3f

* In experiments:

- Enhanced tendency for clustering: [Theurkauff et al, PRL 108, 268303 (2012); Palacci et al., Science 339, 936 (2013)]
- Phase separation: [Buttinoni et al., PRL 2013, 110, 238301]
- self-propelled Janus colloids
- Bacterial colonies: [Liu et al, PRL 122, 248102, (2019)]
- Quincke rollers: [Geyer et al, PRX 9, 031043 (2019)]
  Coexistence between ordered polar active liquid & an arrested solid.

II The instability Mechanism

ABP's or RTP's interacting via quorum-sensing interaction $v(\rho(r))$

① Active particles accumulate where they go slower

feed back loop

② Interactions that slow down self-propulsion

II.1) Spatially varying $v(\vec{r})$

2D, periodic boundary conditions

$$\partial_t P(\vec{r},\theta) = -\vec{\nabla}_{\vec{r}} \cdot \left[v(r)\, \vec{u}(\theta)\, P(\vec{r},\theta,t)\right] + \text{isotropic reorientation terms } \Theta \cdot P$$

ABPs: $\textcircled{H} P = D_r \partial_{\theta\theta} P(\vec{r},\theta)$

RTPs: $\textcircled{H} P = -\alpha P(\vec{r},\theta) + \alpha \int \frac{d\theta'}{2\pi} P(\vec{r},\theta')$

Steady-state $\partial_t P(\vec{r},\theta) = 0$

$\textcircled{\alpha}$ $P(\vec{r},\theta) = f(\vec{r})$ then $\textcircled{H} P = 0$

$\textcircled{\beta}$ $\vec{\nabla}_{\vec{r}} \cdot \left[v(\vec{r})\, \vec{u}(\theta) f(\vec{r}) \right] = 0 \Rightarrow f(\vec{r}) = \frac{K}{v(\vec{r})}$

$$\vec{\nabla}_{\vec{r}} \cdot \Big[\underbrace{K \vec{u}(\theta)}_{\text{no } \vec{r}\text{-dependency}} \Big] = 0$$

$\Rightarrow$ Steady-state $\boxed{P_{ss}(\vec{r},\theta) = \frac{K}{v(\vec{r})}}$

Active particles spend more time when they go slowly

Experiments on light controlled bacteria:

[Frangipane et al, elife 7, e 36608 (2018)]

[Arlt et al, Nat. Com. 9, 1 (2018)]

II.2) From repulsive forces to kinetic slow down

Sometime, interactions between active particles directly lead to a self propulsion speed that depends on the local density: competition for food, quorum-sensing interactions among cells, etc.

[Liu et al, Science 334, p238, (2011)]
[Curatolo et al, Nat. Phys 16, p1152, (2020)]

$\Rightarrow$ model $\dot{\vec{r}}_i = v(\vec{r}_i, [\rho])\,\vec{u}(\theta_i) + \cdots$

Repulsive forces: a mean-field picture

$$\dot{\vec{r}}_i = v_0\,\vec{u}(\theta_i) + \vec{F}_i \;; \quad \vec{F}_i = -\sum_j \vec{\nabla}_{\vec{r}_i} V(\vec{r}_i - \vec{r}_j)$$

$$= \underbrace{\left[v_0 + \vec{F}_i \cdot \vec{u}(\theta_i)\right]\vec{u}(\theta_i)}_{=\text{“}v(\rho)\text{”}\,\vec{u}(\theta_i)} + \underbrace{\left(1 - \vec{u}(\theta_i)\,\vec{u}(\theta_i)\right)\vec{F}_i}_{+\,0}$$

MF + neglect 2nd term.

Repulsive forces lead to a decrease of $v(\rho)$ as

Numerics:

$$v(\rho) \simeq v_0\left(1 - \frac{\rho}{\rho^*}\right)$$ [Fily et al, PRL 2012]

ρ^* ← crowding density

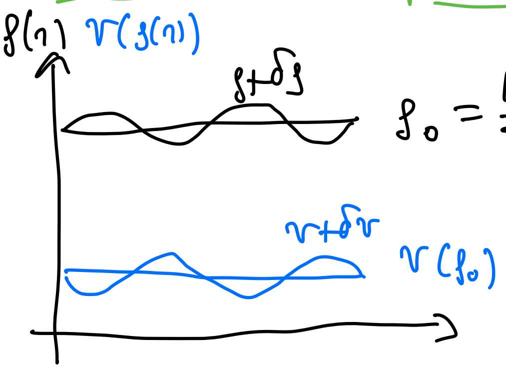
$\Rightarrow$ qualitatively, one can try to model repulsive interactions as quorum-sensing

→ captures MIPS

→ misses lots of things

II.3) The instability mechanism

Feed back loop leading to MIPS:



$\rho_0 = \frac{K}{v_0}$

Perturbation $\rho(r) = \rho_0 + \delta\rho(r)$

$\delta\rho(r) \ll \rho_0$

Since $v(\rho(r)) = v(\rho_0) + \delta v(r)$

$= v(\rho_0) + v'(\rho_0)\,\delta\rho$

Q: where does $\rho(\vec r)$ wants to relax?

$\rho(\vec r)$ is a conserved field $\Rightarrow$ its evolution on large scales is slow

Locally particles want to relax towards $\rho(\vec r) \propto \frac{K}{v(\vec r)}$

$$\frac{K}{v(\rho(r))} = \frac{K}{v(\rho_0)+v'(\rho_0)\delta\rho} = \frac{K}{v(\rho_0)}\cdot\frac{1}{1+\frac{v'}{v}\delta\rho} = \underbrace{\frac{K}{v(\rho_0)}}_{\rho_0}\left(1 - \frac{v'(\rho_0)}{v(\rho_0)}\delta\rho\right)$$

Start from $\rho_0 + \delta\rho$; relax to $\rho_0 - \frac{v'(\rho_0)}{v(\rho_0)}\rho_0\,\delta\rho$

if $|\delta\rho| < \left|-\frac{v'}{v}\rho_0\,\delta\rho\right| \Rightarrow$ perturbation is amplified $\Rightarrow$ instability

linear instability criterion: $\boxed{\frac{v'(\rho_0)}{v(\rho_0)} < -\frac{1}{\rho_0}}$

$\Longleftrightarrow \frac{d}{d\rho_0}\ln[v(\rho_0)\rho_0] < 0 \Leftrightarrow \boxed{\frac{d}{d\rho_0}\rho_0 v(\rho_0) < 0}$

Conclusion: When $v'(\rho_0)$ is sufficiently negative, this hand-waving argument predicts a linear instability. 42

Q: ① can we show this more seriously?
② where does this leads to?

$\Rightarrow$ Build hydrodynamic theory
① for $v(r)$ slowly varying in space
② generalize to $v(r,[\rho])$

III Coarse-grained description of RTPs

III.1) Large-scale diffusive approximation ($v(\vec{r})$)

$P(\vec{r},\theta)$ too much info

$\psi(\vec{r}) = \int d\theta\, P(\vec{r},\theta)$ proba to find the part at $\vec{r}$.

$$\boxed{\partial_t P(\vec{r},\theta) = -\vec{\nabla}\cdot\left[v(\vec{r})\,\vec{u}(\theta)\,P(\vec{r},\theta)\right] - \alpha P(\vec{r},\theta) + \frac{\alpha}{2\pi}\psi(\vec{r})} \qquad (1)$$

$\int (1)\, d\theta$: $\partial_t \psi(\vec{r}) = -\vec{\nabla}\cdot\left[v(\vec{r}) \underbrace{\int d\theta\, \vec{u}(\theta) P(\vec{r},\theta)}_{\equiv \vec{m}(\vec{r})}\right] \underbrace{-\alpha\psi + \alpha\psi}_{0}$

$$\boxed{\partial_t \psi = -\vec{\nabla}\left[v(\vec{r})\,\vec{m}(\vec{r})\right] \quad (2)}$$

$\int (1)\, u_i(\theta)\, d\theta \Rightarrow \partial_t m_i(\vec{r}) = -\partial_j\left[v(\vec{r})\int u_j u_i P\, d\theta\right] - \alpha m_i + 0 \qquad (3)$

$$\int d\theta\, u_j u_i P = \underbrace{\int d\theta \left(u_i u_j - \frac{\delta_{ij}}{2}\right) P}_{Q_{ij}(\vec{r})} + \underbrace{\int d\theta\, \frac{\delta_{ij}}{2} P}_{\frac{1}{2}\psi(\vec{r})}$$

$$(3): \quad \boxed{\partial_t m_i = -\partial_j\left[v(\vec r)\, Q_{ij}(\vec r)\right] - \partial_i\left[\frac{v(r)}{2}\Psi\right] - \alpha m_i} \quad (4)$$

$$\partial_t Q_{ij} = -\alpha Q_{ij} - \partial_h\,[\text{stuff}]$$

Comments: what do $m(\vec r)$ and $Q(\vec r)$ measure?

$$\Psi = \int d\theta\, P \; ; \quad \vec m = \int d\theta\, \vec u(\theta)\, P \; ; \quad Q_{ij} = \int d\theta \left(u_i u_j - \frac{\delta_{ij}}{2}\right) P$$

$$P = f(r) \Rightarrow \Psi = 2\pi f(r) \; ; \quad \vec m = 0 \; ; \quad Q_{ij} = 0$$

$$P = f(r)\,\delta(\theta-\theta_0) \Rightarrow \Psi = f(r) \; ; \quad \underbrace{\vec m = f(\vec r)\,\vec u(\theta_0)}_{\text{magnetisation}} \; ; \quad Q = \frac{f(r)}{2}\begin{pmatrix} \cos 2\theta_0 & \sin 2\theta_0 \\ \sin 2\theta_0 & -\cos 2\theta_0 \end{pmatrix}$$

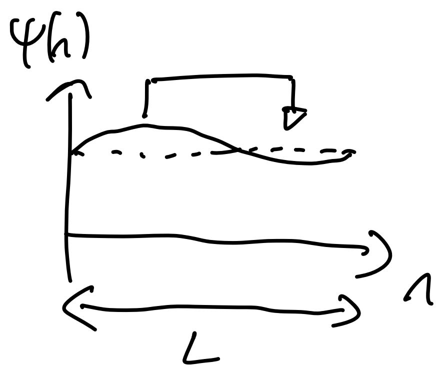
$$P = f(r)\left[\delta(\theta-\theta_0) + \delta(\theta-\theta_0+\pi)\right]$$

$$\Psi = 2 f(r) \; ; \quad \vec m = \vec 0 \; ; \quad Q = \frac{f(r)}{2}\begin{pmatrix} \cos 2\theta_0 & \sin 2\theta_0 \\ \sin 2\theta_0 & -\cos 2\theta_0 \end{pmatrix}$$

$\Psi \to$ local density ; $Q \to$ local nematic order

$\vec m \to$ local magnetisation

Comments: slow and fast fields



$$\boxed{\partial_t \Psi = -\vec\nabla\cdot\left[v(\vec r)\, \vec m(\vec r)\right] \quad (2)}$$

Ψ conserved field $\Rightarrow$ relaxation time diverges with L

$$\partial_t \vec m = -\alpha \vec m + \vec\nabla\cdot[\dots] \qquad (1')$$

4€

$$\underbrace{\partial_t \bar{\bar{Q}}}_{} = -\alpha \bar{\bar{Q}} + \vec{\partial}\cdot[\cdots] \qquad (2')$$

relaxation time $\propto \frac{1}{\alpha}$ finite $\Rightarrow$ on large time scale, $\vec{m}$ & $\bar{\bar{Q}}$ relax to values that are enslaved to $\psi(\vec{r})$

$$(2') \Leftrightarrow 0 = -\alpha \bar{\bar{Q}} + \vec{\partial}\cdot[\cdots] \Rightarrow \bar{\bar{Q}} \sim \mathcal{O}(\nabla)$$

$$(1') \Rightarrow \alpha \vec{m} = -\underbrace{\vec{\partial}\cdot[v \bar{\bar{Q}}]}_{\sim \mathcal{O}(\nabla^2)} - \vec{\partial}\left[\frac{v}{2}\psi(\vec{r})\right] \Rightarrow \boxed{\vec{m}(\vec{r}) = -\vec{\nabla}\left[\frac{v(\vec{r})}{2\alpha}\psi(\vec{r})\right]}$$

$$(1+2) \Rightarrow \boxed{\partial_t \psi(\vec{r}) = \vec{\nabla}\cdot\left[v(\vec{r})\,\vec{\nabla}\left[\frac{v(\vec{r})}{2\alpha}\psi(\vec{r})\right]\right]}$$

$$= \vec{\nabla}\cdot\left[\underbrace{\frac{v^2}{2\alpha}\vec{\nabla}\psi}_{\text{diffusion term}} + \underbrace{\frac{v\vec{\nabla}v}{2\alpha}\psi}_{\text{drift driving particles against } \vec{\nabla}v}\right]$$

Inhomogeneous $v(\vec{r})$

steady-state $\psi(\vec{r}) \propto \frac{1}{v(\vec{r})}$ $\qquad \left[J = \frac{v}{2\alpha}\vec{\partial}(v\psi)\right]$

Langevin: $\partial_t \psi = \vec{\nabla}\left[\vec{\nabla}\left(\frac{v^2}{2\alpha}\psi\right) - \frac{v\vec{\nabla}v}{2\alpha}\psi\right]$

At large times (vs $\frac{1}{\alpha}$), the run and tumble dynamics is equivalent to a Langevin equation:

$$\boxed{\dot{\vec{r}}_i = F(\vec{r}_i) + \sqrt{2D(\vec{r}_i)}\,\vec{\eta}_i}$$

when $D(\vec{r}) = \frac{v^2(\vec{r})}{2\alpha(\vec{r})}$; $F = \frac{v\vec{\nabla}v}{2\alpha} = \frac{1}{2}\vec{\nabla}D$

Comment: * In the Ito formalism, F leads to large v } D wins.
D —— small v }

less transparent...

* Strato leads to $\vec{F} = 0$ ooo

III.2) Collective dynamics of N RTPs

A) Non-interacting in the presence of $v(x)$ in 1D

$$\rho(x,t) = \sum_{i=1}^{N} \delta(x - x_i(t))$$

← sole time dependency of ρ with time

From $\dot{x}_i = \underbrace{F(x_i)}_{=\frac{1}{2}\partial_x D} + \sqrt{2D(x_i)}\,\eta_i \xrightarrow{\text{stochastic calculus}} \frac{d}{dt}\rho(x,t)$

$$\dot{\rho}(x,t) = -\partial_x\Big[\underbrace{\rho(x,t)\,F(x)}_{\frac{1}{2}\rho\,\partial_x D(x)} - \partial_x\big(D(x)\,\rho(x)\big) + \Lambda(x,t)\Big] \qquad (*)$$

← GWN field

$\langle \Lambda(x,t)\rangle = 0$

$\langle \Lambda(x,t)\,\Lambda(x',t')\rangle = 2D(x)\,\rho(x)\,\delta(x-x')\,\delta(t-t')$

$$= -\partial_x\Big[-\frac{1}{2}\rho(x)\,D'(x) - D(x)\,\rho'(x) + \Lambda(x,t)\Big]$$

$$= \partial_x\Big[\rho(x)\,D(x)\Big[\frac{1}{2}\frac{D'(x)}{D(x)} + \frac{\rho'(x)}{\rho(x)}\Big] + \sqrt{2D(x)\,\rho(x)}\,\xi(x,t)\Big] \qquad \langle\xi\rangle = 0$$

$\langle \xi(x,t)\,\xi(x',t')\rangle = \delta(x-x')\,\delta(t-t')$

$$= \partial_x\Big[\rho(x)\,D(x)\,\partial_x\Big[\underbrace{\ln\sqrt{D(x)} + \ln\rho(x)}_{\mu}\Big] + \sqrt{2D(x)\,\rho(x)}\,\xi(x,t)\Big]$$

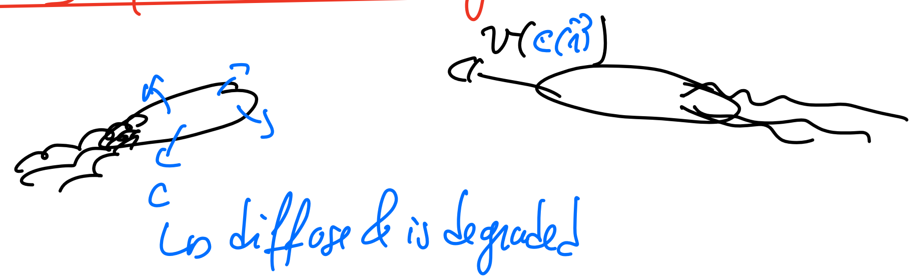
$$(*) \Leftrightarrow \dot{\rho} = +\partial_x\Big[\rho D\,\partial_x\mu + \sqrt{2\rho D}\,\xi(x,t)\Big] \qquad (**)$$

If $\boxed{\mu = \frac{\delta \hat{f}}{\delta \rho}}$ then (**) is an equilibrium theory with flux-free steady-state distribution and $P \propto e^{-\hat{f}}$

$$\boxed{\text{Here: } \mu = \frac{\delta \hat{f}}{\delta \rho} \; ; \; \hat{f} = \int dx \; \underbrace{\rho(\ln \rho - 1)}_{-\text{ entropy}} + \underbrace{\rho(x) \ln \sqrt{D(x)}}_{\text{potential energy}}}$$

$D(x) = \frac{v^2}{2\alpha}$

B) Quorum-sensing interactions



adapt v to concentration of c.

$$\dot{\vec{r}}_i = v\left(c(\vec{r}_i)\right) \vec{u}(\theta_i)$$

$$\dot{c}(\vec{r}) = \underbrace{D_c \Delta c(\vec{r})}_{\text{diff.}} \underbrace{- \gamma C(\vec{r})}_{\text{degradation}} + \underbrace{\beta \rho(\vec{r}, t)}_{\text{production}}$$

Fast-variable treatment on $c \Rightarrow c(\vec{r}, [\rho])$

[O'Byrne, Tailleur, PRL 2020]

$\dot{c} = 0 \Rightarrow c = G * \rho$ where $D_c \Delta G - \gamma G = -\beta \delta(\vec{r})$

$$G * \rho(x) = \int dx' G(x') \rho(x - x') = \int dx' G(x') \sum_n \frac{(-x')^n}{n!} \rho^{(n)}(x) \simeq \sum_n c_n (\partial_x)^n \rho(x)$$

① local approximation $c \propto \rho \Rightarrow v(\vec r,[\rho]) = v(\rho(\vec r))$

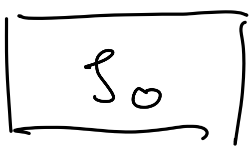
Again $\mu = \dfrac{\delta \hat F}{\delta \rho}$; $\hat F = \int dx \, \underbrace{f(\rho(x))}_{\text{free energy density}}$

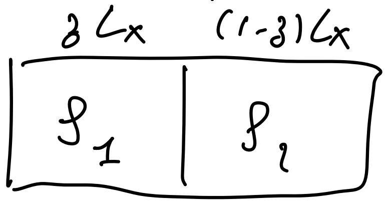
$$f(\rho) = \rho(\ln \rho - 1) + \int^{\rho} ds \, \ln v(s) + c^{st} \cdot \rho$$

Within this approximated framework, we know everything $\Rightarrow$ condition for phase separation.

$P[\rho] \propto e^{-\hat F[\rho]} \Rightarrow$ which ρ extremalizes $\hat F$?

$\rho(\vec r, t) = \rho_0$ vs $\rho(\vec r, t)$ phase-separated

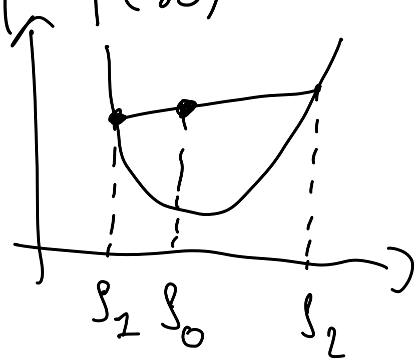




$\hat F = L^d f(\rho_0)$

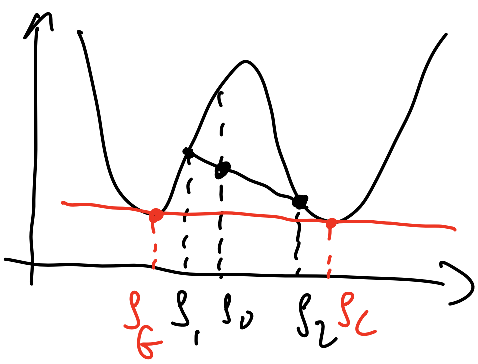
$\hat F = L^d \left[\xi f(\rho_1) + (1-\xi) f(\rho_2) \right]$

If $f(\rho_0)$ convex, $f(\rho_0) < \xi f(\rho_1) + (1-\xi) f(\rho_2)$



$\Rightarrow$ Homogeneous

Otherwise



$$f(\rho_0) > z\, f(\rho_1) + (1-z)\, f(\rho_2)$$

non-convex $\Rightarrow$ phase separation

When does this stop?

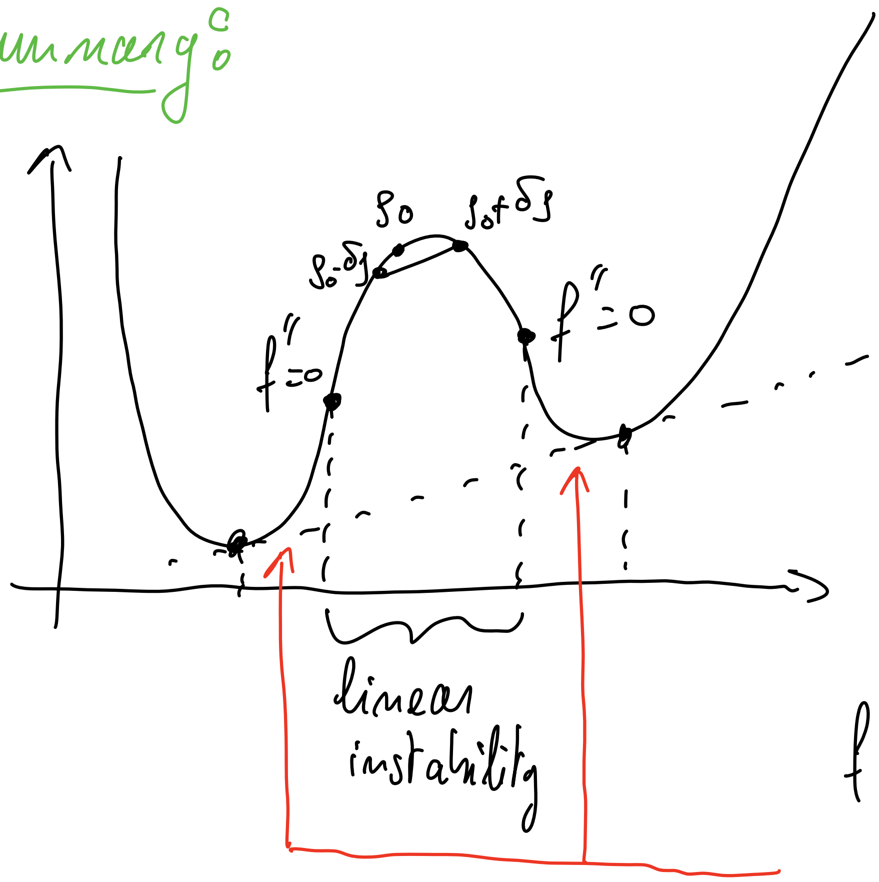
Common-tangent construction.

Non-convexity : interval such that $f''(\rho) < 0$

$$\Leftrightarrow \frac{v'}{v} + \frac{1}{\rho} < 0$$

hand-waving argument was right!

Summary:



$f''>0 \Rightarrow$ no linear instability

$\Rightarrow$ nucleation

Looks all good but ... phase separation ⇒ interface
⇒ higher order gradients
⇒ generically breaks equilibrium mapping.

② Semi-local approximation

$\dot{c}(\vec{r},t) = D_c \Delta c - \gamma c + \beta \rho(\vec{r},t)$

$r \equiv \sqrt{\frac{D_c}{\gamma}} \sim$ how far c diffuses before dying out.

gradient expansion: $c = c_0 + c_2 \Delta \rho$

$$= \frac{\beta}{\gamma}\rho + \frac{D_c \beta}{\gamma^2}\Delta\rho = \frac{\beta}{\gamma}\left(\rho + \frac{D_c}{\gamma}\Delta\rho\right)$$

$$v(c) \to v\left(\rho + \frac{D}{\gamma}\Delta\rho\right) \simeq v(\rho) + r^2 \Delta\rho \, v'(\rho)$$

$$\ln v = \ln v(\rho) + \frac{v'(\rho)}{v(\rho)} r^2 \Delta\rho$$

dynamics of $\rho(\vec{r},t)$

$$\partial_t \rho = \vec{\nabla}\cdot\left[\rho D \vec{\nabla}\left[\ln\rho + \ln v(\rho) - K(\rho)\Delta\rho\right] + \sqrt{2\rho D}\,\xi\right]$$

$$-K(\rho)\Delta\rho \overset{?}{=} \frac{\delta \hat{f}_\Delta}{\delta\rho} \to \text{No}$$

Non-eq gradient terms break detailed balance

Eq. theory: qualitatively right, but quantitatively wrong regarding e.g. coexisting densities.

Generalized free energy:

Change of variable $R(\rho)$ such that $R'(\rho) \equiv \frac{1}{\kappa(\rho)}$

Then $\mu = \frac{\delta \hat{f}[R]}{\delta R}$; $\hat{f}[R] = \int d^d r \, \Phi(R(\rho(\vec{r}))) + \frac{\kappa}{2\kappa'} (\nabla R)^2$

$$\frac{d\Phi}{dR} = \ln\left[\rho(R)\, v(\rho(R))\right]$$

Common-tangent construction on $\Phi(R)$ works!

[Solon et al, NJP 2018]

Summary:

$$\text{QSAPs} \xrightarrow[\text{long-time dynamics}]{\text{gradient expansion}} \text{Stochastic PDE for } \rho(\vec{r},t)$$

$$\big\downarrow \text{ Mean-field treatment}$$

$$\text{Lattice-based models} \xrightarrow{\text{exact}} \text{Phase diagram}$$

[M. Kourbane-Houssene, PRL 120, 268003 (2018)]

Still a lot of questions:

→ beyond mean-field
→ coarsening dynamics
→ pairwise forces much harder / richer
etc...