Defect-driven melting of active fluids

Suraj Shankar

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Symmetry, Thermodynamics and Topology in Active Matter
KITP, 9th April, 2020

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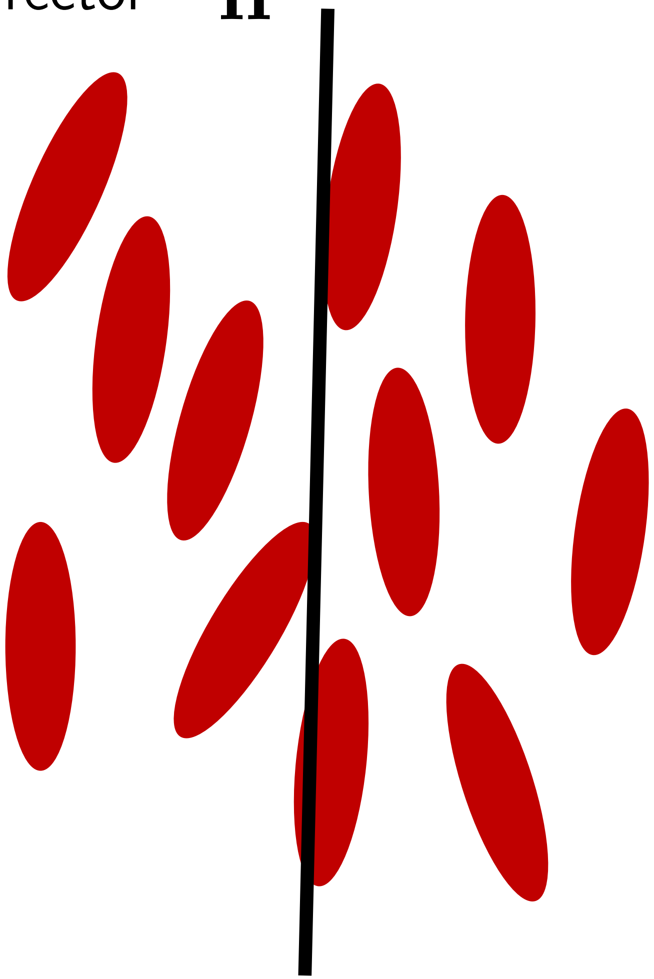
Two Types of Order

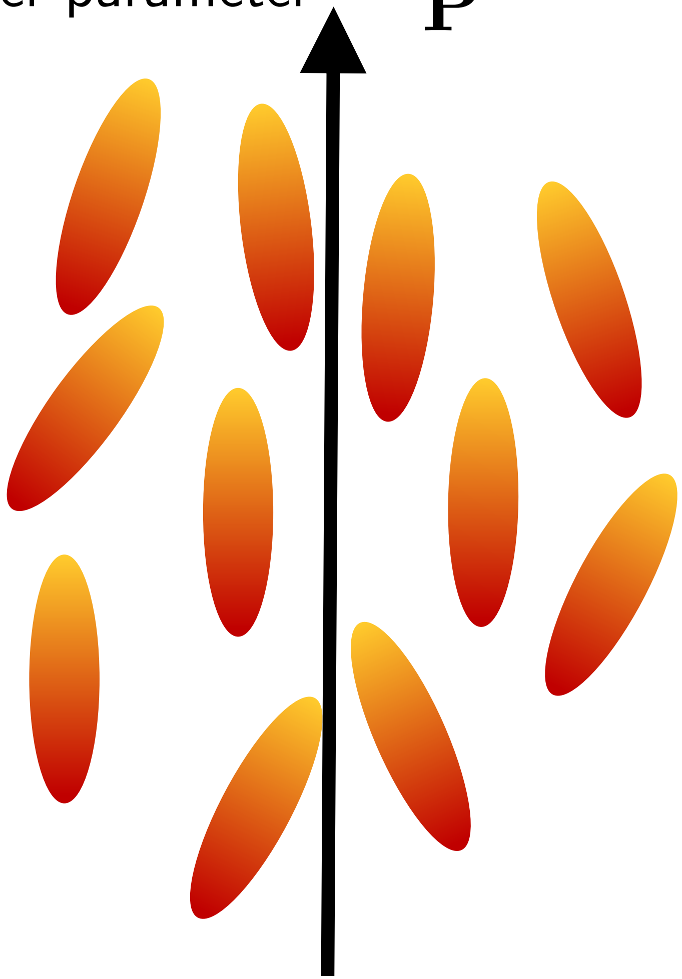
Order parameter

$$Q_{ij} = \frac{S}{2}\left(n_i n_j - \frac{\delta_{ij}}{2}\right)$$

(in two dimensions)



Nematic order



Polar order

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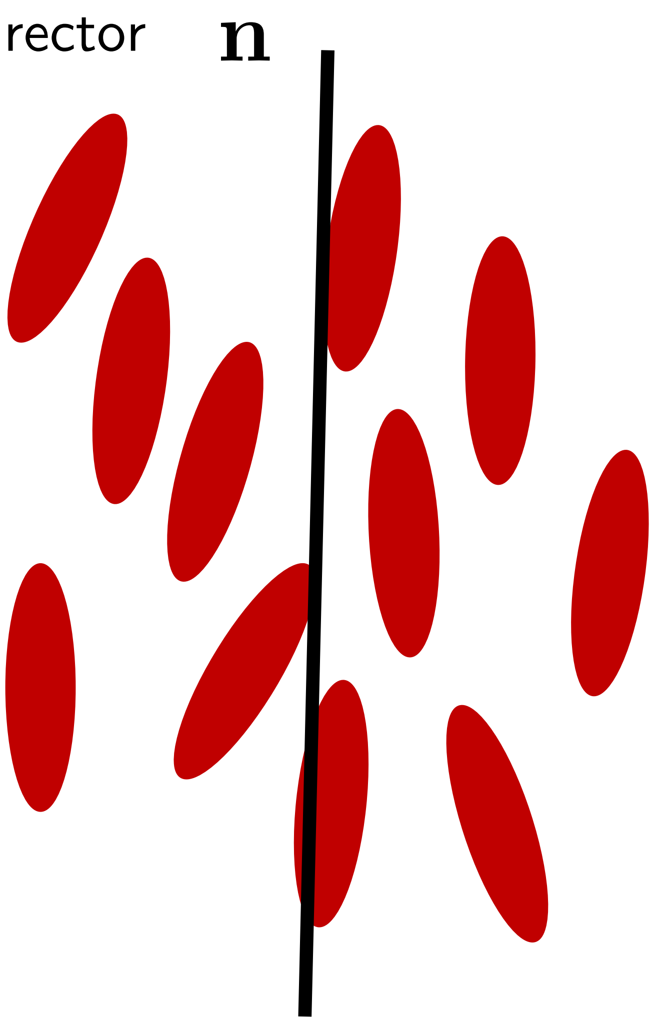
Two Types of Order

Nematic director



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(in two dimensions)

Nematic order

Order parameter

Polar order

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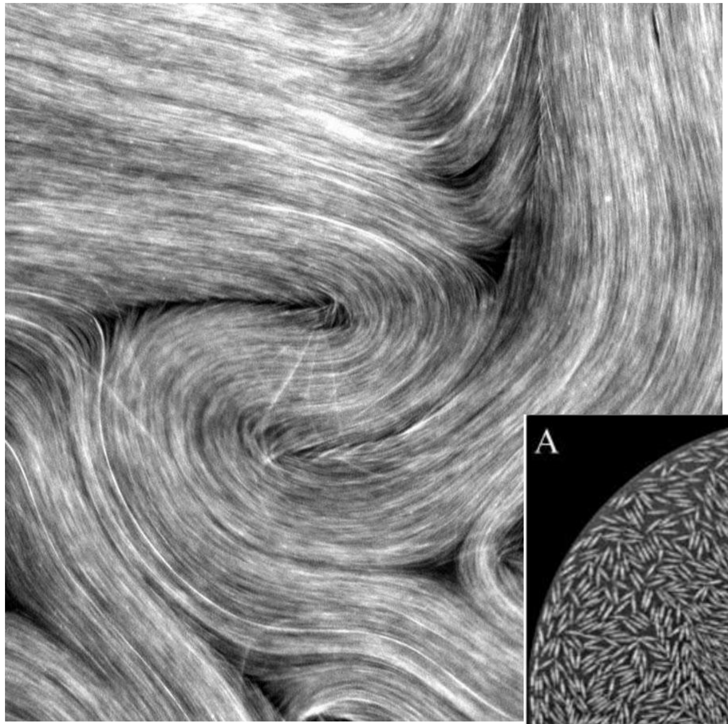
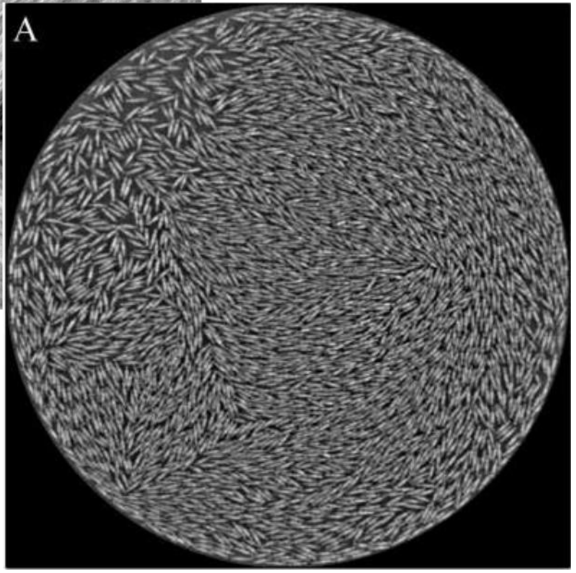
Active Nematics

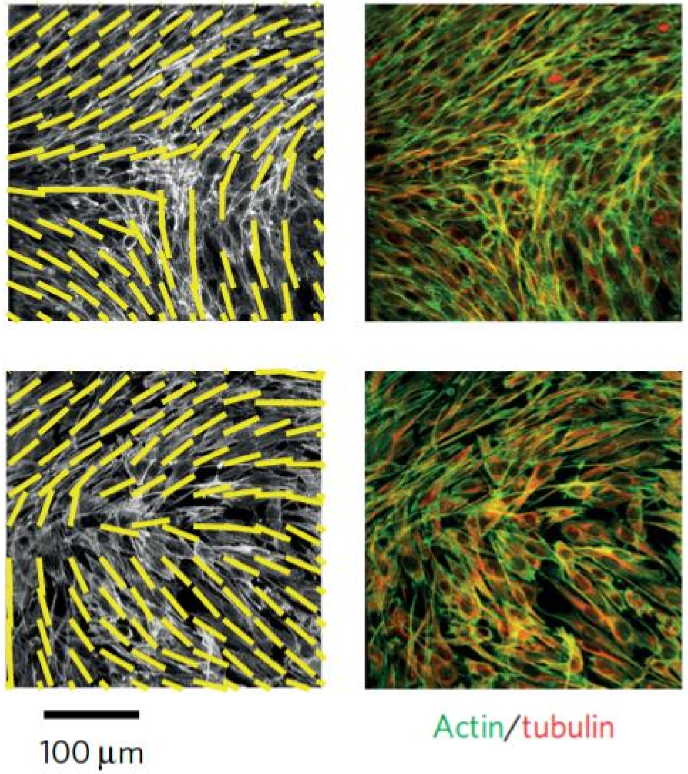
Nematically ordered collections of **self-driven** particles

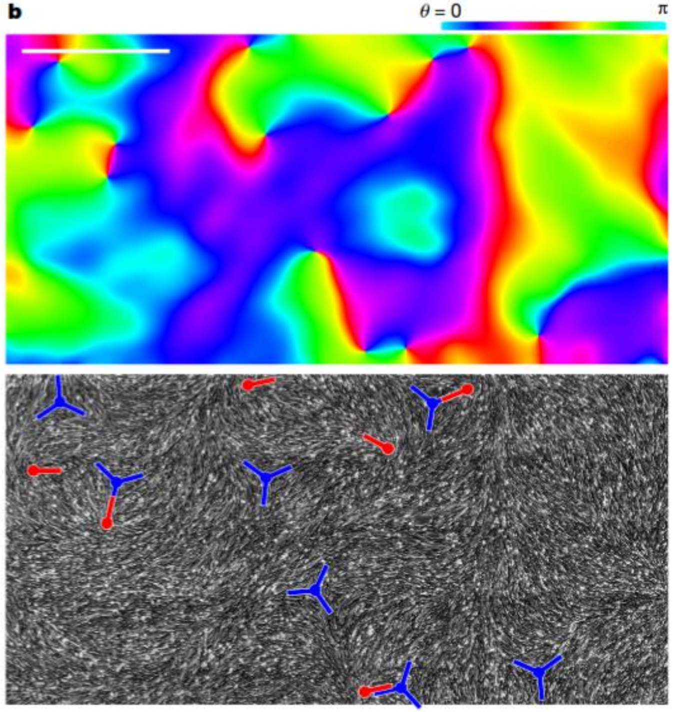
Recent review: Doostmohammadi, Nat. Comm. 2018



Kinesin - Microtubule bundle nematic film
Sanchez *et al.*, Nature 2012 ...







Cellular nematics - Duclos *et al.*, Nat. Phys. 2017; Saw *et al.* Nature 2017; Kawaguchi *et al.*, Nature 2017...

2D Vibrated rods Narayan *et al.*, Science 2007

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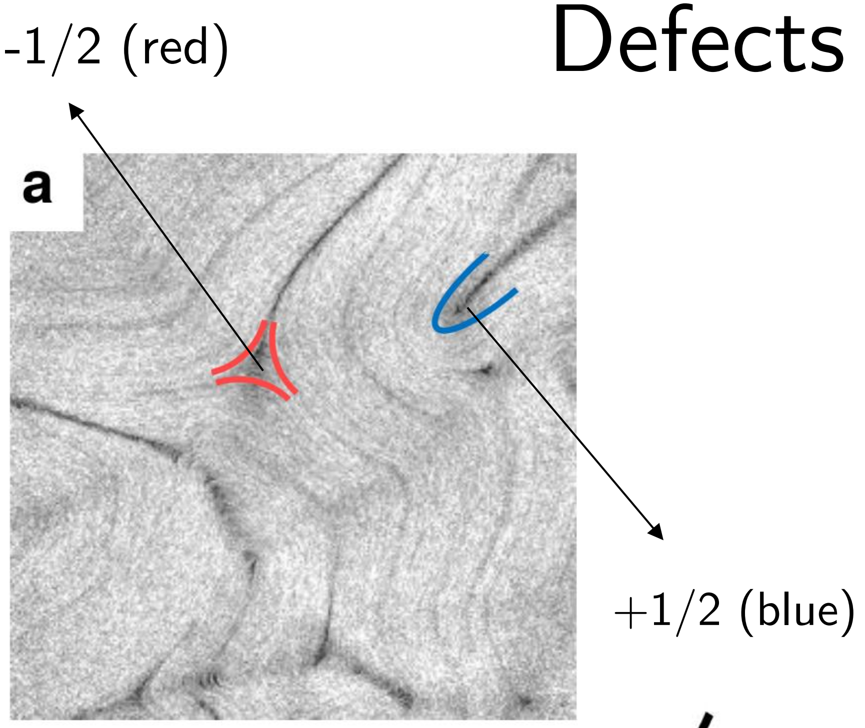
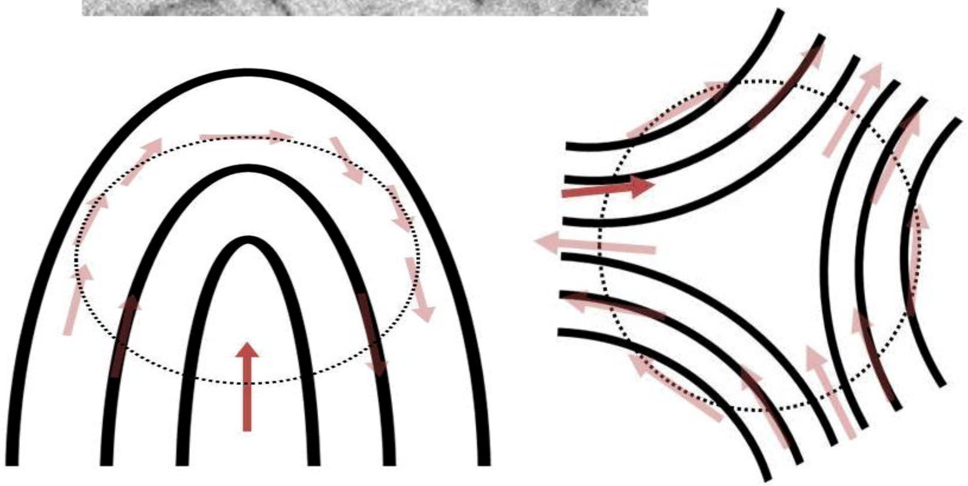
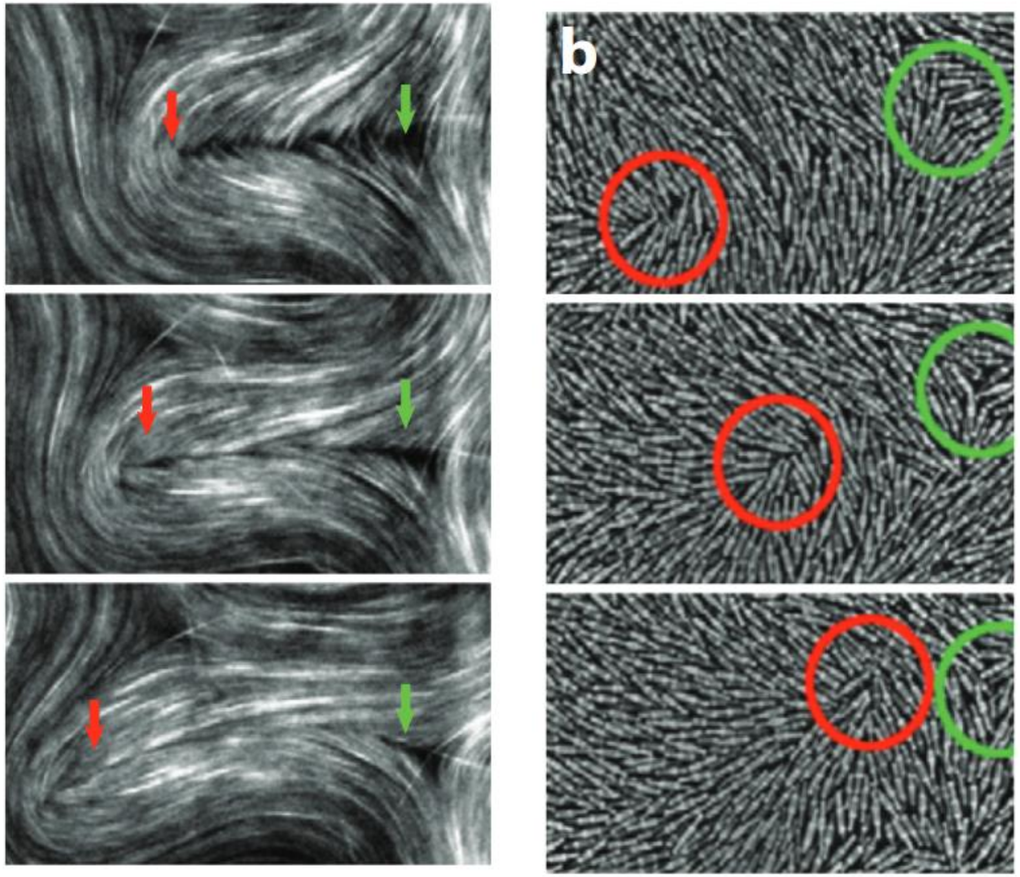
Defects in 2D Active Nematics





+1/2 disclination

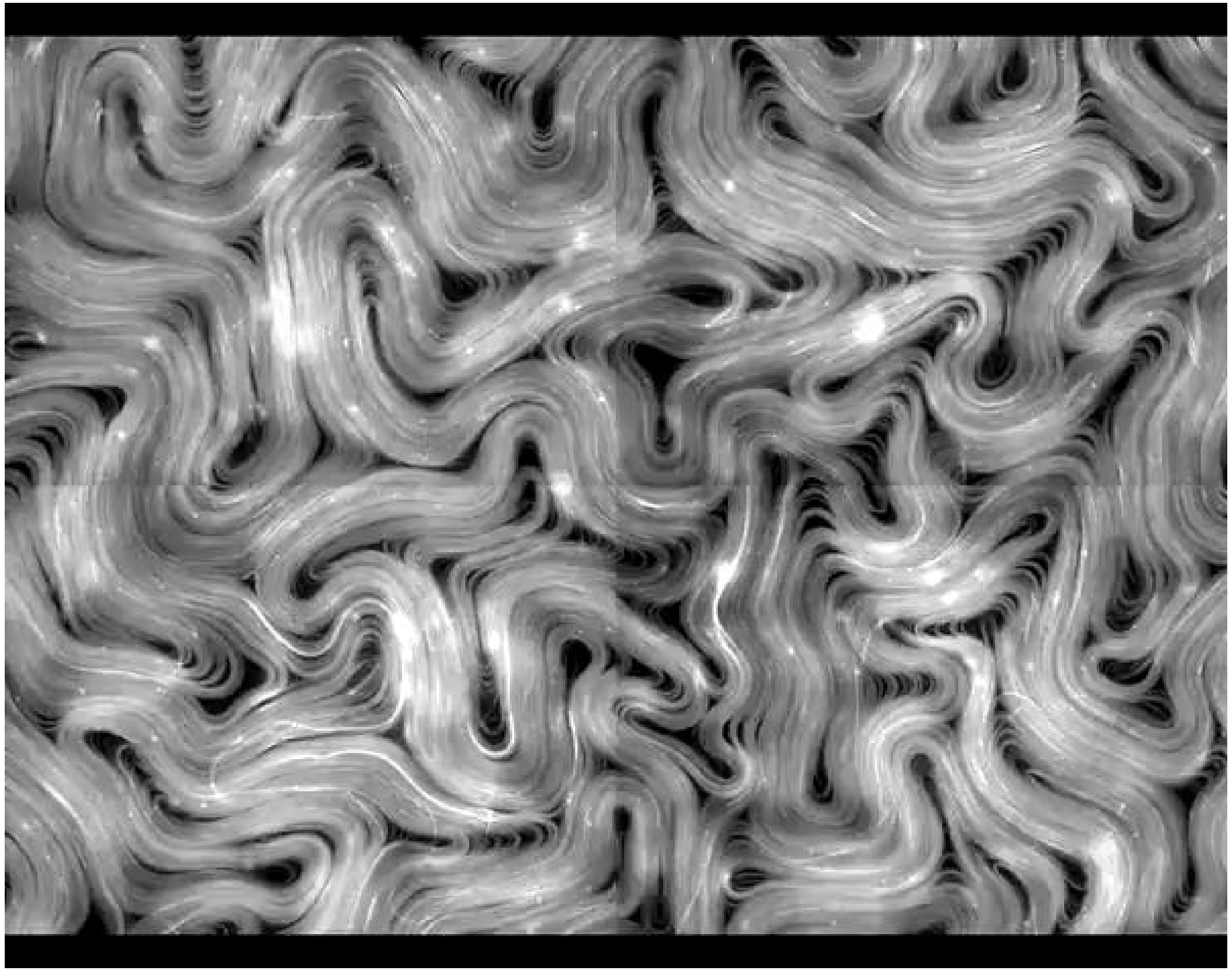
-1/2 disclination



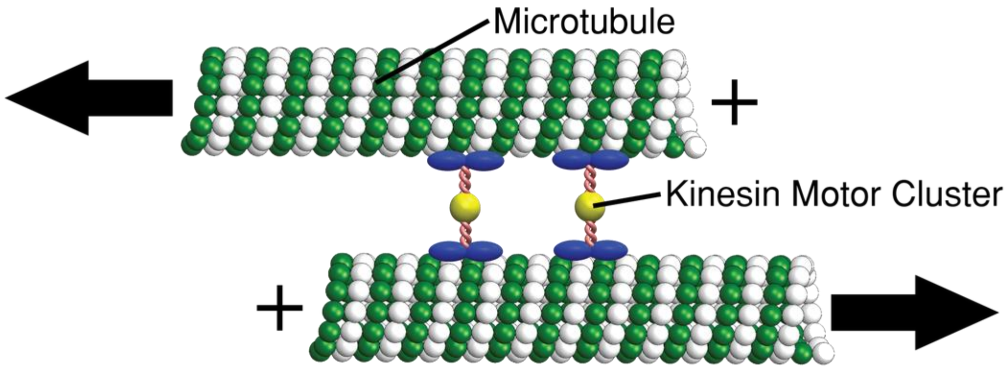
+1/2 disclinations are motile in active systems

Giomi *et al.*, PRL 2013; Giomi *et al.*, Phil Trans. R. Soc. 2014; Pismen PRE 2013; Sanchez *et al.*, Nature 2012; Narayan *et al.*, Science 2007...

Active Nematic Chaos



Microtubule + Kinesin motor complex at oil-water interface



Sanchez *et al.*, Nature 2012

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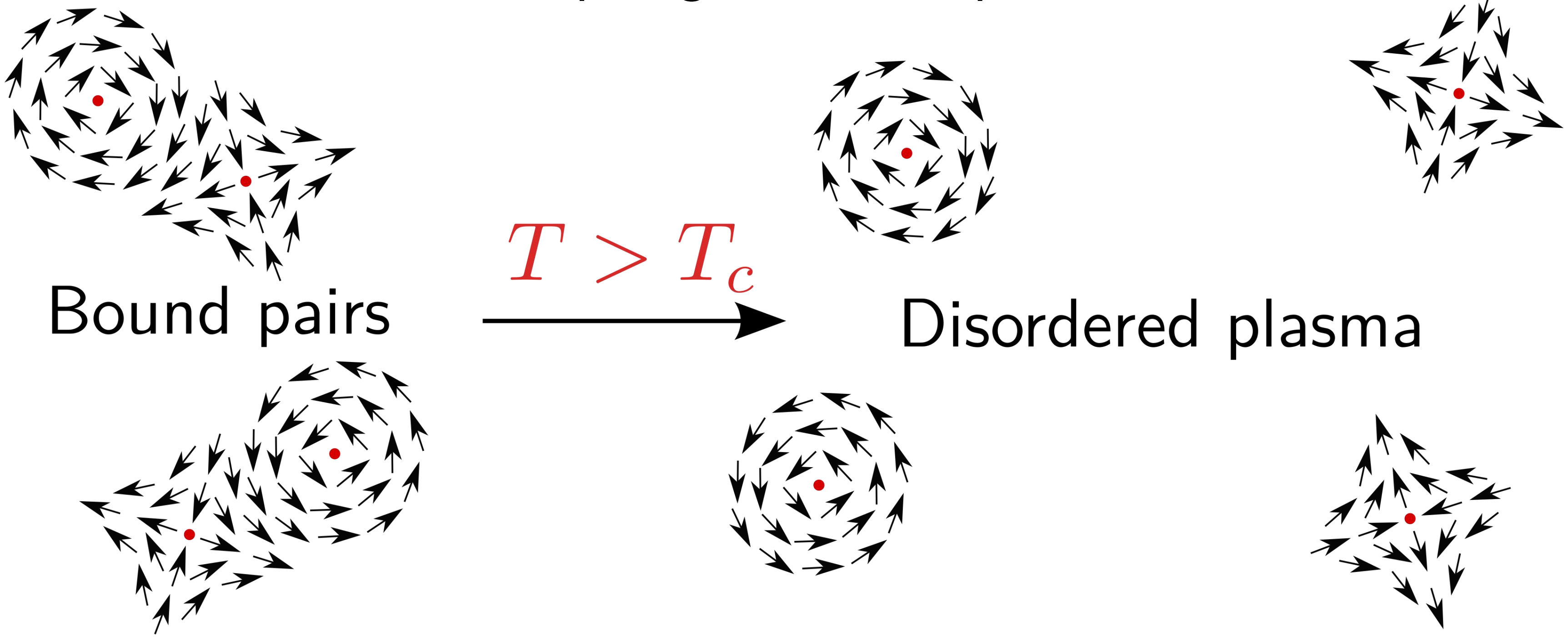
Berezinskii-Kosterlitz-Thouless (BKT) transition

Continuous order-disorder transitions in 2D via defect unbinding

Entropic unbinding of
topological defect pairs



Berezinskii, Sov. J. Exp and Theor. Phys. 1971;
Kosterlitz, Thouless, J. Phys. C 1973; Kosterlitz, J. Phys. C, 1974

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Berezinskii-Kosterlitz-Thouless (BKT) transition

Continuous order-disorder transitions in 2D via defect unbinding

Is there an active BKT transition?


Berezinskii, Sov. J. Exp and Theor. Phys. 1971;
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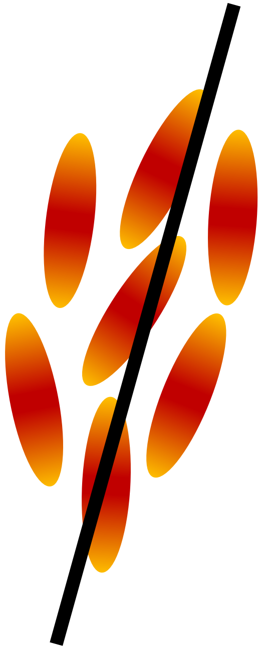
From $\mathbf{Q}$ Dynamics to Defect Dynamics

Start from the active dynamics of the liquid crystal alignment tensor $\mathbf{Q}$

$$\partial_t \mathbf{Q} + \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{Q} + [\boldsymbol{\Omega}, \mathbf{Q}] = \lambda(\boldsymbol{\nabla}\mathbf{u})_{ST} + \frac{1}{\gamma}[a_2 - a_4|\mathbf{Q}|^2]\mathbf{Q} + \frac{K}{\gamma}\nabla^2\mathbf{Q}$$

Flow coupling **Ordering Potential** **Elasticity**



$\mathbf{n}$ Nematic director

Order parameter

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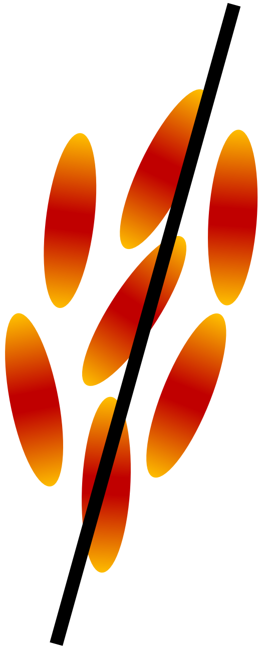
Flow coupling — **Ordering Potential** — **Elasticity**



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$\mathbf{u}$ is the flow velocity

$$\Gamma\mathbf{u} = \boldsymbol{\nabla}\cdot(\alpha\mathbf{Q})$$

Friction — **Active stress**

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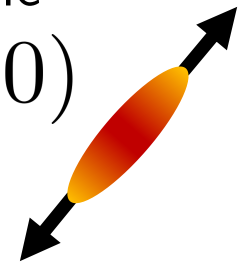
Flow coupling **Ordering Potential** **Elasticity**

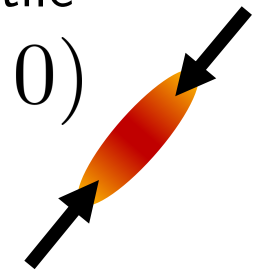
Extensile

$(\alpha < 0)$



Contractile

$(\alpha > 0)$



$\mathbf{u}$ is the flow velocity

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Friction **Active stress**

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Flow coupling **Ordering Potential** **Elasticity**

Extensile Contractile

$\mathbf{u}$ is the flow velocity

Solve for a single moving defect solution perturbatively in activity and the defect speed

Obtain equations of motion for both the position and orientation of defects

Shankar *et al.*, PRL 2018

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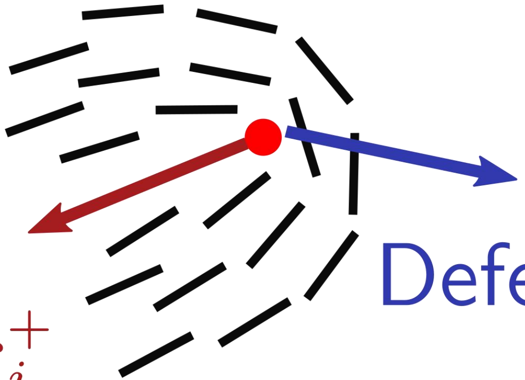
Defects as Quasiparticles

+1/2 disclination

$$\partial_t \mathbf{r}_i^+ = v\mathbf{e}_i + \mu \mathbf{F}_i$$

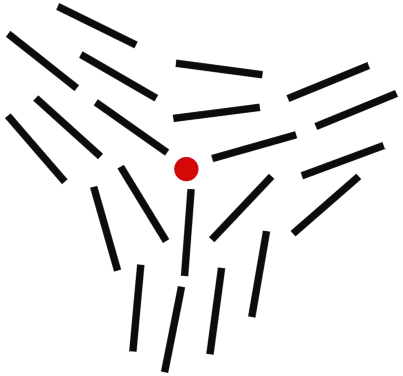
$$v \propto \frac{\alpha}{\Gamma a}$$

+1/2 self-propelling speed $= |v|$



$\mathbf{v}_i \equiv \partial_t \mathbf{r}_i^+$
Defect velocity

$\mathbf{e}_i = \boldsymbol{\nabla} \cdot \mathbf{Q}|_{\mathbf{r}_i^+}$
Defect orientation



-1/2 disclination

$$\partial_t \mathbf{r}_i^- = \mu \mathbf{F}_i$$

$\mathbf{F}_i$ - Elastic force

Shankar *et al.*, PRL 2018

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Motility Driven Defect Unbinding

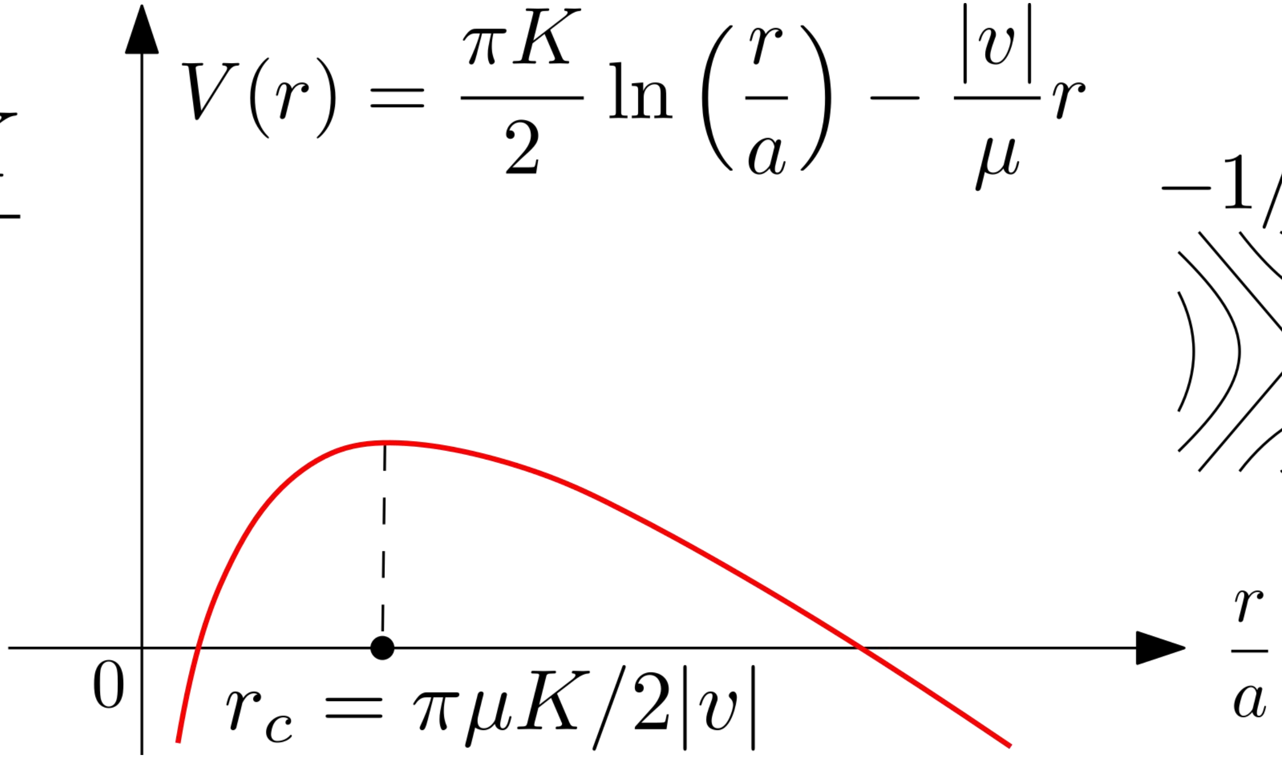
Simplified 1D model for a defect pair

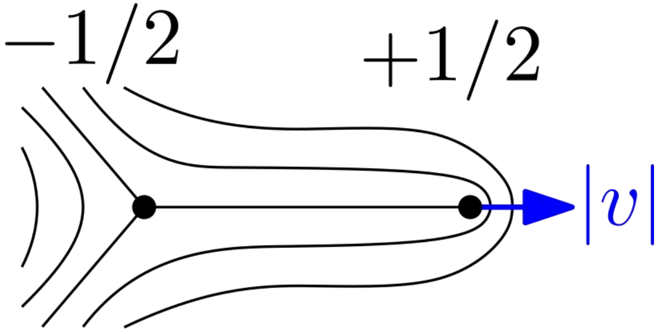
$$\dot{r} = |v| - \mu\frac{\pi K}{2r}$$

$$\downarrow$$

$$\dot{r} = -\partial_r V(r)$$

$$V(r) = \frac{\pi K}{2}\ln\left(\frac{r}{a}\right) - \frac{|v|}{\mu}r$$





Elasticity (K) balances self-propulsion ($|v|$)

Shankar *et al.*, PRL 2018
Giomi *et al.*, PRL 2013

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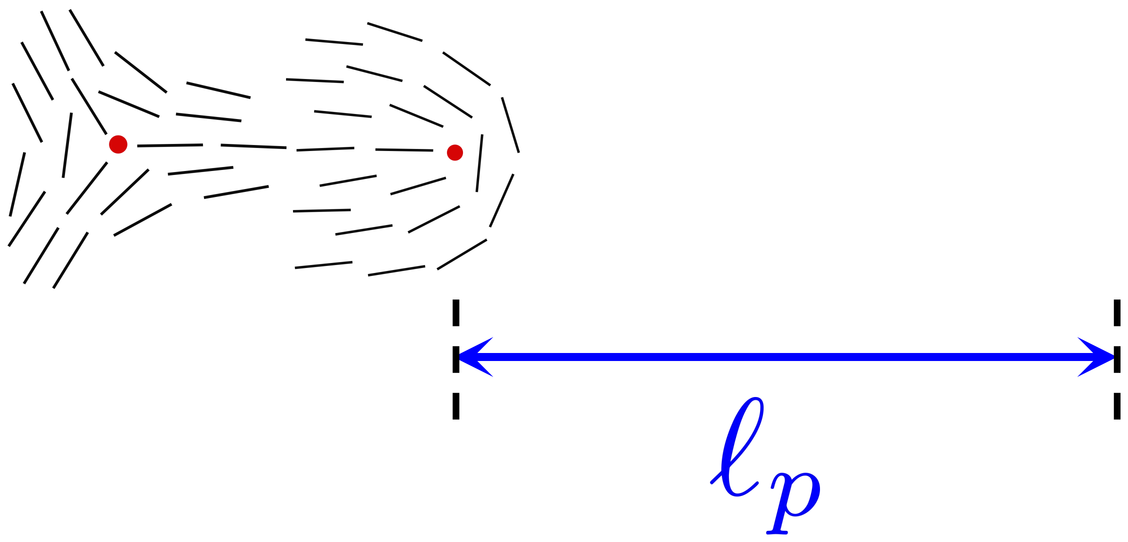
"Motile" BKT Transition

Including rotational diffusion D_R for defects

Persistence length

Distance to barrier

$$\ell_p = \frac{|v|}{D_R} \gtrsim r_c$$



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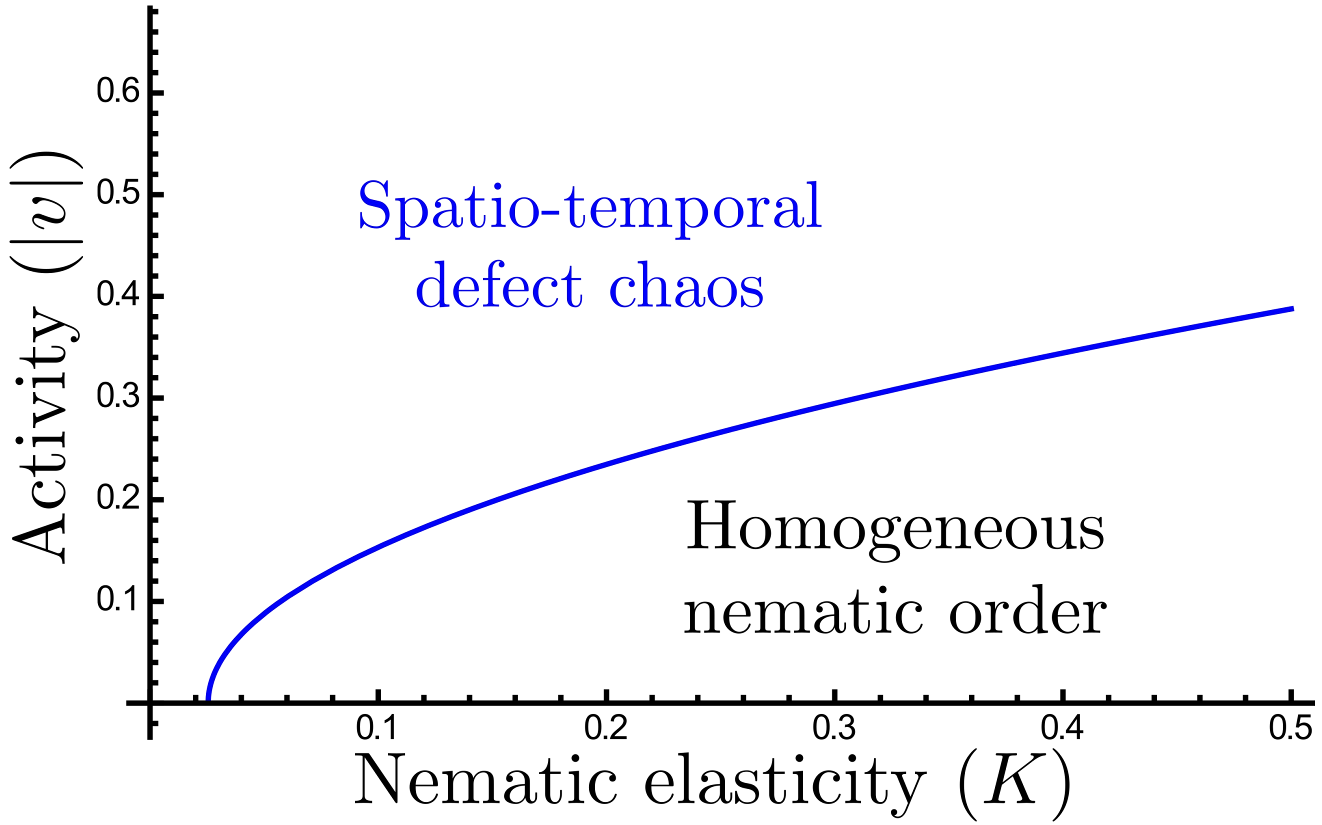

Shankar *et al.*, PRL 2018

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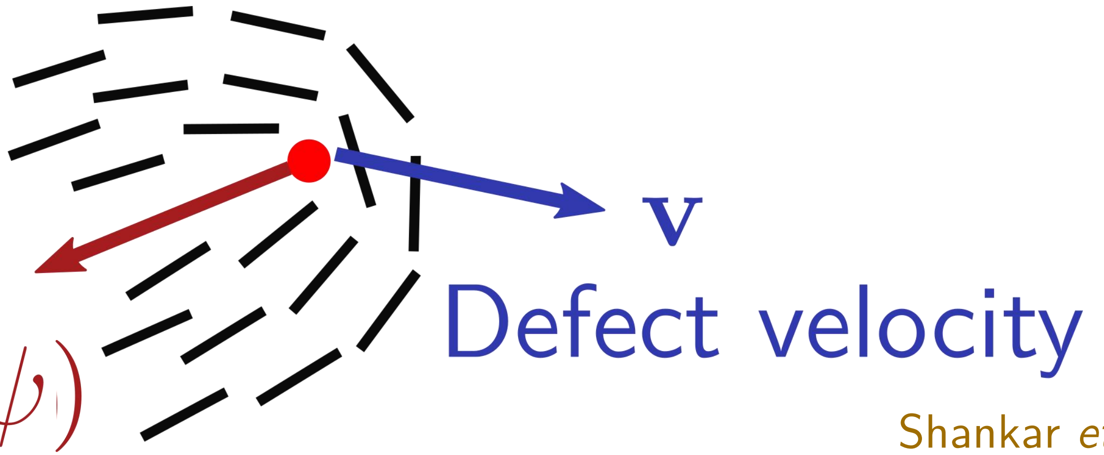
Defect Orientational Torques

Angular dynamics of the $+1/2$ defect

Active torque

$$\omega \equiv \partial_t \psi \propto v(\mathbf{v} \times \hat{\mathbf{e}})$$

- Contractile stress (v>0) favours ***self anti-alignment***
- Extensile activity (v<0) favours ***self alignment***



$$\hat{\mathbf{e}} = (\cos\psi, \sin\psi)$$

Defect orientation

Shankar *et al.*, PRL 2018
Also see: Vromans, Giomi, SM 2016; Tang, Selinger, SM 2017

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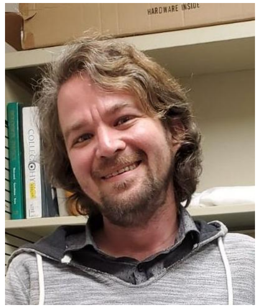
Defect Orientational Torques

Dogic lab
UCSB

Linnea Lemma



Link Morgan

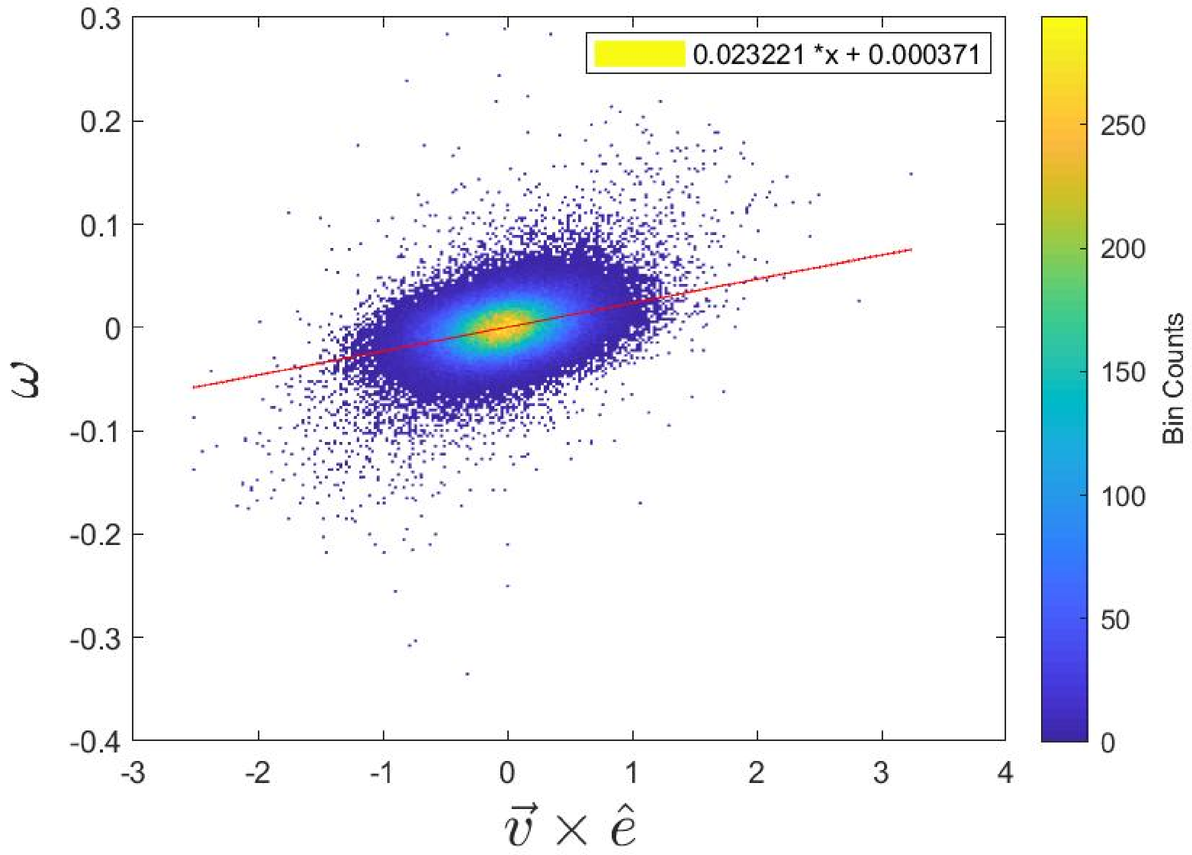
Angular dynamics of the $+1/2$ defect

Active torque

$$\omega \equiv \partial_t \psi \propto v(\mathbf{v} \times \hat{\mathbf{e}})$$

Extensile activity - $v<0$

Angular velocity is positively correlated with **v** x **e**!?!



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Defect Orientational Torques

Angular dynamics of the $+1/2$ defect

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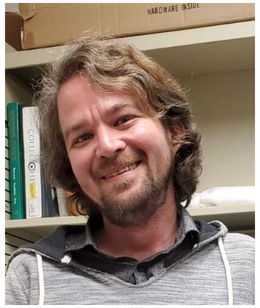
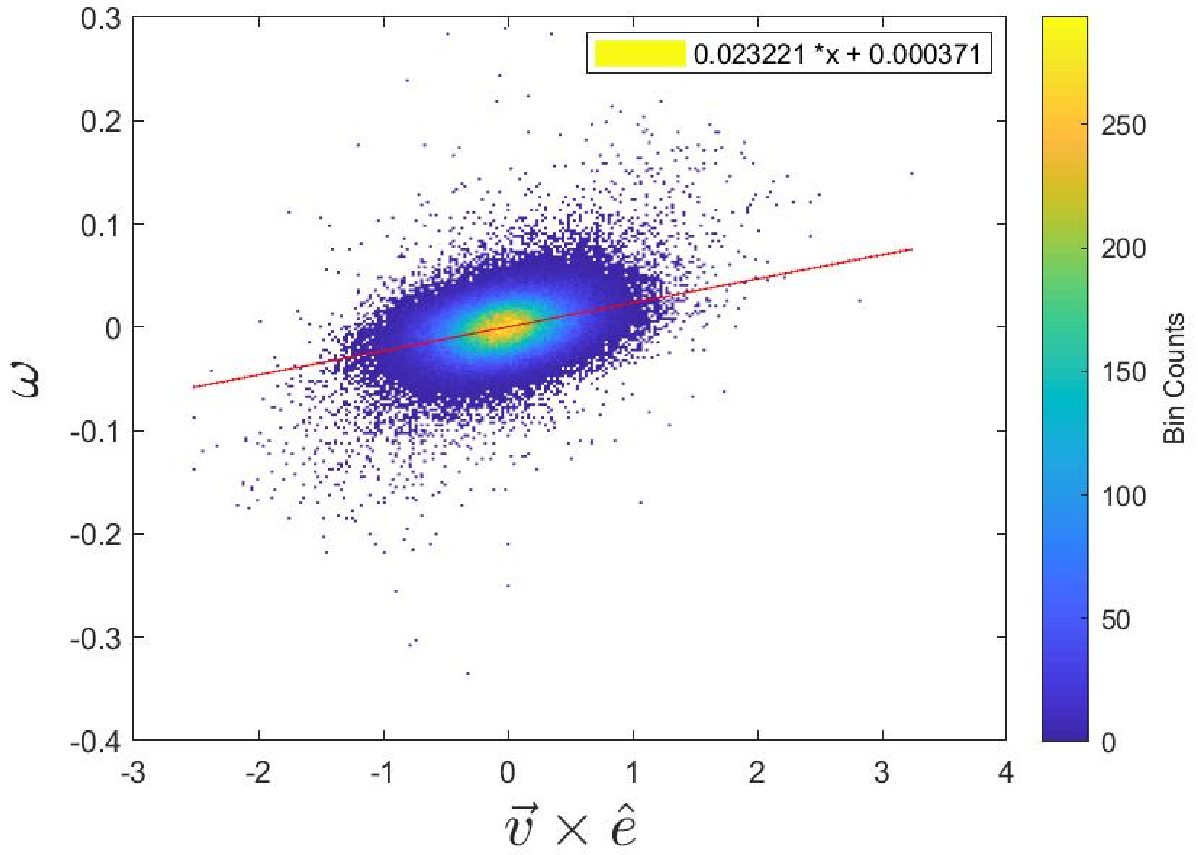


Linnea Lemma Link Morgan

Active torque

$$\omega \equiv \partial_t \psi \propto v(\mathbf{v} \times \hat{\mathbf{e}})$$

What's missing?



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Defect Orientational Torques

Angular dynamics of the $+1/2$ defect

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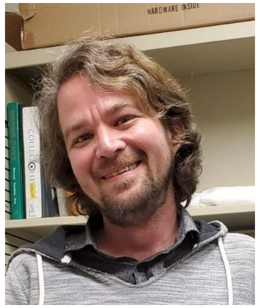


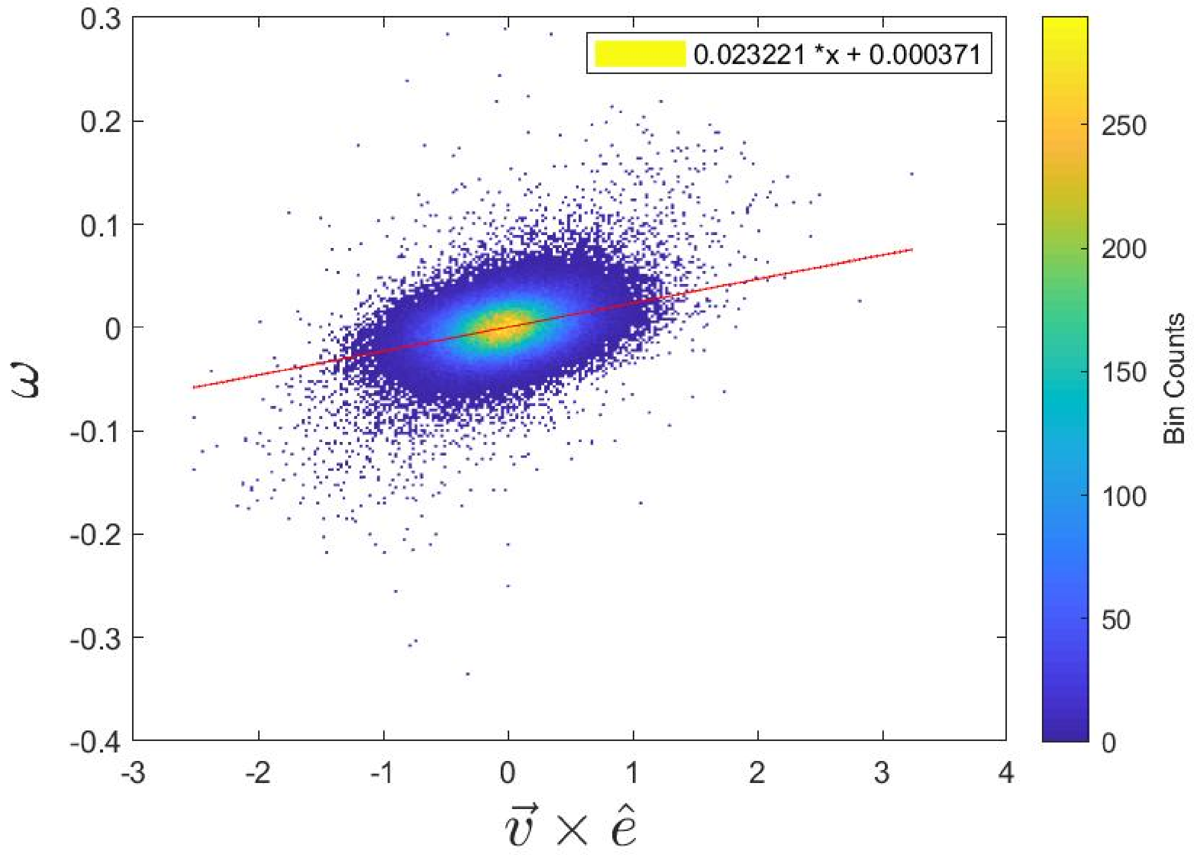
Link Morgan

Active torque

$$\omega \equiv \partial_t \psi \propto v(\mathbf{v} \times \hat{\mathbf{e}})$$

What's missing?

- Viscous effects
- Incompressibility



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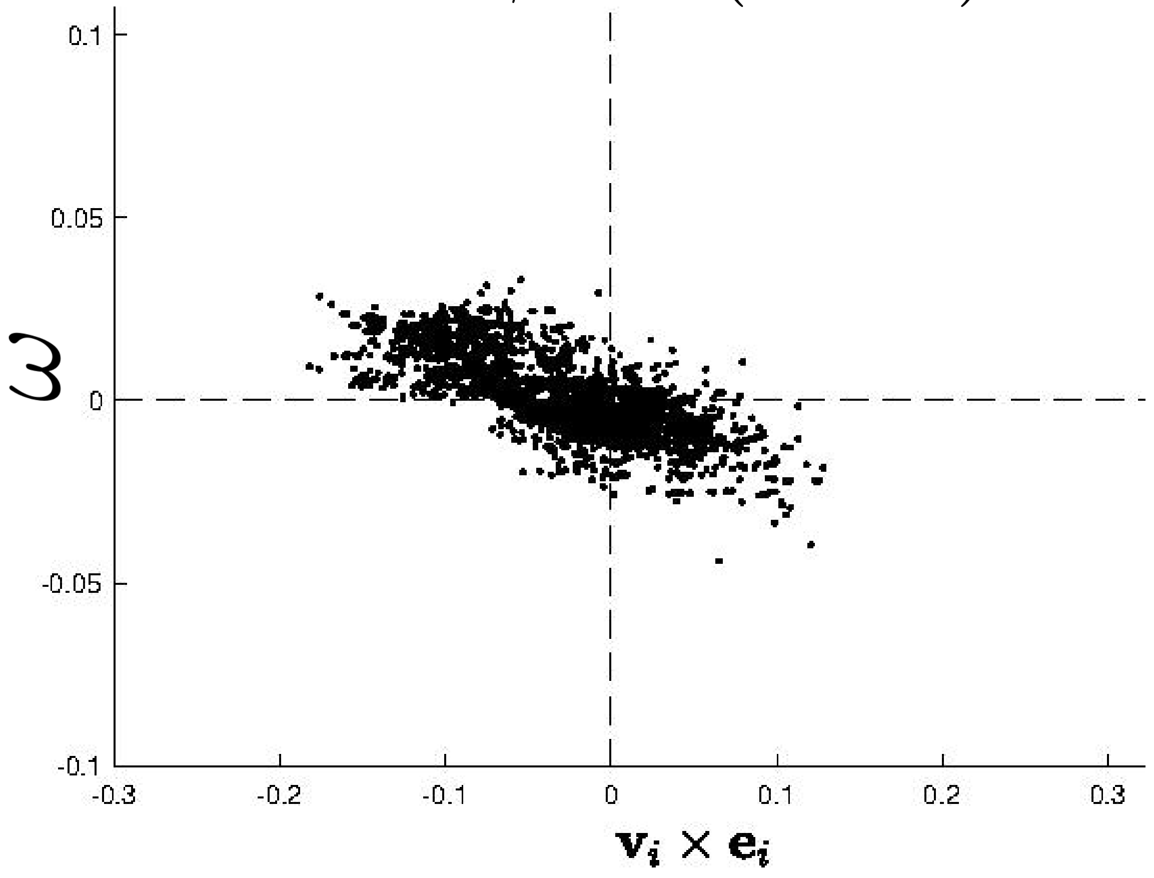
Incompressibility Changes Active Torque

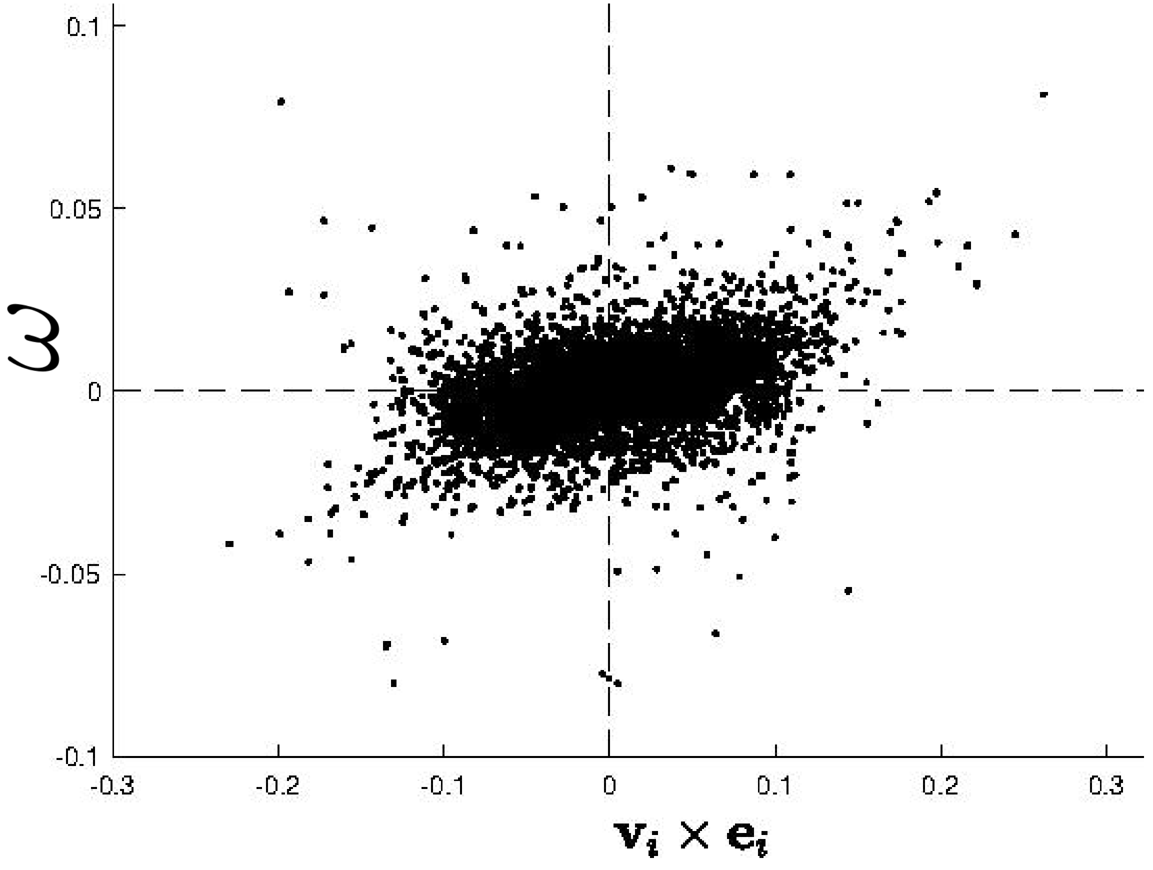
Numerical simulations of continuum equations with just friction

Supavit Pokawanvit
UCSB

$$\omega \equiv \partial_t \psi \propto v(\mathbf{v} \times \hat{\mathbf{e}})$$



Compressible (extensile)



Incompressible (extensile)

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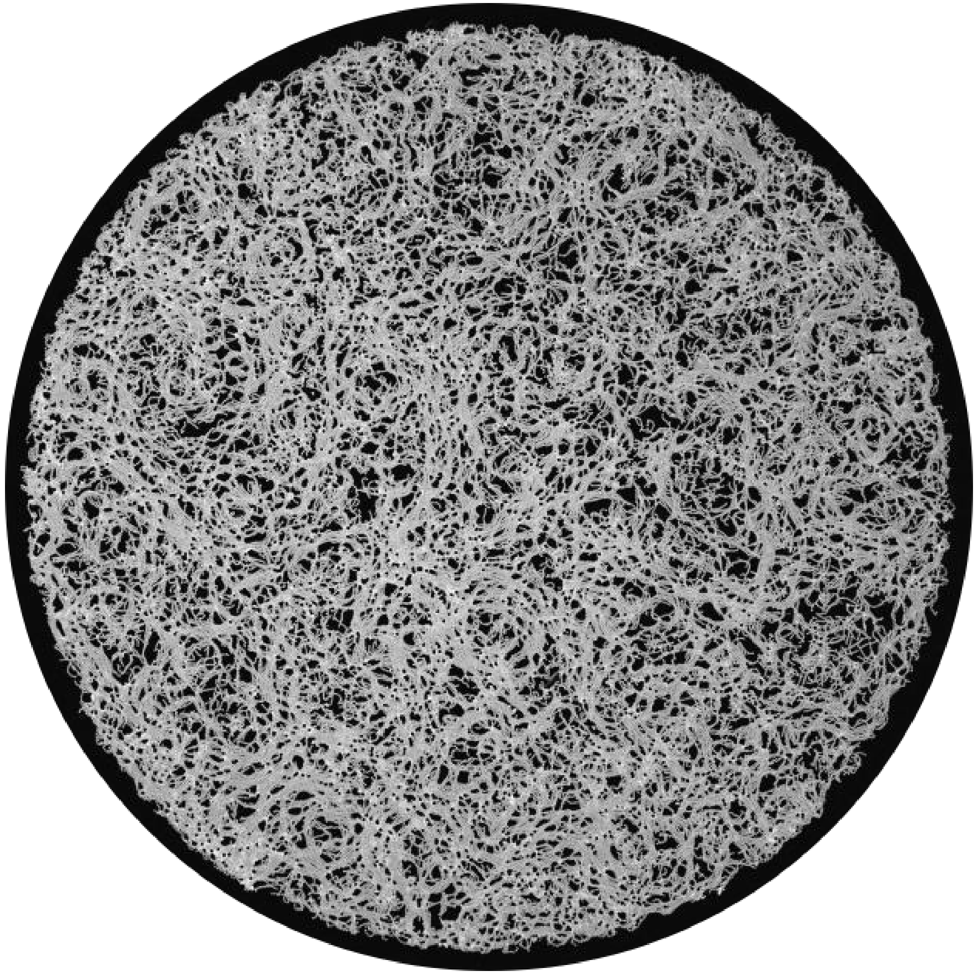
Some Open Questions

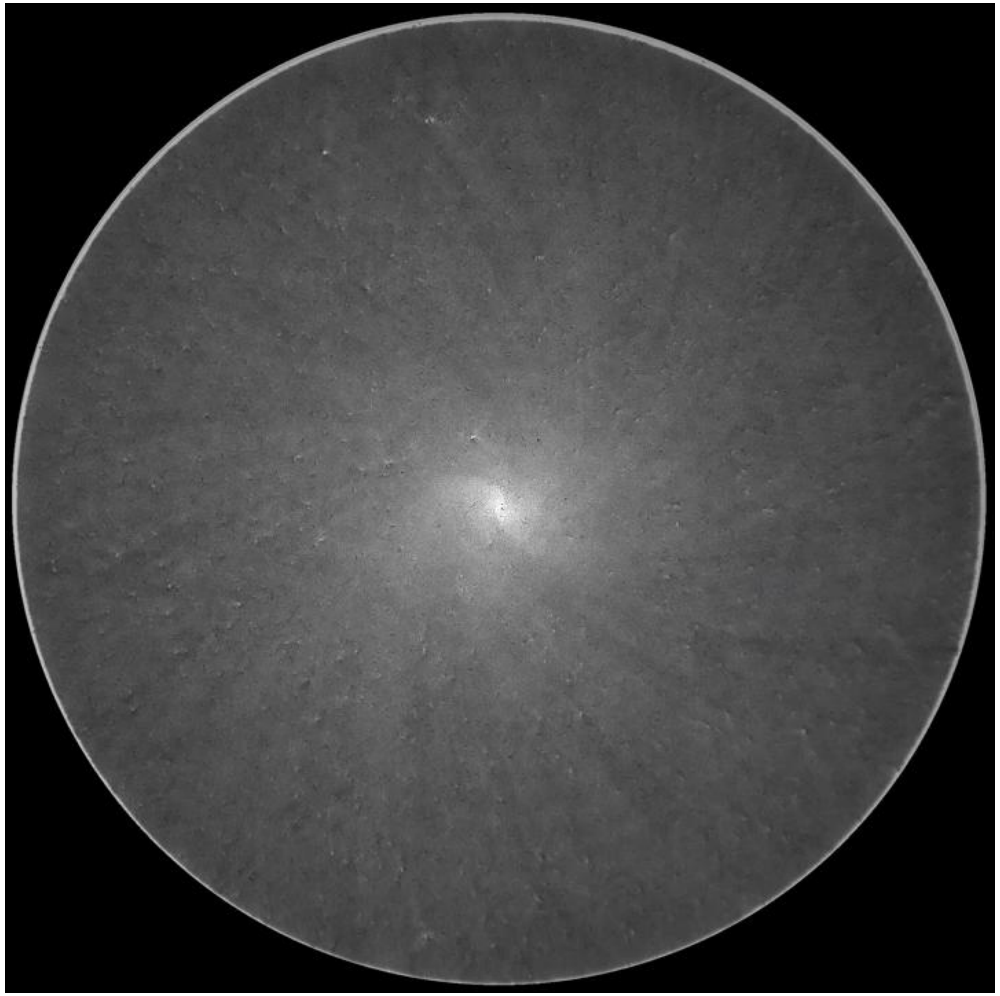
- How do viscous effects modify these torques? Can we understand this (along with the effect of incompressibility) theoretically?
- Does this change in the torque sign explain the symmetry of defect ordered states - nematic versus polar defect ordering?
- Can we tune the sign of the torque continuously? What role do density fluctuations play?

Defect Unbinding in Active Polar Fluids



Chardac, Shankar *et al.*, arXiv:2002.12893

Quincke Colloidal Flocks

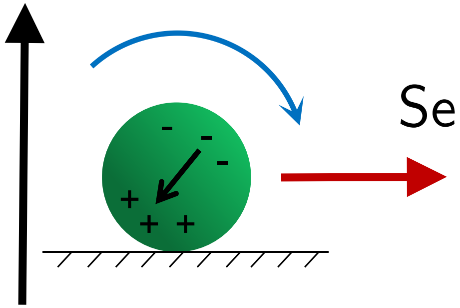


Denis Bartolo

Amelie Chardac

ENS Lyon

$E > E_Q$



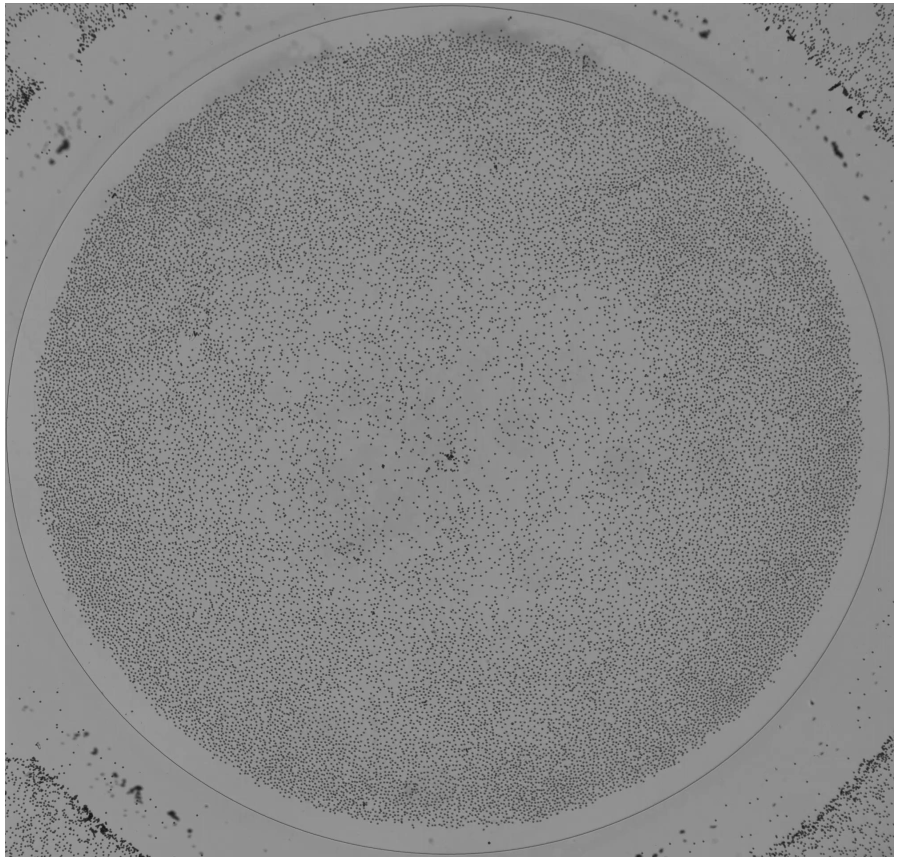
Self-propulsion speed - v_0

Quincke roller

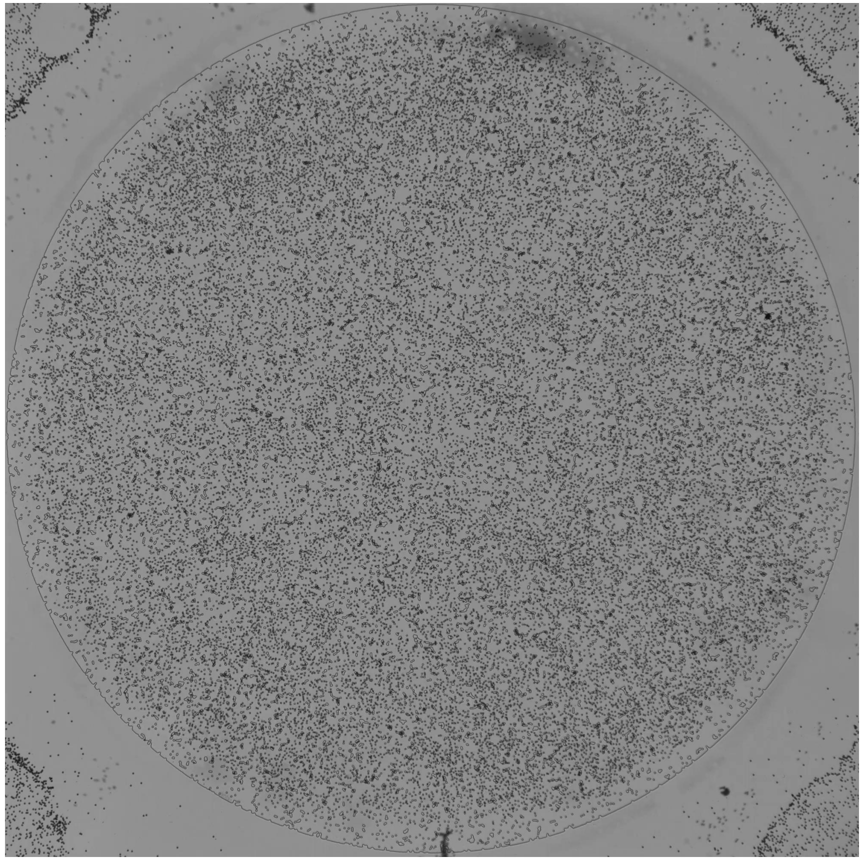
Also see Bricard *et al.*, Nature 2013

Flocking through Disorder

$\phi_0 = 0\%$



$\phi_0 = 15\%$



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Melting a Flock

How does a flock melt under quenched disorder?

Ordered flock —?→ **Isotropic gas**

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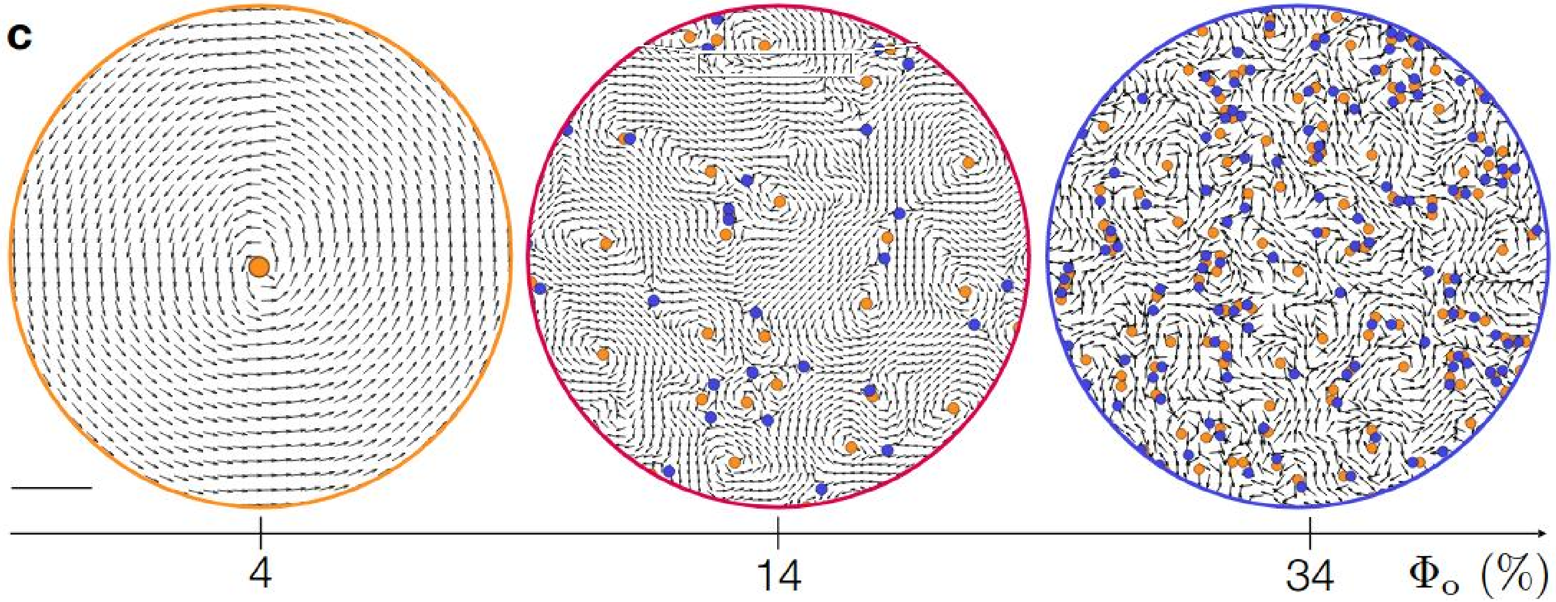
Melting a Flock

How does a flock melt under quenched disorder?

Ordered flock → **Isotropic gas**

Polar order   **Vortex glass**   Gas



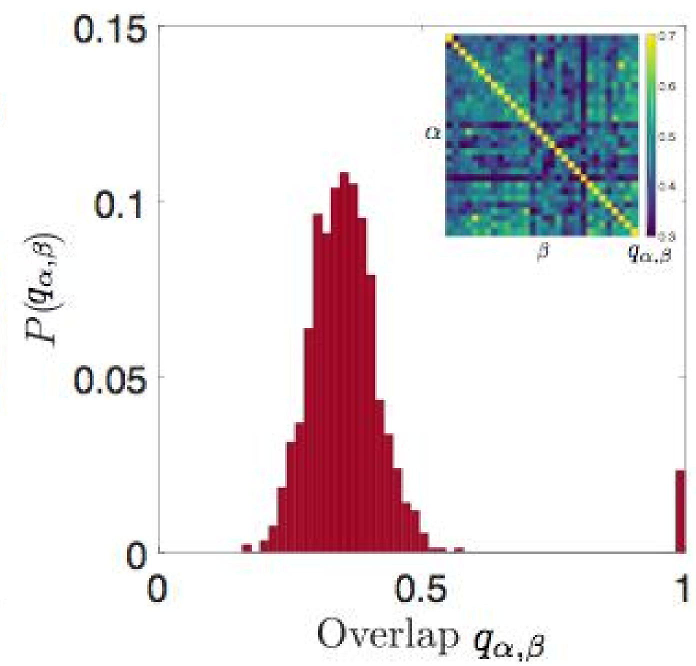
Chardac, Shankar *et al.*, arXiv:2002.12893

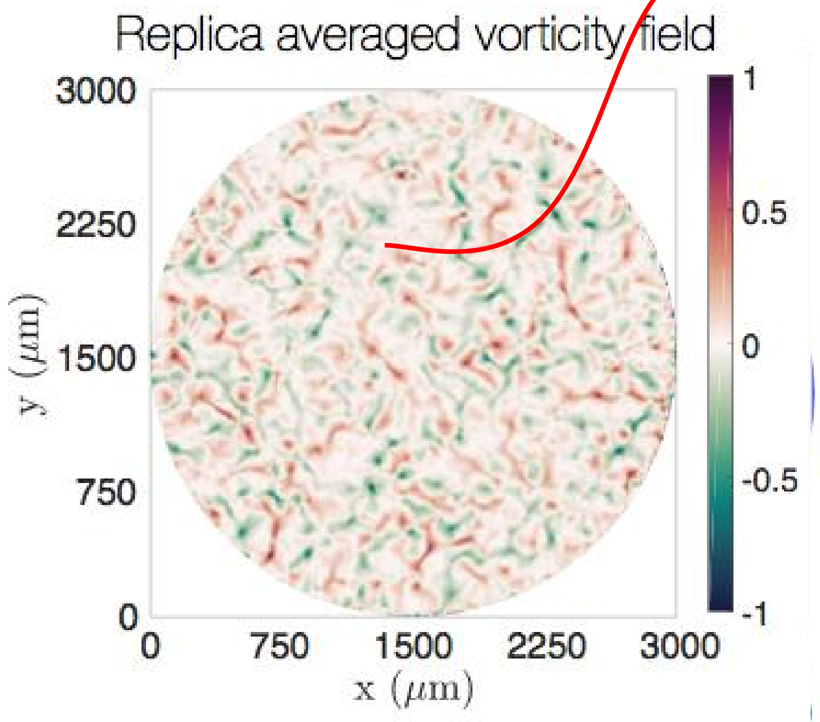
Melting a Flock

How does a flock melt under quenched disorder?

Ordered flock → **Isotropic gas**

Frozen Topological defects!





$$q_{\alpha\beta} = \langle \mathbf{p}_\alpha \cdot \mathbf{p}_\beta \rangle_{\mathbf{r}}$$

Chardac, Shankar *et al.*, arXiv:2002.12893

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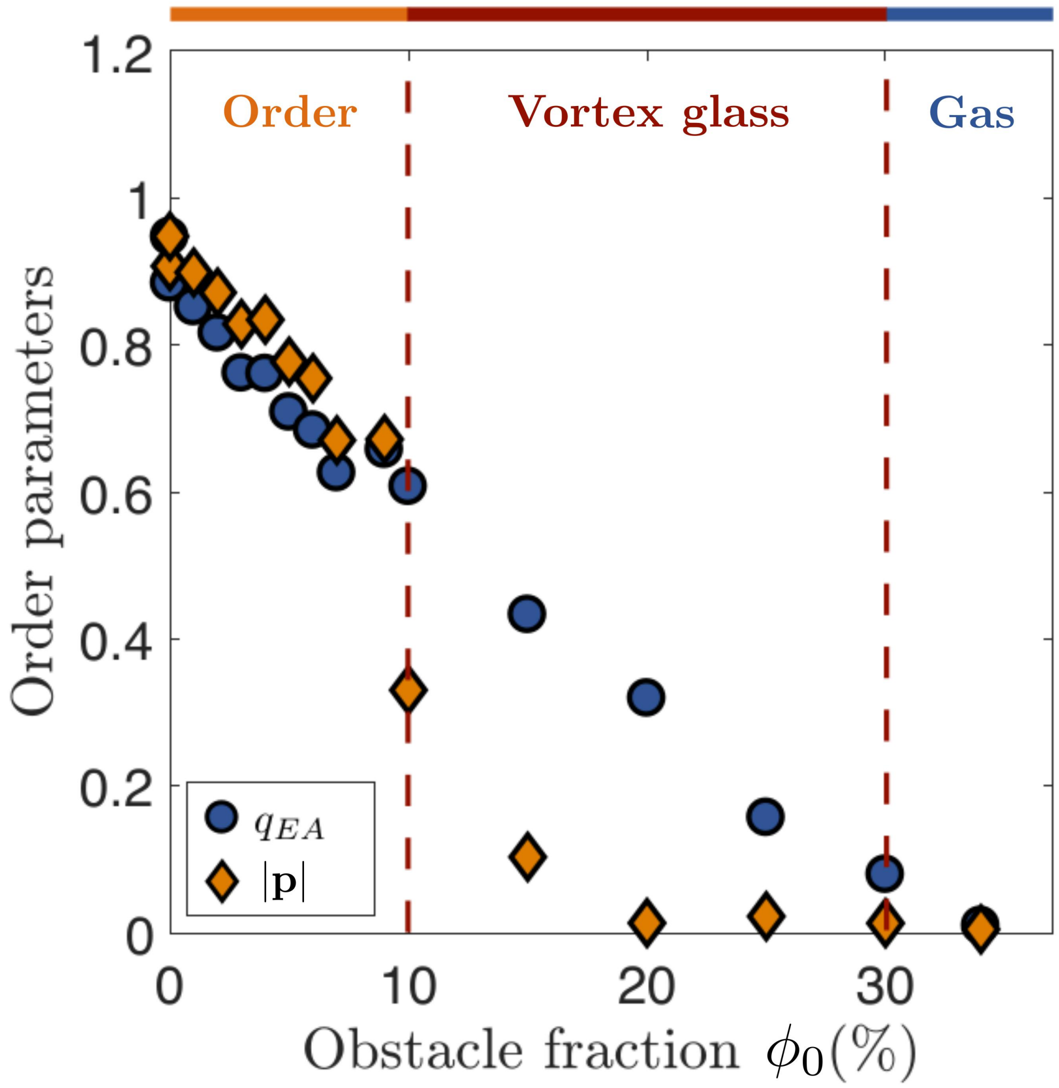
Puzzles

- Loss of long ranged polar order (LRO) by proliferating pinned vortices

- Intermediate phase has finite overlap and persistent collective motion with no net flow.

Why two transitions?
Can we understand it in terms of topological defects?



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Toner - Tu with Quenched Disorder

$$\partial_t \rho + \nabla \cdot \mathbf{p} = 0$$

ρ : Density field

$\mathbf{p} = \rho \mathbf{u}$: Polarization order parameter

active advection

polar order

$$\partial_t \mathbf{p} + \lambda \mathbf{p} \cdot \nabla \mathbf{p} = [a(\rho - \rho_c) - b|\mathbf{p}|^2]\mathbf{p} + K\nabla^2 \mathbf{p} - \chi \nabla \rho - \beta \nabla \Phi$$

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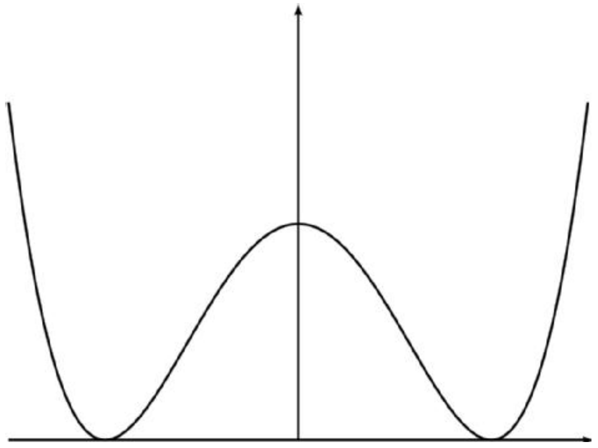
$\rho > \rho_c$



$|\mathbf{p}|$

Double well "potential"

Chardac, Shankar *et al.*, arXiv:2002.12893

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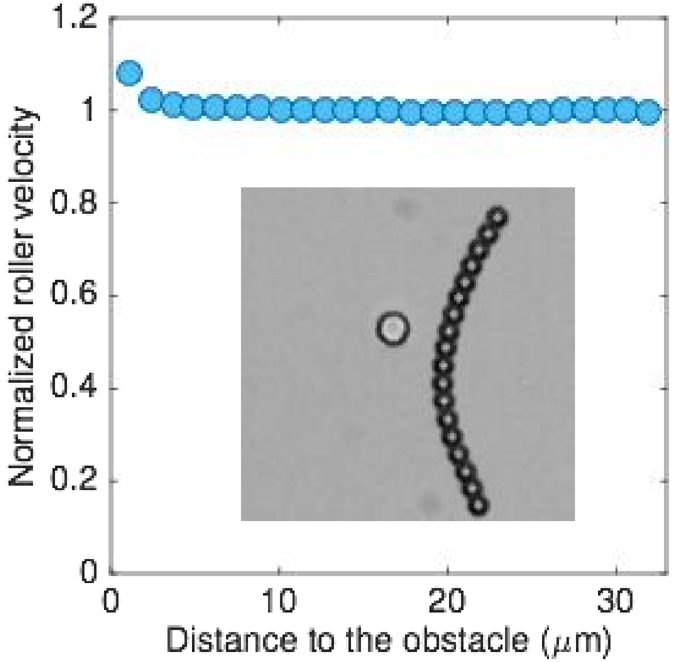
active advection polar order

$$\partial_t \mathbf{p} + \lambda \mathbf{p} \cdot \nabla \mathbf{p} = [a(\rho - \rho_c) - b|\mathbf{p}|^2]\mathbf{p} + K\nabla^2 \mathbf{p} - \chi \nabla \rho - \beta \nabla \Phi$$

quenched obstacles



Obstacles repel at constant speed: potenial disorder!

$$\overline{\nabla \Phi(\mathbf{r}) \nabla' \Phi(\mathbf{r}')} = \phi_0 \nabla \nabla' \delta(\mathbf{r} - \mathbf{r}')$$

Chardac, Shankar *et al.*, arXiv:2002.12893

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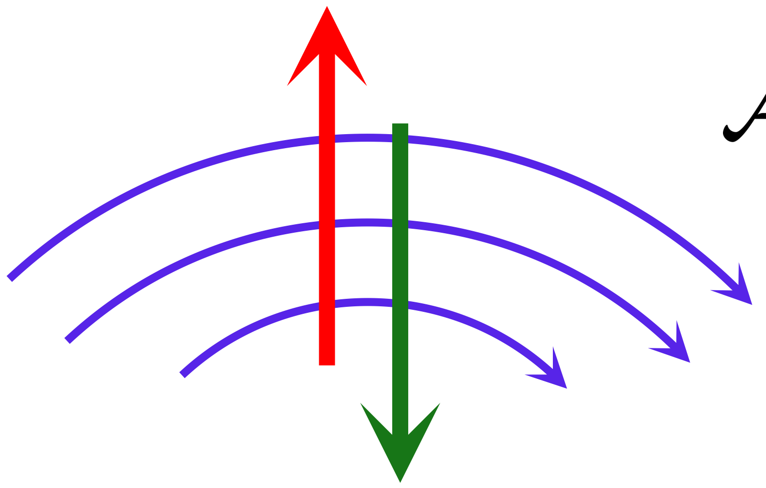
Obstacles create Background Charge

Deep in the ordered state, $|\mathbf{p}| = \text{fixed}$

$$\mathbf{p} = |\mathbf{p}|(\cos\theta, \sin\theta)$$

Balance **advective fluxes** and **pressure fluxes** from disorder

$$\lambda \mathbf{p}\cdot\nabla\mathbf{p} \sim -\beta\nabla\Phi$$



$$\mathcal{A} \equiv [\nabla\theta]_d = -\frac{\beta}{\lambda}\epsilon\cdot(\mathbf{1} - \hat{\mathbf{p}}\hat{\mathbf{p}})\cdot\nabla\Phi$$

$$\mathcal{Q} = \nabla\times\mathcal{A}$$

Map to a random charge problem!!

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Vortex Nucleation & Proliferation

Generalized Kosterlitz-Thouless argument: Elastic penalty versus optimal disorder gain

$$E_{el} = \int \mathrm{d}^2 r K |\nabla\theta|^2 \sim K \ln(R/a)$$

$$E_{dis} = \int \mathrm{d}^2 r K \nabla\theta \cdot \mathcal{A} \sim \frac{\beta\phi_0}{\lambda} K \ln(R/a)$$

→ Nucleating a single vortex is favourable for

$$\phi_0 > \phi_c \sim \lambda/\beta$$

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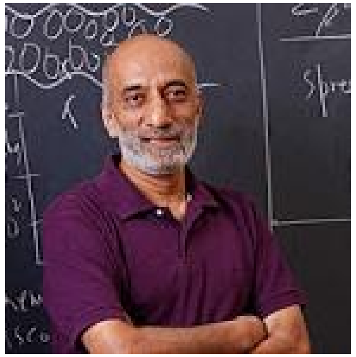

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Thanks!