Continuum Theories of active liquid crystalline fluids

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Scope of today’s talk

- **Pedagogical theory talk**
  - literature, experimental systems not detailed

- **Active fluids: World view and context**

- **Story 1**: active polar fluid (solitary waves)

- **Story 2**: active nematic fluid (defect ordered nematic)

- Things to be done, coming attractions….
Introduction and Context

Traditional non-equilibrium materials

- Driven at the boundary: Macroscopic Drive
- Energy cascades down to the microscale – dissipation/temperature
- Thermodynamics gives me a theoretical handle on what happens

\[ (u=V \text{ at } y=h) \]
\[ (u=0 \text{ at } y=0) \]
Introduction and Context

Active Materials

• Driven at the microscale
• Energy cascades up to the macroscale
• Rules of the game? Design principles?
Introduction and Context

Why should I care?

Interesting from a fundamental point of view:

• Liberation from the constraints of equilibrium

• Need to invent theory – Fluctuation-dissipation, regression etc out the window.

• New Physics: Long range order in 2D, Anamolous fluctuations, Novel instabilities and pattern formation,
Interesting from a more real world point of view:

- Physical Scaffold of Biological Systems
- Properties dynamically changed by coupling to regulation
**Introduction and Context**

**Theoretical paradigm-Symmetry and Hydrodynamics**

- Prototype active fluid: Particles that consume fuel from environment and produce forces

- Classify fluids based on symmetry

- Symmetry of activity

- Symmetry of interactions

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**Diagram Notes:**

- Polar
- Dipolar/Nematic
- Don’t care/isotropic
- Polar

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Partial Order: Mathematics, Simulations and Applications, IPAM, Jan 2016
Introduction and Context

Examples

Polar drive /isotropic interactions

Polar drive /Polar interactions

Nematic drive /Nematic interactions
Story 1: Active Polar Fluid

- Polar activity and polar interactions
- Move through a medium – Force=velocity
- Macroscopic theory – Hydrodynamics

Dynamics of Conserved Quantities and Broken Symmetry Variables

Density of Particles

\[ \rho(r, t) \]

Polarization (Velocity)

\[ P(r, t) \]

\[
\frac{\partial P}{\partial t} + \lambda_1 (P \cdot \nabla P) = -D_R (a_2 + P^2 a_4) P - w_0 \nabla \rho + (D_s - D_b) \nabla (\nabla \cdot P) \\
+ D_b \nabla^2 P + \lambda_2 P (\nabla \cdot P) + \frac{\lambda_3}{2} \nabla P^2
\]

Toner and Tu 1995
Active Polar Fluid

- Start with an equilibrium polar fluid
  \[ \partial_t P = - \frac{\delta F}{\delta P} \]

- Gradient descent dynamics on some free energy landscape

- Under some imposed inhomogeneous flow
  \[ \partial_t P + \lambda_1 (P \cdot \nabla P) = - D_b \nabla (\nabla \cdot P) \]

- Active fluid has self generated flow
  \[ u = \mu_T F_{act} = \lambda P \]
  \[ \omega = \mu_R \tau_{act} = \lambda' \nabla \times P \]
  \[ \llbracket E \rrbracket \sim \mu_S \nabla F_{act} \sim \nabla P \]
Story 1: Active Polar Fluid

- Extensively studied equation that has rich phenomenology

- Applicable to self propelled particle systems with “Vicsek” like interactions – Actin filament motility assay, quinke rotors, chemotactic bacteria, self-propelled rods…. 

- Focus on one particular phenomenon – solitary waves
Story 1: Active Polar Fluid

\[ \partial_t \rho = - \nabla \cdot (w_0 \rho \mathbf{P} - D \nabla \rho) \]

\[ \partial_t \mathbf{P} = - D_R (a_2 + P^2 a_4) \mathbf{P} \]

Low density $a_2 > 0$ and $\mathbf{P} = 0$

High density $a_2 < 0$ and $\mathbf{P} = \sqrt{-\frac{a_2(\rho)}{a_4(\rho)}}$
Story 1: Active Polar Fluid

Stripe Phase

- Not a pattern but rather solitonic wave trains
- Initial conditions determine widths/number of stripes

\[ \partial_t \rho = -\nabla \cdot w_0 \rho P \]

\[ \partial_t \rho P = -w_0 \nabla \rho \]

Recent work along these lines: Solon PRL 2014
Story 1: Active Polar Fluid

Stripe Phase

$\sqrt{\frac{-a_2(\rho_h)}{a_4(\rho_h)}}$

NB: Not a complete story, works only close to the critical point
Story 1: Active Polar Fluid
Story 2: Active Nematic Fluid

Dynamics of Conserved Quantities and Broken Symmetry Variables

Density of Particles

\[ \rho (\mathbf{r}, t) \]

Nematic Order Parameter

\[ Q_{\alpha\beta} (\mathbf{r}, t) = \left\langle \hat{u}_\alpha \hat{u}_\beta - \frac{1}{2} \delta_{\alpha\beta} \right\rangle \]
Story 2 : Active Nematic Fluid

• Start with an equilibrium nematic fluid

\[ \partial_t Q_{\alpha\beta} = -\frac{\delta F}{\delta Q_{\alpha\beta}} \]

• Gradient descent dynamics on some free energy landscape

\[ \partial_t Q_{\alpha\beta} + u \cdot \nabla Q_{\alpha\beta} + \Omega_{\alpha\gamma} Q_{\gamma\beta} - Q_{\alpha\gamma} \Omega_{\gamma\beta} + E_{\alpha\gamma} Q_{\gamma\beta} = -\frac{\delta F}{\delta Q_{\alpha\beta}} \]

• Active fluid has self generated flow

\[ u = \mu T F_{act} = \lambda C \nabla \cdot \langle \vec{Q} \rangle \]

\[ \omega = \mu R \tau_{act} = \lambda R \nabla \times \nabla \cdot \langle \vec{Q} \rangle \]

\[ E_{\alpha\beta} \propto \mu E \lambda \partial_\gamma F_\beta \]
Story 2: Active Nematic Fluid

- The dynamical equation of interest

\[ \partial_t Q_{ij} = -\gamma \frac{\delta F}{\delta Q} + \frac{\lambda_C}{\rho} [\partial_k Q_{kl}] \partial_t Q_{ij} \]

\[ -\frac{\lambda_R}{2\rho} \left( Q_{ik} \partial_k \partial_l Q_{jl} - Q_{ik} \partial_j \partial_l Q_{kl} - Q_{kj} \partial_i \partial_l Q_{kl} + Q_{kj} \partial_k \partial_l Q_{il} \right) \]

- Need dynamics for the density

\[ \partial_t \rho = D \nabla^2 \rho + D_Q \nabla \nabla : Q \]
Story 2: Active Nematic Fluid

- Close to the critical density – “similar phenomenology”
- Symmetry does not allow for propagating waves
- Instead you get bands of nematic high density regions

Story 2 : Active Nematic Fluid

• What happens to the homogeneous nematic state at high densities?

• Onset controlled by the active torque

\[ \psi = \frac{\lambda_R - 2D_\delta}{D_E \cdot f(\rho_0)} > 1 \]

Active torque - (bend-splay)

Goes to zero at the critical point
Story 2: Active Nematic Fluid

- What happens to Random Initial Conditions?

- Initialize in an isotropic state and integrate the equations

![Graph showing defect density vs. bend instability parameter for different densities](image)
Story 2 : Active Nematic Fluid

• Defect Ordered Nematic

Movie 1

Movie 2
Story 2: Active Nematic Fluid

- Turbulent Defective nematic
Coming Attractions/Weird things that real systems do

• The defect order in the experimental system is nematic

• Confinement does weird things: Movie
Summary

• Active fluids sorted by symmetry

• Two stories

• Solitary waves in polar systems

• Defective states in nematic systems

• More things to understand than understood
Active Nematic Fluid – Context

Active nematic suspension

\[ \partial_t Q_{\alpha\beta} + u \cdot \nabla Q_{\alpha\beta} + \Omega_{\alpha\gamma} Q_{\gamma\beta} - Q_{\alpha\gamma} \Omega_{\gamma\beta} + E_{\alpha\gamma} Q_{\gamma\beta} = -\frac{\delta F}{\delta Q_{\alpha\beta}} \]

\[ \nabla^2 u = \nabla \cdot \sigma^{act} \]

\[ \sigma^{act}_{ij} = \alpha Q_{ij} \]

\[ \nabla^2 u + \zeta u = \nabla \cdot \sigma^{act} \]

- Same director dynamics
- Stokes equation
- Same active stress
- Screening/damping
- Same theory with \[ \lambda_C = \lambda_R \]

Many experts in the audience: Marchetti et al, Yeomans et al…
Active Nematic Fluid – Context

Dry Active nematic

\[ \partial_t Q_{ij} = - (\alpha + \beta \text{Tr} (Q^2)) Q_{ij} + \nabla^2 Q_{ij} + \partial_i \partial_j \rho \]

\[ \partial_t \rho = \nabla^2 \rho + \partial_i \partial_j Q_{ij} \]

• This theory with \( \lambda_c = \lambda_R = 0 \)
  \( D_\delta = 0 \)

• Valid close to critical density

• Phase separation, chaos giant number fluctuations

• Unchanged here

Many experts in the audience: Ramaswamy et al, Toner et al, Bertin et al, Aranson et al, Shi et al, Chate et al…