}\underbrace{\sum_{i=1}^{N}\kappa_i^t\left(\mathbf{n}_i^t\cdot\nabla\right)f_s\left(\mathbf{r}_i^t-\mathbf{x}\right)}_{T1}+\underbrace{\frac{v_0^{\,2}}{2}\sum_{i=1}^{N}\left(\mathbf{n}_i^t\cdot\nabla\right)\left(\mathbf{n}_i^t\cdot\nabla\right)f_s\left(\mathbf{r}_i^t-\mathbf{x}\right)}_{T2}$$

$$T_2=\frac{v_0^2}{2}\partial_\alpha\partial_\beta\left(\rho\,[\mathbf{Q}]_{\alpha\beta}\right)+\frac{v_0^2}{4}\nabla^2\rho$$

Multiplicative noise treatment

T1 is a noise term $$\omega(\mathbf{x},t) \equiv \sum_{i=1}^{N} \kappa_i^t (\mathbf{n}_i^t \cdot \nabla) f_s(\mathbf{r}_i^t - \mathbf{x})$$

With correlations $$\langle \omega(\mathbf{x},t)\omega(\mathbf{y},t')\rangle = v_0^2 \delta(t-t') \sum_{i=1}^{N} (\mathbf{n}_i^t \cdot \nabla)(\mathbf{n}_i^t \cdot \nabla) f_s(\mathbf{r}_i^t - \mathbf{x}) f_s(\mathbf{r}_i^t - \mathbf{y})$$

$$\approx v_0^2 \delta(t-t') f_s(\mathbf{y}-\mathbf{x}) \sum_{i=1}^{N} (\mathbf{n}_i^t \cdot \nabla)(\mathbf{n}_i^t \cdot \nabla) f_s(\mathbf{r}_i^t - \mathbf{x})$$

over the coarse graining scale s

$$\approx v_0^2 \delta(t-t') \delta(\mathbf{y}-\mathbf{x}) \partial_\alpha \partial_\beta \left([\mathbf{Q}]_{\alpha\beta} + \frac{\delta_{\alpha\beta}}{2} \right) \rho$$

It has the same correlations as $$\widetilde{T}_1 \equiv v_0 \nabla \cdot \sqrt{\rho}\, \mathbf{n}\, \zeta$$

(see D.S. Dean, J. Phys A (1996))

Coarse grained nematic tensor evolution

$$\mathbf{Q}_j^{t+\Delta t} = \mathbf{R}_{\theta_j^t}(\eta) \frac{\left\langle \mathbf{Q}_i^t \right\rangle_{i\sim j}}{\sqrt{2}\left\| \left\langle \mathbf{Q}_i^t \right\rangle_{i\sim j} \right\|} \mathbf{R}_{\theta_j^t}(\eta)^T$$

$$\mathbf{Q}(\mathbf{x},t)\rho(\mathbf{x},t) = \sum_{i=1}^{N} f_s\left(\mathbf{r}_i^t - \mathbf{x}\right)\mathbf{Q}_i^t$$

- Expand rotation matrix for small noise

$$\mathbf{R}_\theta = \left(1 - \frac{\theta^2}{2}\right)\mathbf{I} + \theta\,\mathbf{A} \qquad \mathbf{A} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

- Gradient expansion as for density

- Expand the normalization term up to second order (for sufficintly large total density)

Coarse grained Langevin equations

$$\partial_t \rho = \frac{a_2}{2}\nabla^2\rho + a_2\partial_\alpha\left(\rho\,\partial_\beta[\mathbf{Q}]_{\alpha\beta}\right) + a_2\partial_\alpha\left([\mathbf{Q}]_{\alpha\beta}\partial_\beta\rho\right) + \sqrt{2a_2}\nabla\cdot\sqrt{\rho}\,\mathbf{n}\xi$$

$$\partial_t \mathbf{Q} = \left[g(\rho) - \frac{b_2}{\rho}\|\mathbf{Q}\|^2\right]\mathbf{Q} + b_1\sqrt{\rho}\nabla^2\mathbf{Q} + \frac{b_1}{4\sqrt{\rho}}\boldsymbol{\Gamma}\rho + \frac{b_3}{\sqrt{\rho}}\boldsymbol{\Xi}$$

with: $$g(\rho,\sigma^2) = \frac{1}{\sqrt{\rho}}\left(\rho - \eta^2 + \ldots\right)$$

$$[\mathbf{Q}]_{\alpha\beta} = [\mathbf{n}]_\alpha[\mathbf{n}]_\beta - \frac{\delta_{\alpha\beta}}{2}$$

$$[\Gamma]_{11} = -[\Gamma]_{22} = \partial_1\partial_1 - \partial_2\partial_2 \qquad [\Gamma]_{12} = [\Gamma]_{21} = 2\partial_1\partial_2$$

Coarse grained Langevin equations

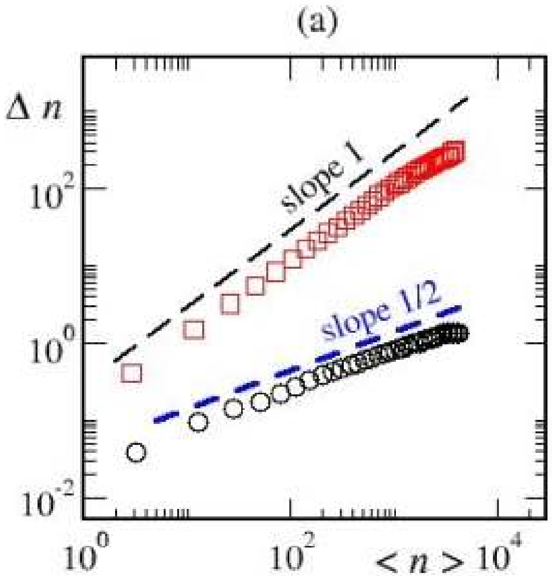
$$\partial_t \rho = \frac{a_2}{2}\nabla^2\rho + a_2\partial_\alpha\left(\rho\,\partial_\beta[\mathbf{Q}]_{\alpha\beta}\right) + a_2\partial_\alpha\left([\mathbf{Q}]_{\alpha\beta}\partial_\beta\rho\right) + \sqrt{2a_2}\nabla\cdot\sqrt{\rho}\,\mathbf{n}\xi$$

$$\partial_t \mathbf{Q} = \left[g(\rho) - \frac{b_2}{\rho}\|\mathbf{Q}\|^2\right]\mathbf{Q} + b_1\sqrt{\rho}\nabla^2\mathbf{Q} + \frac{b_1}{4\sqrt{\rho}}\mathbf{\Gamma}\rho + \frac{b_3}{\sqrt{\rho}}\Xi$$

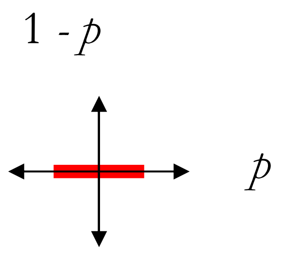
Multiplicative Noise

Alignment

Out of equilibrium current term (cannot be derived from a correct symmetry Franck free energy term) – Violates fluctuation dissipation



A pedagogical check: back to Brownian particles



$$\mathbf{r}_j^{t+\Delta t} = \mathbf{r}_j^{t} + \Delta t\, \kappa_j^t\, \mathbf{w}_j^t \qquad \mathbf{w}_j^t = \begin{cases} \mathbf{n}_j^t & \text{w.p.} \quad p \\ \mathbf{n}_{\perp j}^t & \text{w.p.} \quad 1 - p \end{cases}$$

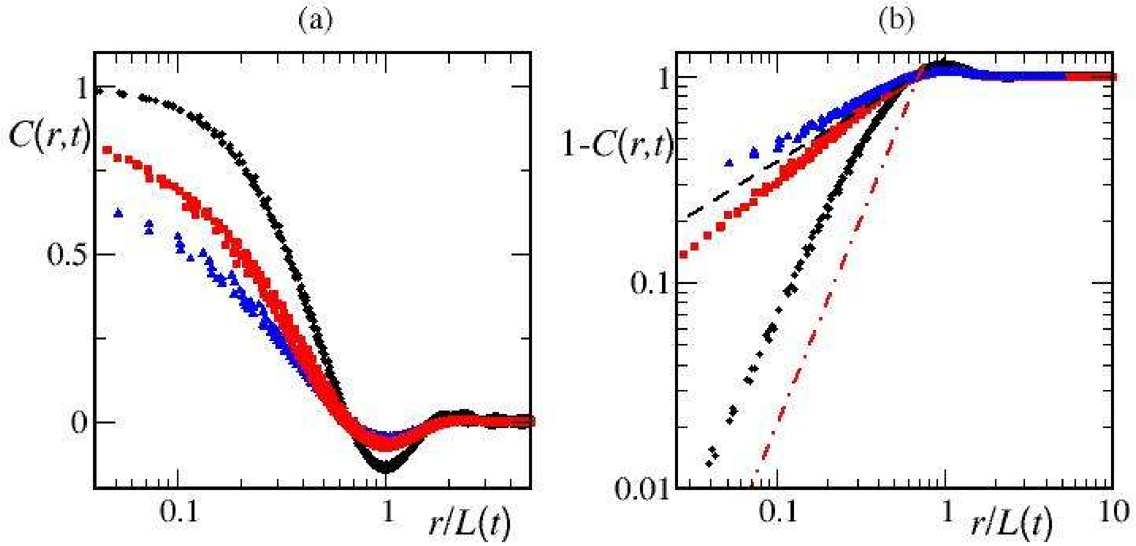
Since $\qquad [\mathbf{n}_\perp]_\alpha [\mathbf{n}_\perp]_\beta = -[\mathbf{Q}]_{\alpha\beta} + \dfrac{\delta_{\alpha\beta}}{2}$

$$\partial_t \rho = \frac{a_2}{2}\nabla^2 \rho + a_2(2p-1)\partial_\alpha \partial_\beta \left(\rho\, [\mathbf{Q}]_{\alpha\beta}\right) + \sqrt{a_2}\nabla \cdot \sqrt{\rho}\, \mathbf{q}$$

with $\qquad \left\langle [\mathbf{q}(\mathbf{x},t)]_\alpha [\mathbf{q}(\mathbf{x},t)]_\beta \right\rangle \approx v_0^2 \delta(t-t')\delta(\mathbf{y}-\mathbf{x}) \left((2p-1)[\mathbf{Q}]_{\alpha\beta} + \dfrac{\delta_{\alpha\beta}}{2} \right)$

$p = 1/2$ Brownian particles!!

Comparison with microscopic behavior: Coarsening

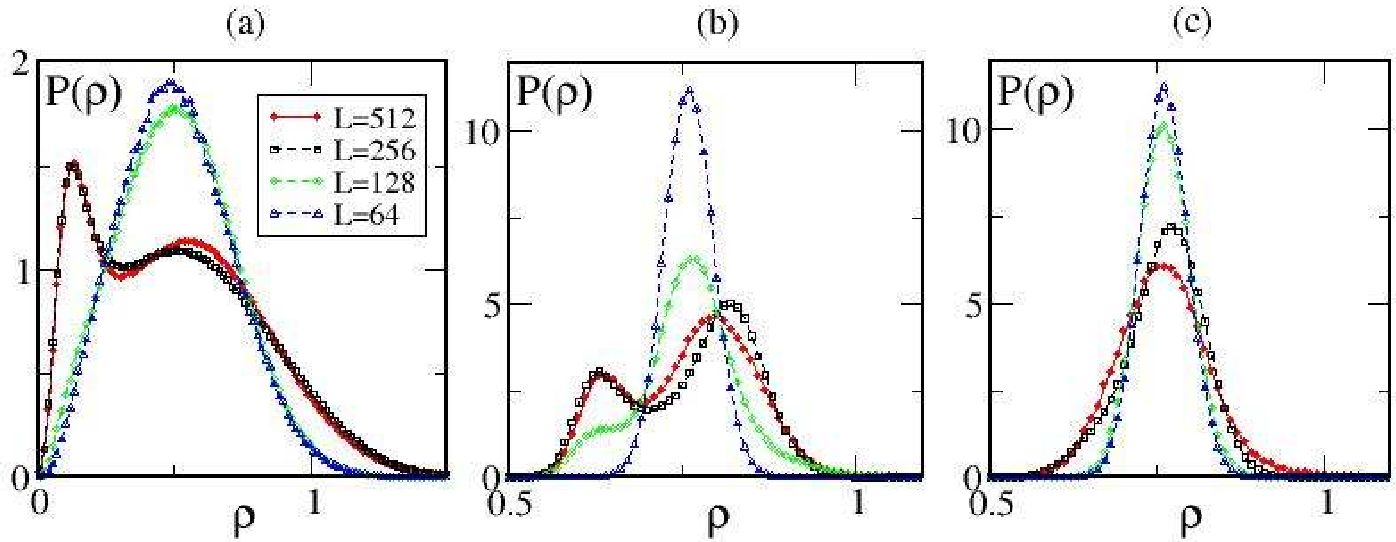


Microscopic active nematics

Langevin equations

Deterministic version of mesoscopic dynamics

Comparison with microscopic behavior: Segregation



Microscopic dynamics

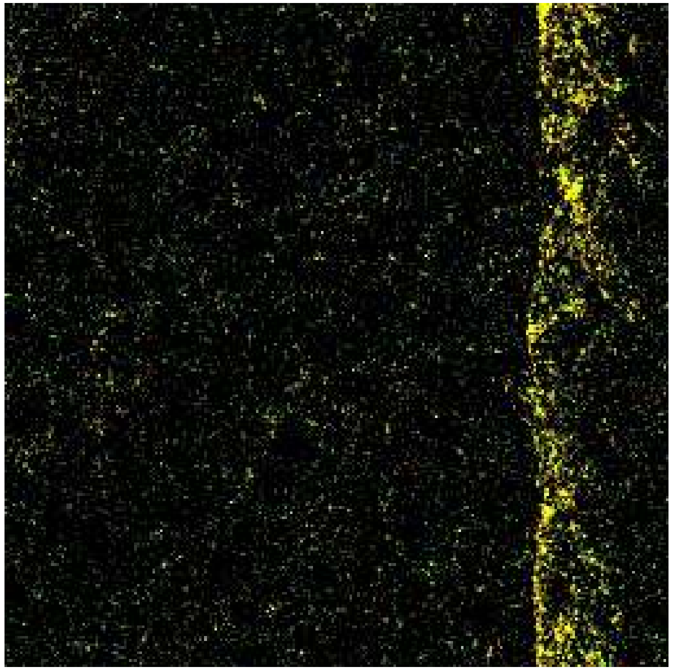
Langevin dynamics
multiplicative noise

Langevin dynamics
additive noise

Segregation in other self propelled particles models

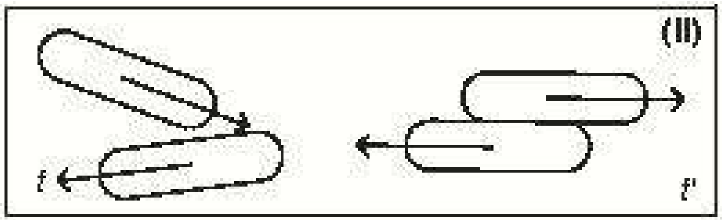
Vicsek model, as noise is raised towards the order-disordered transition

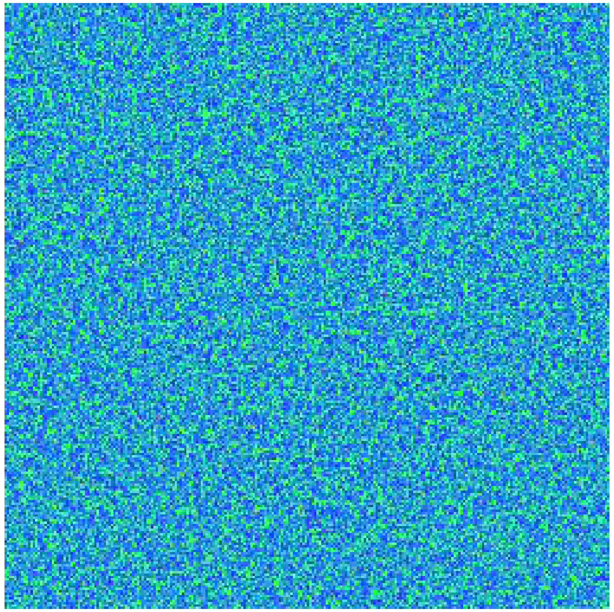
- Ordered, spatially homogeneous
- Band regime
- Disordered phase

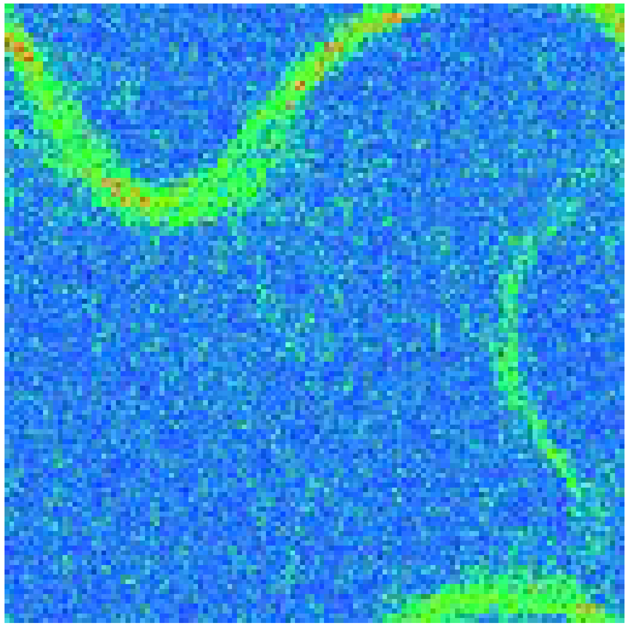


Weakly interacting solitary objects

Polar particles with nematic interactions







(with F. Peruani, M. Baer)

Conclusions

- Ensembles of active particle have genuine non-equilibrium features
- Captured by simple models
- Giant number density fluctuations, superdiffusion,
- Segregation phenomena with non-sharp interfaces
- Correct noise correlations are needed in a Langevin description