Pressure and phase separation in active matter

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Active matter

Stored energy $\rightarrow$ Mechanical energy

Self-propelled particles
Active matter

Stored energy ➔ Mechanical energy
Self-propelled particles

Found at all scales in living systems

sub-cellular  cellular  macroscopic
Active matter

Stored energy $\rightarrow$ Mechanical energy
Self-propelled particles

Found at all scales in living systems

sub-cellular  cellular  macroscopic

Active matter $=\,$ Assemblies of active particles
Active matter

- **Nonequilibrium** systems (reversed energy cascade) → **Rich phenomenology**
- Simple models → **Universality**
- Numerous experiments
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Vibrated disks

Artificial self-propelled particles

Janus colloids
Active matter

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- **Simple models** → **Universality**
- **Numerous experiments**

- Vibrated disks
- **Artificial self-propelled particles**
- **Janus colloids**

- **Precisely controlled interactions**

- **Bacterial patterns**
- **Robot swarms**
Active matter

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- Simple models → Universality
- Numerous experiments

- Vibrated disks
- Janus colloids
- Artificial self-propelled particles
- Bacterial patterns
- Precisely controlled interactions
- Robot swarms

Smart materials?
Outline

Pressure in active fluids

Motility-induced phase separation
Active forces

Cell cortex

Wound healing
Active forces

Cell cortex  Wound healing

**Much simpler:** active fluid in a box

→ Mechanical pressure
From passive to active pressure

Equilibrium fluid:

\[ P = \frac{F_{\text{wall}}}{S} = - \frac{\text{Tr} \sigma}{d} = - \frac{\partial F}{\partial V} \bigg|_N \]
From passive to active pressure

- Equilibrium fluid:

\[
P = \frac{F_{\text{wall}}}{S} = -\frac{\text{Tr} \sigma}{d} = - \left. \frac{\partial \mathcal{F}}{\partial V} \right|_N = f(\rho_0, T)
\]

extensive \( \mathcal{F} \) ➔ Equation of state
From passive to active pressure

- Equilibrium fluid:
  \[ P = \frac{F_{\text{wall}}}{S} = -\frac{\text{Tr} \sigma}{d} = -\frac{\partial F}{\partial V} \bigg|_N = f(\rho_0, T) \]
  Extensive \( F \) \rightarrow Equation of state

- Active fluid: no free energy
  \[ P = \frac{F_{\text{wall}}}{S} = ? \]
Mechanical pressure: $P = \int_0^\infty dx \rho(x) V'_w(x)$

Particles confined by a potential $V_w$
Mechanical pressure

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Mechanical pressure: $P = \int_0^\infty dx \rho(x) V'_w(x)$

- Ideal gas: $\rho(x) = \rho_0 e^{-V_w(x)/kT}$ $\rightarrow$ $P = \rho_0 kT$
Mechanical pressure

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Mechanical pressure: $P = \int_0^{\infty} dx \rho(x) V'_w(x)$

- Ideal gas: $\rho(x) = \rho_0 e^{-V_w(x)/kT} \rightarrow P = \rho_0 kT$

$P$ independent of $V_w \rightarrow$ Equation of state $P(\rho_0, T)$
ABPs et RTPs

- Constant velocity $v$ (no momentum conservation)
- Two mechanisms for reorientation

Run and Tumble Particles (RTP) Active Brownian Particles (ABP)

$\alpha =$tumble rate  
$D_r =$rotational diffusion
ABPs et RTPs

- Constant velocity $v$ (no momentum conservation)
- Two mechanisms for reorientation

Run and Tumble Particles (RTP) Active Brownian Particles (ABP)

$\alpha =$ tumble rate

$D_r =$ rotational diffusion

- Two effects from the wall

$\Gamma_w \cdot -\nabla V_w = \text{Force} + \text{Torque}$
Ideal active gas

Master equation $\rightarrow$ Compute $P = \int_0^\infty dx \rho(x) V'_w(x)$
Ideal active gas

Master equation $\rightarrow$ Compute $P = \int_0^{\infty} dx \rho(x) V'_w(x)$

Ideal gas: exact expression

$$P = \rho_0 k T_{\text{eff}} - \frac{v}{D_r + \alpha} \int_0^{\infty} dx \int_0^{2\pi} d\theta \Gamma_w(x, \theta) \sin(\theta) P(x, \theta)$$

$$k T_{\text{eff}} = \frac{v^2}{2(D_r + \alpha)}$$
Ideal active gas

Master equation \rightarrow \text{Compute } P = \int_0^\infty dx \rho(x) V'_w(x)

Ideal gas: exact expression

\[ P = \rho_0 kT_{\text{eff}} - \frac{v}{D_r + \alpha} \int_0^\infty dx \int_0^{2\pi} d\theta \Gamma_w(x, \theta) \sin(\theta) \mathcal{P}(x, \theta) \]

\[ kT_{\text{eff}} = \frac{v^2}{2(D_r + \alpha)} \]

- $P$ depends on the interaction with the wall: No equation of state
Self-propelled ellipses

- **Ellipses**, axes $a$ and $b$, rotational diffusion
  
  Harmonic wall $V_w(x) = \lambda \frac{(x-x_w)^2}{2}$

\[
\Gamma_w = \lambda \kappa \sin(2\theta)
\]

\[
\kappa = \frac{a^2 - b^2}{8}
\]

\[
P \approx \rho_0 v^2 \lambda \kappa \left[ 1 - e^{-\lambda \kappa Dr} \right]
\]
Self-propelled ellipses

- **Ellipses**, axes $a$ and $b$, rotational diffusion
  
  Harmonic wall $V_w(x) = \frac{\lambda (x-x_w)^2}{2}$

- **Torque**: $\Gamma_w = \lambda \kappa \sin(2\theta)$
  
  $\kappa = \frac{(a^2 - b^2)}{8}$
Self-propelled ellipses

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- Torque: $\Gamma_w = \lambda \kappa \sin(2\theta)$
  $\kappa = \frac{(a^2 - b^2)}{8}$

\[ P \approx \frac{\rho_0 v^2}{2\lambda \kappa} \left[ 1 - e^{-\frac{\lambda \kappa}{D_t}} \right] \]
When $\Gamma_w$ increases, $P$ decreases

When $\Gamma_w$ increases, $P$ decreases.
Active ideal gas - Summary

- **Spherical** particles ($\Gamma_w = 0$): equation of state

- **Non-spherical** particles $\rightarrow$ Torques $\rightarrow$ No equation of state
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Other ways to lose the equation of state?
Active ideal gas - Summary

- **Spherical** particles ($\Gamma_w = 0$): equation of state
- **Non-spherical** particles $\rightarrow$ Torques
  $\rightarrow$ No equation of state

Other ways to lose the equation of state?

$\rightarrow$ Spherical particles with interactions
Hard-core interactions

![Graph showing the equation of state for hard-core interactions and WCA potential. The graph plots pressure (P) against density (ρ0) for different values of λ (λ = 2, 4, 6, 0.1, 1, 10). The graph includes a line for non-interacting systems.](image-url)
Hard-core interactions

Equation of state
Quorum sensing interactions

$\rho_0$ with $P$ in the range of $0$ to $50$ and $\lambda$ in the range of $0.1$, $1$, and $10$.

Quorum sensing $v(\rho)$, $\rho$ local density.
Quorum sensing interactions

Quorum sensing interactions involve the communication between cells based on their local density. The figure shows the relationship between the local density $\rho$ and the pressure $P$, with different values of $\lambda$. The equation of state is not specified.

No Equation of state
No equation of state
Confusing
Need a simple test
Alignment

No equation of state
No equation of state

Confusing → Need a simple test
A simple test

- Place an asymmetric mobile partition in the middle of a cavity
- Equilibrium $\rightarrow$ the partition is static
A simple test - All cases

Non-interacting spherical ABPs
Non-interacting elliptic ABPs
ABPs interacting via WCA potential
ABPs interacting via $v(\bar{\rho})$

No equation of states $\rightarrow$ Spontaneous compression •
Self-organization at the edges

- Force balance

In equilibrium $F_1 = F_2$
Self-organization at the edges

- Force balance

Active particles $F_1 \neq F_2$
Self-organization at the edges

- Force balance

Active particles $F_1 \neq F_2$

Force exerted by the substrate
Curved walls

Active particles accumulate in curved regions

Curved walls

Active particles accumulate in curved regions

(Di Leonardo et al., PNAS 2010)

Inhomogeneous pressure:

\[ \langle P \rangle \]

Equation of state in average:

\[ J_y = -\mu F_y^{20/33} \]
Curved walls

Inhomogenous pressure:

\[ \langle P \rangle \]

Wall

\[ \text{Equation of state in average} \]
Curved walls

Inhomogenous pressure:

\[ \langle P \rangle \]

Equation of state in average

\[ J_y = -\mu F_y \]

Ratchet

non-universal
Semi-flexible filament in an active bath

Instability for $q < q_i(T, \kappa_s, \kappa_b)$
Free filament

Free filament

Free filament


- Macroscopic motion without external symmetry breaking
- Sorting mechanism
The existence of a "pressure" is not trivial in active systems. 
$P$ depends in general on the probe.
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- $P$ depends in general on the probe.

**Unusual properties**

- Anisotropic pressure: $P(\theta)$ if $\nu(\theta)$
- Inhomogeneous pressure: $P(x)$ if $\nu(x)$
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$P$ depends in general on the probe.

**Unusual properties**
- Anisotropic pressure: $P(\theta)$ if $v(\theta)$
- Inhomogeneous pressure: $P(x)$ if $v(x)$

**Special cases with equation of state**
- Thermodynamics of active systems

- Currents, ratchets, instabilities
Outline

Pressure in active fluids

Motility-induced phase separation
Motility-induced phase separation (MIPS)

Phase separation: dilute/fast vs dense/slow

Buttinoni et al, PRL 2013
Liu et al, Science 2011
Motility-induced phase separation (MIPS)

Phase separation: dilute/fast vs dense/slow

Feedback loop: Collisions/interactions


⇒ Particles slow down ⇒ Increase in density
Motility-induced phase separation (MIPS)

Phase separation: dilute/fast vs dense/slow

Buttinoni et al, PRL 2013
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Feedback loop: Collisions/interactions
\[ \Rightarrow \text{Particles slow down} \Rightarrow \text{Increase in density} \]

Cohesive matter without attractive interactions
Motility-induced phase separation (MIPS)

Phase separation: dilute/fast vs dense/slow

Feedback loop: Collisions/interactions

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Cohesive matter without attractive interactions

How can we understand the phase coexistence?
Microscopic models

Pairwise interactions

\[-\nabla V (r_i - r_j)\]

Fily and Marchetti (PRL 2012), Redner et al (PRL 2013),
Stenhammar et al (PRL 2013), Mallory et al (PRE 2014),
Takatori et al (PRL 2014), Solon et al (PRL 2015)...

Quorum sensing

Tailleur and Cates (PRL 2008), Solon et al (EPJ 2015)

Similar to liquid-gas
phase separation
Microscopic models

Pairwise interactions

\[-\nabla V \left( r_i - r_j \right)\]


Quorum sensing

\[v(\rho)\]

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Microscopic models

Pairwise interactions

$$-\nabla V(r_i - r_j)$$


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$$v(\rho)$$

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Similar to liquid-gas phase separation

Similar to liquid-gas phase separation
Liquid-gas phase separation in equilibrium

Cahn-Hilliard equation

\[ \frac{\partial \rho}{\partial t} = \nabla \cdot M(\rho) \nabla \frac{\delta F[\rho]}{\delta \rho}, \quad F = \int d\vec{r} \left[ f(\rho) + \frac{c(\rho)}{2} |\nabla \rho|^2 \right] \]
Liquid-gas phase separation in equilibrium

Cahn-Hilliard equation

\[
\frac{\partial \rho}{\partial t} = \nabla \cdot M(\rho) \nabla \left[ f'(\rho) + \frac{c'}{2} |\nabla \rho|^2 - c \Delta \rho \right]
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\[ \bar{J} = 0 \implies f'(\rho) + \frac{c'}{2} |\nabla \rho|^2 - c \Delta \rho = \text{Cst.} = \mu \]
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- \( f'(\rho_g) = f'(\rho_\ell) \)
- equality of chemical potential
Liquid-gas phase separation in equilibrium

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  equality of chemical potential

- \(\mu \int_{x_g}^{x_\ell} \nabla \rho \, dx = \int_{x_g}^{x_\ell} f'(\rho) \nabla \rho \, dx + \int_{x_g}^{x_\ell} \left[ \frac{c'}{2} |\nabla \rho|^2 - c \Delta \rho \right] \nabla \rho \, dx = 0\)
Liquid-gas phase separation in equilibrium

Cahn-Hilliard equation

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\[f'(\rho_g) = f'(\rho_\ell)\]

equality of chemical potential

\[\mu(\rho_\ell - \rho_g) = f(\rho_\ell) - f(\rho_g)\]

equality of pressure \( P = \rho f' - f \)
Cahn-Hilliard equation

$$\frac{\partial \rho}{\partial t} = \nabla \cdot M(\rho) \nabla \left[ f'(\rho) + \frac{c'}{2} |\nabla \rho|^2 - c \Delta \rho \right]$$

$$\bar{J} = 0 \implies f'(\rho) + \frac{c'}{2} |\nabla \rho|^2 - c \Delta \rho = \text{Cst.} = \mu$$

- $f'(\rho_g) = f'(\rho_\ell)$
  equality of chemical potential

- $\mu(\rho_\ell - \rho_g) = f(\rho_\ell) - f(\rho_g)$
  equality of pressure $P = \rho f' - f$
Nonequilibrium phase separation

Most general for a scalar conserved field

\[
\frac{\partial \rho}{\partial t} = \nabla \cdot M(\rho) \nabla \left[ \mu_0(\rho) + \lambda(\rho) |\nabla \rho|^2 - \kappa(\rho) \Delta \rho \right]
\]
Nonequilibrium phase separation

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- \[\mu_0(\rho_g) = \mu_0(\rho_\ell)\]
  equality of chemical potential
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- \( \mu_0(\rho_g) = \mu_0(\rho_\ell) \)
  
  equality of chemical potential

- \( \mu(\rho_\ell - \rho_g) = f(\rho_\ell) - f(\rho_g) + \int_{x_g}^{x_\ell} \left[ \lambda |\nabla \rho|^2 - \kappa \Delta \rho \right] \nabla \rho \, dx \)

\[ \frac{df}{d\rho} = \mu_0 \]

\( \neq 0 \)
Nonequilibrium phase separation

Most general for a scalar conserved field

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\frac{\partial \rho}{\partial t} = \nabla \cdot M(\rho) \nabla \left[ \mu_0(\rho) + \lambda(\rho) |\nabla \rho|^2 - \kappa(\rho) \Delta \rho \right]
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- \[\mu_0(\rho_g) = \mu_0(\rho_\ell)\]
  equality of chemical potential

- \[\mu(\rho_\ell - \rho_g) = f(\rho_\ell) - f(\rho_g) + \int_{x_g}^{x_\ell} [\lambda |\nabla \rho|^2 - \kappa \Delta \rho] \nabla \rho \, dx\]
  \[\frac{df}{d\rho} = \mu_0\]
  Uncommon tangent construction
Generalized thermodynamic constructions

\[ \mu = \mu_0(\rho) + \lambda(\rho) |\nabla \rho|^2 - \kappa(\rho) \Delta \rho \]

\[ \mu \int_{x_g}^{x_l} \nabla \rho \, dx = \int_{x_g}^{x_l} \mu_0(\rho) \nabla \rho \, dx + \int_{x_g}^{x_l} \left[ \lambda(\rho) |\nabla \rho|^2 - \kappa(\rho) \Delta \rho \right] \nabla \rho \, dx \]
Generalized thermodynamic constructions

\[ \mu = \mu_0(\rho) + \lambda(\rho)|\nabla \rho|^2 - \kappa(\rho)\Delta \rho \]

\[ \mu \int_{x_g}^{x_\ell} \nabla R \, dx = \int_{x_g}^{x_\ell} \mu_0(\rho) \nabla R \, dx + \int_{x_g}^{x_\ell} [\lambda(\rho)|\nabla \rho|^2 - \kappa(\rho)\Delta \rho] \nabla R \, dx \]

Effective density \( R(\rho) \) s.t. \( R'' = -\frac{2\lambda + \kappa'}{\kappa} R' \)
Generalized thermodynamic constructions

\[
\mu = \mu_0(\rho) + \lambda(\rho)|\nabla \rho|^2 - \kappa(\rho) \Delta \rho
\]

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\mu \int_{x_g}^{x_\ell} \nabla R \, dx = \int_{x_g}^{x_\ell} \mu_0(\rho) \nabla R \, dx + \int_{x_g}^{x_\ell} [\lambda(\rho)|\nabla \rho|^2 - \kappa(\rho) \Delta \rho] \nabla R \, dx
\]

Effective density \( R(\rho) \) s.t. \( R'' = \frac{-2\lambda + \kappa'}{\kappa} R' \)

\[
\mu (R_\ell - R_g) = \phi(R_\ell) - \phi(R_g), \quad \frac{d\phi}{dR} = \mu_0
\]

Common tangent construction
Generalized thermodynamic constructions

\[ \mu = \mu_0(\rho) + \lambda(\rho)|\nabla \rho|^2 - \kappa(\rho) \Delta \rho \]

\[ \mu \int_{x_g}^{x_\ell} \nabla R \, dx = \int_{x_g}^{x_\ell} \mu_0(\rho) \nabla R \, dx + \int_{x_g}^{x_\ell} [\lambda(\rho)|\nabla \rho|^2 - \kappa(\rho) \Delta \rho] \nabla R \, dx \]

Effective density \( R(\rho) \) s.t. \( R'' = -\frac{2\lambda + \kappa'}{\kappa} R' \)

\[ \mu(R_\ell - R_g) = \phi(R_\ell) - \phi(R_g), \quad \frac{d\phi}{dR} = \mu_0 \]

Common tangent construction

Thermodynamic pressure:
\[ P = \mu_0 R - \phi \rightarrow \text{Equal-area construction} \]
Quorum sensing interactions

Particles moving at velocity $v(\rho)$

$$\frac{\partial \rho}{\partial t} = \nabla \cdot M(\rho) \nabla \left[ \mu_0(\rho) - \kappa(\rho) \Delta \rho \right], \quad \mu_0 = \log(\rho v), \quad \kappa(\rho) = -\ell^2 \frac{v'}{v}$$
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$\implies$ effective density $R(\rho) = -\int^\rho \frac{1}{\kappa(u)} du$
Quorum sensing interactions

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$$\frac{\partial \rho}{\partial t} = \nabla \cdot M(\rho) \nabla \left[ \mu_0(\rho) - \kappa(\rho) \Delta \rho \right], \quad \mu_0 = \log(\rho v), \quad \kappa(\rho) = -\ell^2 \frac{v'}{v}$$

$\implies$ effective density $R(\rho) = -\int_\rho^\infty \frac{1}{\kappa(u)} du$
Pairwise interactions

- More difficult. **No expression for the interfacial terms.**
  → measured numerically

![Graph showing pairwise interactions](image)

- Equation (11)
- Equilibrium

(b) Simulations
- Eq. (11)
- Equilibrium
Conclusions

- MIPS described by a generalized Cahn-Hilliard equation including non-equilibrium interfacial terms
- Equilibrium relations are recovered after defining an effective density
- The phase diagram depends on the interfacial terms
References

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- Joakim Stenhammar (Lund)
- Raphael Wittkowski (Dusseldorf)
- Aparna Baskaran (Brandeis)
- Yaouen Fily (Brandeis)

Pressure is not a state function for generic active fluids
Solon, Fily, Baskaran, Cates, Kafri, Kardar, Tailleur

Pressure and Phase Equilibria in Interacting Active Brownian Spheres
Solon, Stenhammar, Wittkowski, Kardar, Kafri, Cates, Tailleur

Active particles on curved surfaces: Equation of state, ratchets, and instabilities
Nikola, Solon, Kafri, Kardar, Tailleur, Voituriez

Generalized Thermodynamics of Phase Equilibria in Scalar Active Matter
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Thank you for your attention