ACTIVE MODEL B

Michael Cates (Edinburgh Univ.) KITP Mar 13, 2014

Motility-induced phase separation

Density-dependent swim speed

Free energy mapping for local $v(\rho)$

J Tailleur + MEC, PRL 100, 208301 (2008); EPL 101, 20010 (2013)

Gradient terms: No free energy mapping

Coarsening kinetics surprisingly unaltered

Phase coexistence surprisingly altered

Minimal ϕ^4 model : Active Model B

J Stenhammar, A Tiribocchi, D. Marenduzzo, R. Allen + MEC, PRL 111, 145702 (2013)

J Stenhammar et al, Soft Matter (2014) in press

R Wittkowski et al, arXiv:1311.1256

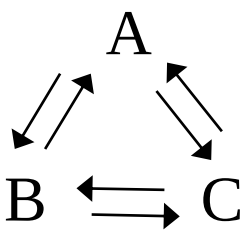
+ work in progress

Active vs Passive Matter

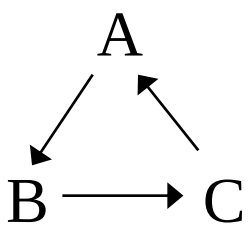
Detailed Balance = Time Reversal Symmetry

Restored for steady state in isolated system

With DB



Without DB



Unique Boltzmann SS

Evaluate $Z = \Sigma \exp[-\beta H]$

Minimize $\beta F = -\log Z$

Find SS by hand

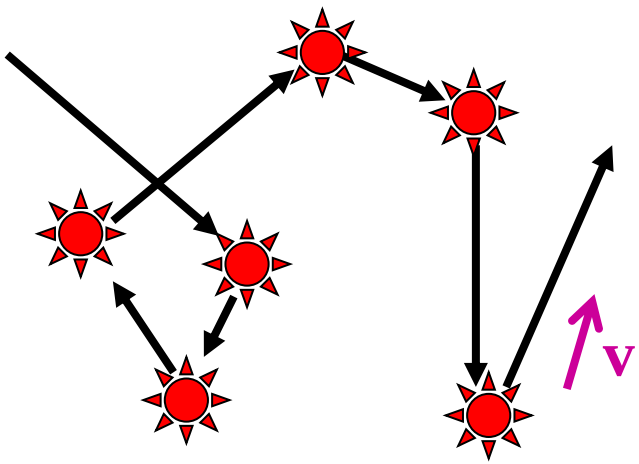
Map onto DB if lucky

Few general principles

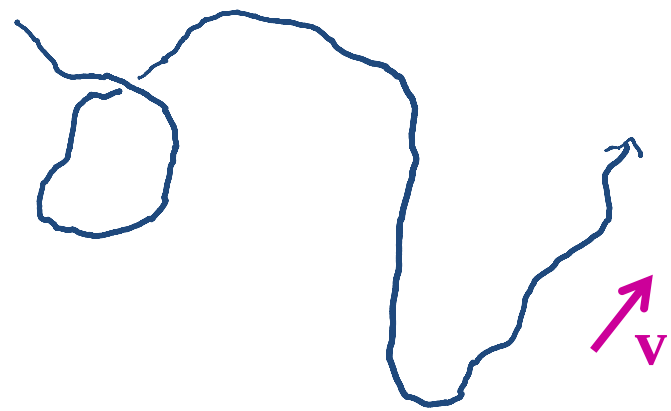
e.g. Brownian motion

e.g. bacterial swimming

Bacteria = RTPs vs ABPs = Synthetic swimmers



swim speed v, tumble rate α



swim speed v, rotational diffusivity D_r

Coarse Graining ⇒ Random walks in d dimensions

$$D = \frac{v^2 \tau}{d}$$

Rotational relaxation time:

$$\tau = (\alpha + (d-1)D_r)^{-1}$$

JT+MEC, EPL 101, 20010 (2013)

Spatially varying motility parameters

$$v = v(\mathbf{r}) \ , \quad \alpha = \alpha(\mathbf{r}) \ , \quad D_r = D_r(\mathbf{r})$$

Explicit coarse-graining gives EOM for 1-body probability density

$$\dot{\rho} = -\nabla \cdot \mathbf{j}$$

$$\mathbf{j} = -D_r \nabla \rho + \mathbf{V} \rho$$

$$D(\mathbf{r}) = v^2/2d$$

$$\mathbf{V}/D = -\nabla (\ln v(\mathbf{r}))$$

Equivalent to isothermal Brownian particle in external potential:

$$\beta U(\mathbf{r}) = \ln v(\mathbf{r})$$

M Schnitzer et al, Symp. Soc. Gen. Microbiol., 46, 15 (1990); PRE 48,2553 (1993)

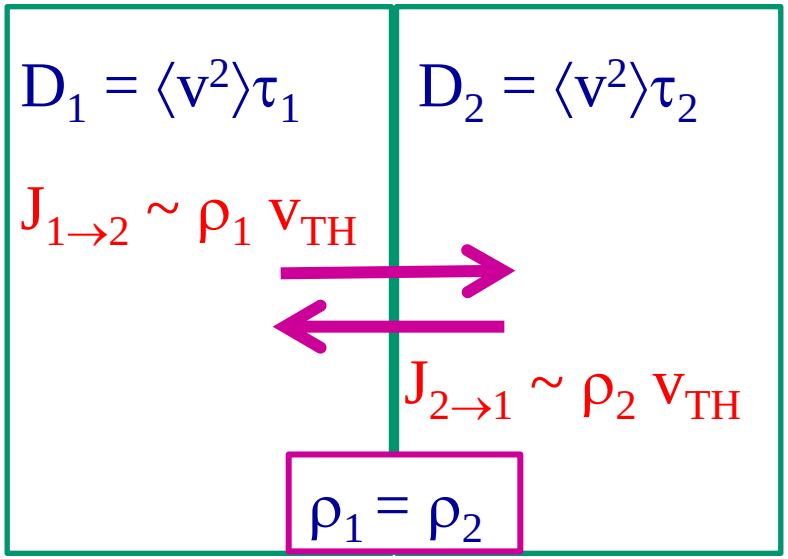
Steady-state solution

$$\rho_{ss}(\mathbf{r}) \propto \exp[-\beta U(\mathbf{r})] = \frac{1}{v(\mathbf{r})}$$

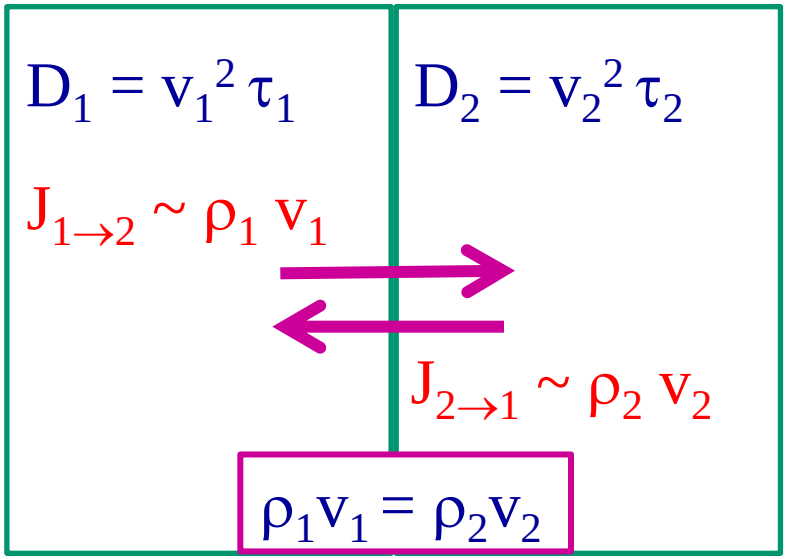
Active particles accumulate where they move slowest

1D illustration:

isothermal Brownian



Active



Coarse Graining: From Microscopics to Diffusion-Drift

MEC and J Tailleur, EPL 101 20010 (2013), PRL 100 218103 (2008)

So far, one particle ⇔ Brownian motion in $\beta U(\mathbf{r}) = -\ln v(\mathbf{r})$

$$j = -D\nabla\rho + V\rho$$

$$D(r) = v^2/2d$$

$$V/D = -\nabla(\ln v(r))$$

⇒ for N independent Brownian particles:

coarse grained collective density $\rho(r) = \sum_i \delta(r - r_i)$

$$\partial\rho/\partial t = -\nabla\cdot J$$

$$J(r) = -D(r)\nabla\rho + V(r)\rho + (2D(r)\rho)^{1/2}\xi$$

$$\xi = \text{unit white noise (Ito)}$$

e.g., D S Dean, J. Phys. A L613 (1996)

Coarse Graining: From Microscopics to Diffusion-Drift

MEC and J Tailleur, EPL 101 20010 (2013), PRL 100 218103 (2008)

Allow spatial dependence of v, τ to be mediated by ρ itself

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot J$$

$$J(r) = -D[\rho]\nabla\rho + V[\rho]\rho + (2D[\rho]\rho)^{1/2}\xi$$

where

$$\left.\begin{aligned} D([\rho;r) &= v^2\tau/d \\ V([\rho;r) &= -D\nabla(\ln v) \end{aligned}\right\} \quad \begin{aligned} v &= v([\rho;r) \\ \tau &= \tau([\rho;r) \end{aligned}$$

Density-Dependent Swimming Speed

J. Tailleur + MEC, PRL 100, 218103 (2008), EPL 101, 20010 (2013)

Equivalent to interacting Brownian particles iff

$$\frac{V([\rho]; r)}{D([\rho]; r)} = \nabla \ln \rho - \beta F_{ex}(r) \quad \text{where} \quad \beta F_{ex} = \frac{\delta F_{ex}[\rho]}{\delta \rho(r)}$$

$\Rightarrow$ a colloidal fluid with free energy

$$\boxed{F[\rho] = \int \rho(\ln \rho - 1)\, dr + F_{ex}[\rho]}$$

units: $\beta = 1$

Density-Dependent Swimming Speed

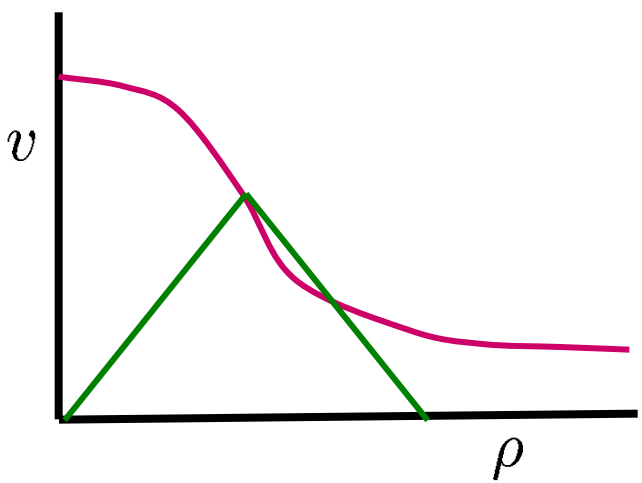
J. Tailleur + MEC, PRL 100, 218103 (2008), EPL 101, 20010 (2013)

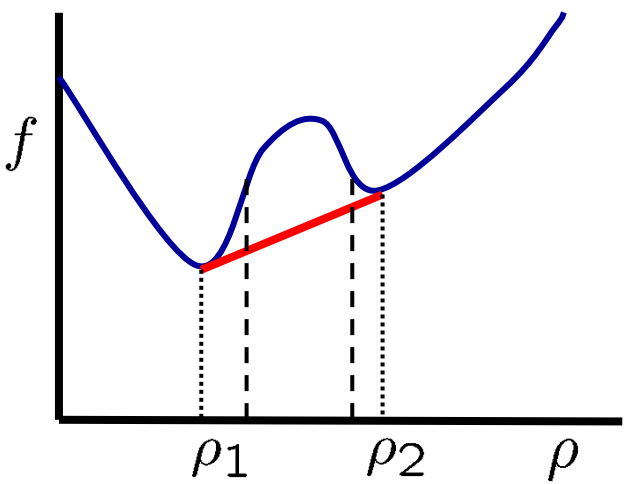
If $v([\rho],\mathbf{r}) \approx v(\rho(\mathbf{r}))$ is local:

$$f(\rho) = \rho(\ln\rho - 1) + \int_0^{\rho} \ln v(s)\,ds$$

spinodal instability

$$\frac{d^2 f}{d\rho^2} < 0 \quad \Leftrightarrow \quad \frac{d\ln v}{d\ln\rho} < -1$$

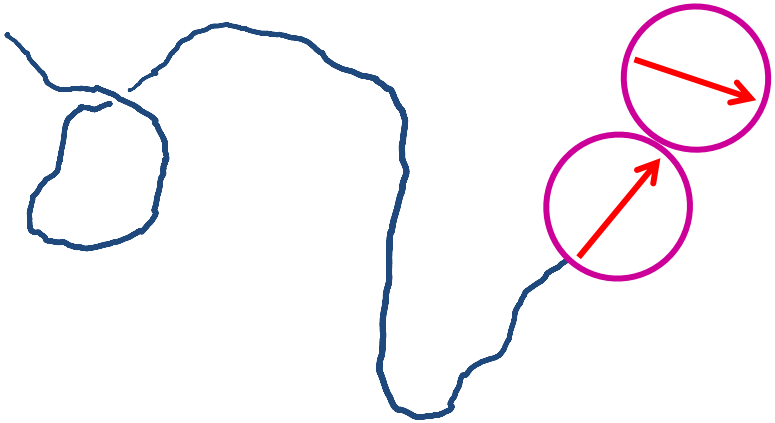


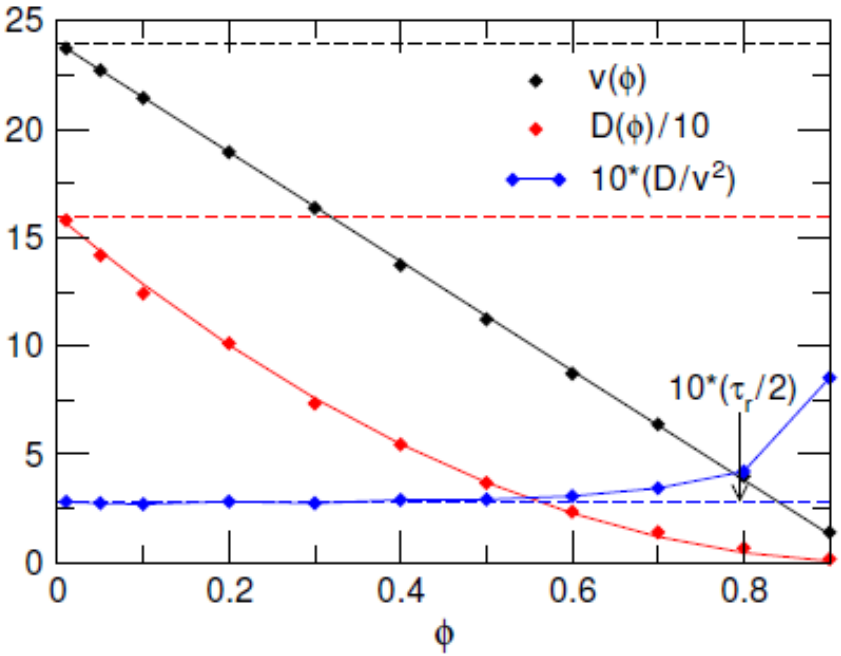


coexistence condition: common tangent on $f(\rho)$

Case Study: Spherical ABPs + Collisions

Y Fily, M C Marchetti, PRL 108 235702 (2012)
GS Redner, A Baskaran, M F Hagan, PRL 110 057701 (2013)
J Stenhammar et al, PRL 111, 145702 (2013)
A. Wysocki, R. G. Winkler and G. Gompper, arXiv:1308.6423





average projected velocity v = **v.u**

$$v(\rho) = v_0(1 - \rho/\rho_m)$$

no rotation in collision: τ unaffected

Phase Separation Kinetics

J. Stenhammar et al, PRL 111, 145702 (2013)

Mapping with local approximation $v([\rho],\mathbf{r}) \approx v(\rho(\mathbf{r}))$:

DB system unstable towards phase separation ✓

But model has:

Infinitely sharp interfaces, no surface tension

$\Rightarrow$ no driving force for domain growth ✗

need nonlocal terms to describe kinetics

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Phase Separation Kinetics

J. Stenhammar et al, PRL 111, 145702 (2013)

Consider slight nonlocality:

$$v([\rho]; r) = v(\rho(r))$$

$$\rho(r) = \rho(r) + \delta^2 r^2 \rho$$

ρ sampled on "persistence length" $\delta = \delta_0 \sqrt{v(\rho)}$

$\delta_0 = O(1)$

$$\frac{V}{D} = \nabla \cdot (\ln v(\rho)) = \nabla \cdot \mu_{ex}$$

$$\boxed{\mu_{ex} = \ln v(\rho) + \frac{\delta^2}{v}\frac{dv}{d\rho}\nabla^2\rho - \frac{\delta F}{\delta\rho}}$$

Gradient terms break Detailed Balance once again!

Phase Separation Kinetics

J. Stenhammar et al, PRL 111, 145702 (2013)

Resulting model:

$$\dot{\rho} = -\nabla.\mathbf{J}$$

$$\mathbf{J} = -D(\rho)\rho\nabla\mu + \text{noise}$$

$$\mu(\rho) = \ln\rho + \ln v(\rho) - \kappa(\rho)\nabla^2\rho \boxed{- \frac{d\kappa(\rho)}{d\rho}\frac{(\nabla\rho)^2}{2}}$$

$$v(\rho) = v_0(1 - A\rho)$$ (+ hardcore correction)

$$\kappa(\rho) = -\gamma_0^2\tau_r^2 v(\rho)\frac{dv(\rho)}{d\rho}$$

compare:

$$\boxed{\mathcal{F} = \int \left(f(\rho) + \frac{\kappa(\rho)}{2}\nabla(\rho)^2\right) d^3\mathbf{r}}$$

DB restoring term

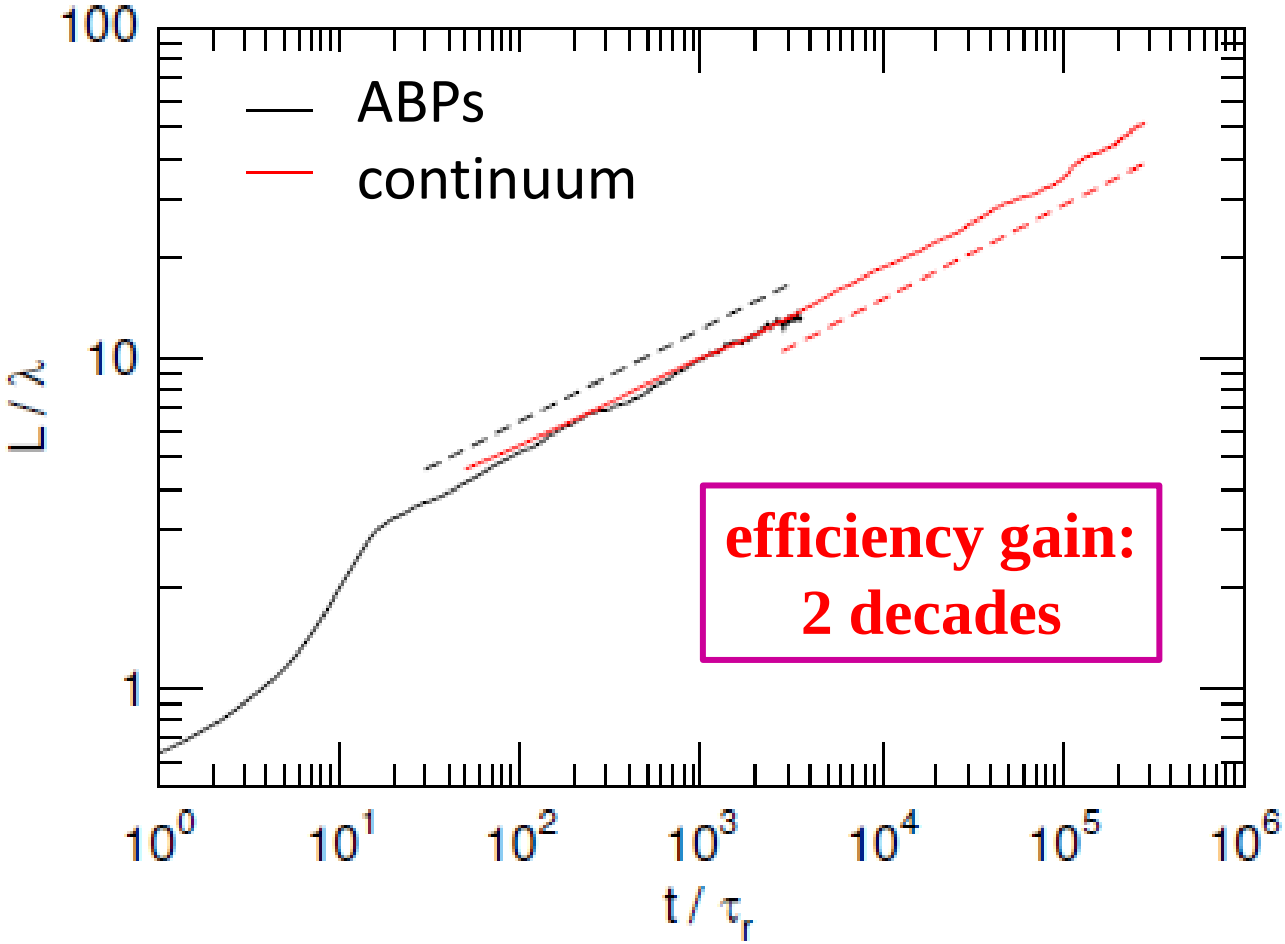
Scaling of domain size L(t)

J Stenhammar et al, PRL 111, 145702 (2013)

fit parameter γ_0

curves join up!

exponent 0.28



Scaling of domain size L(t)

J Stenhammar et al, PRL 111, 145702 (2013)

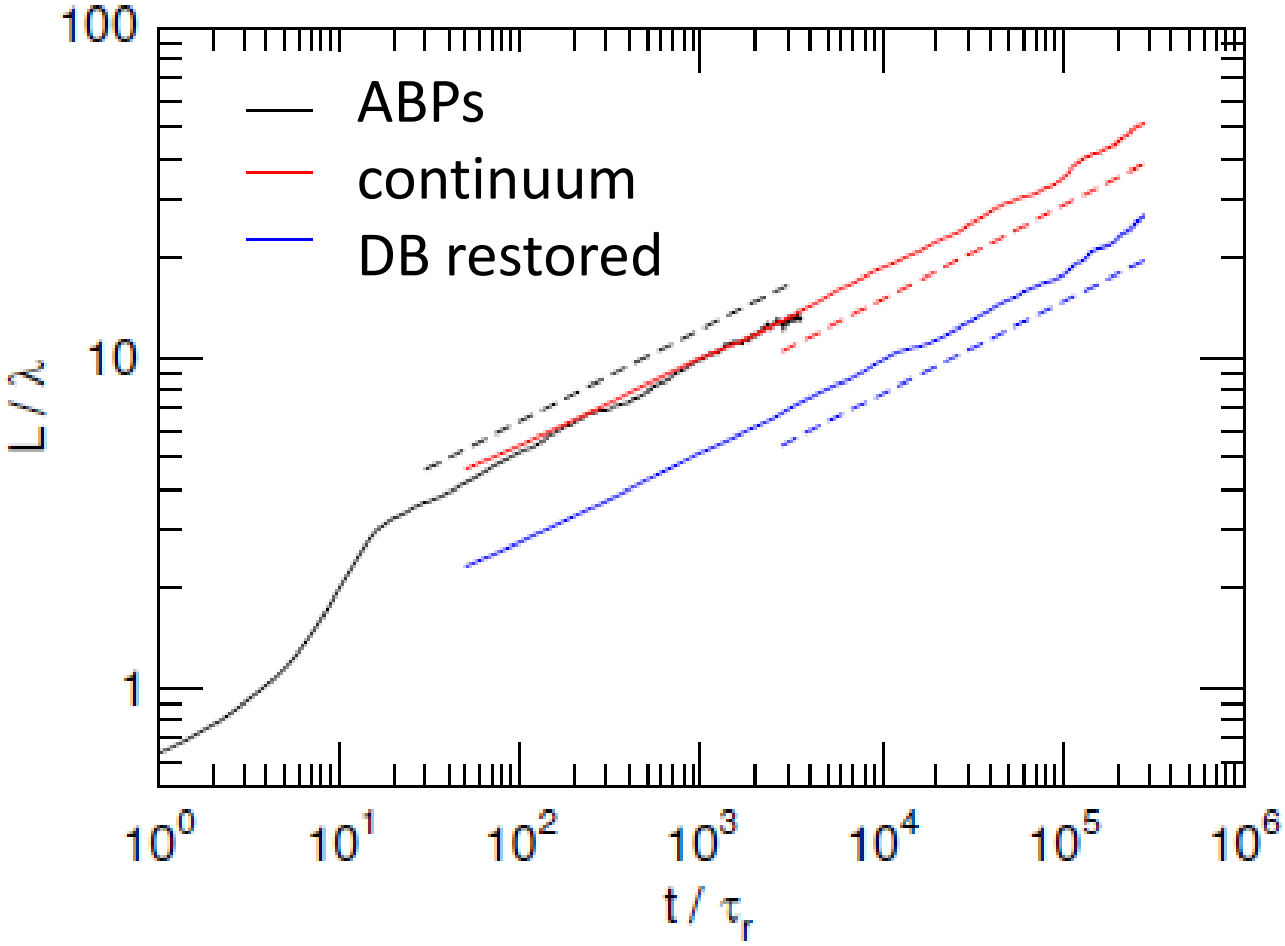
fit parameter γ_0

curves join up!

exponent 0.28

cf passive 0.33
(model B)

DB violation
not responsible
for exponent shift



ABPs: The Story So Far

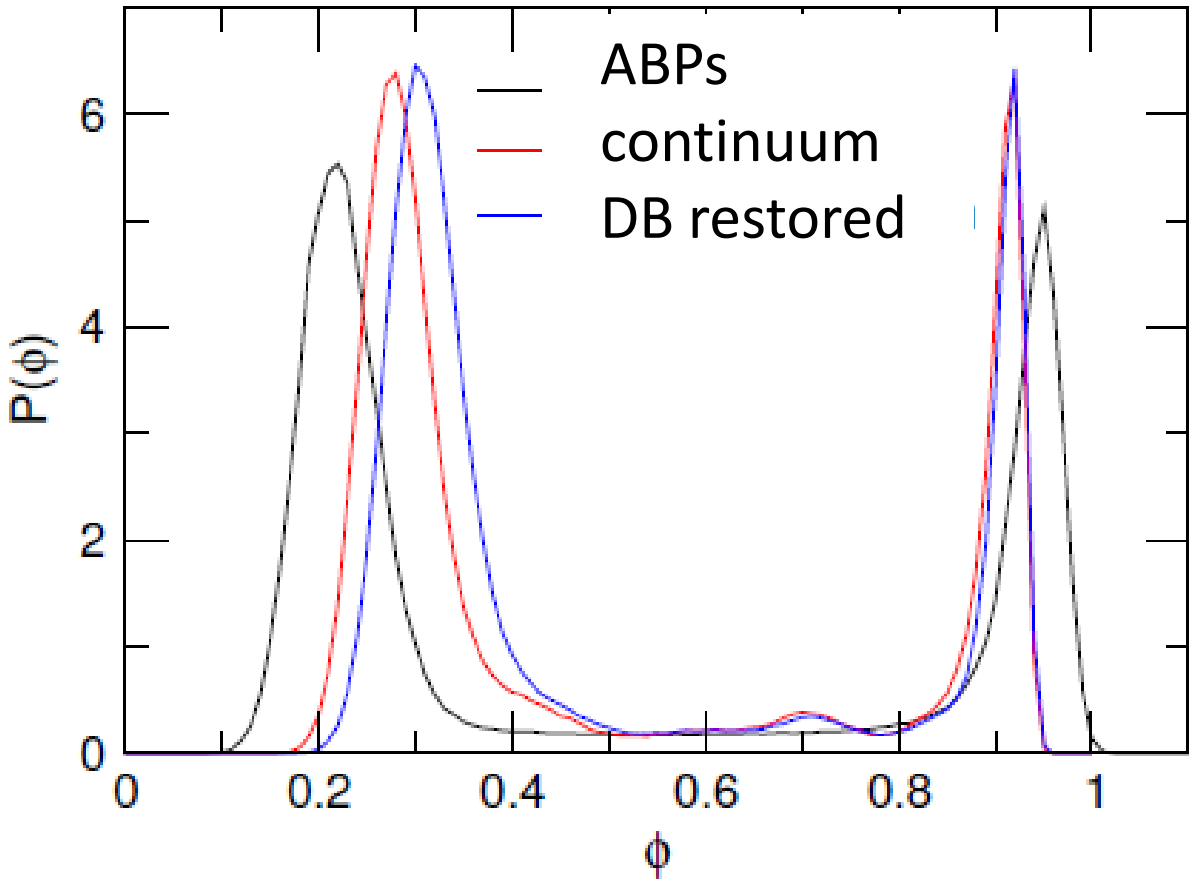
J Stenhammar et al, PRL 111, 145702 (2013)

- Free energy mapping is broken at square gradient level
- Near perfect agreement of continuum and ABP simulations
- DB violations have little effect on phase separation kinetics
- Modest exponent shift: $D(\rho)$ not DB violations
- But.....

ABPs: The Story So Far

J Stenhammar et al, PRL 111, 145702 (2013)

- DB violations do affect phase diagram!



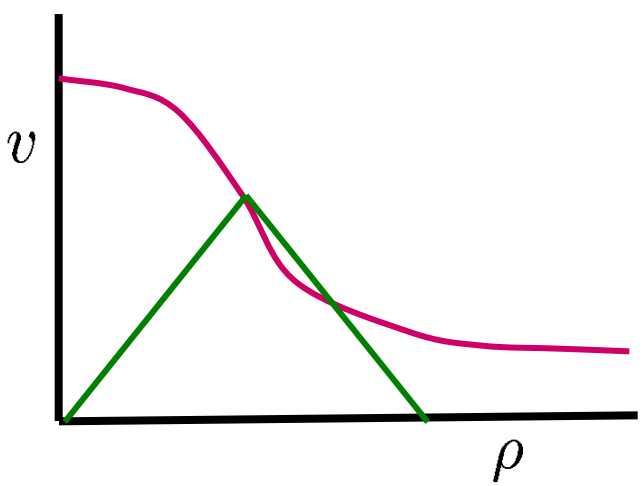
Small but clear shift in coexisting densities with/without DB

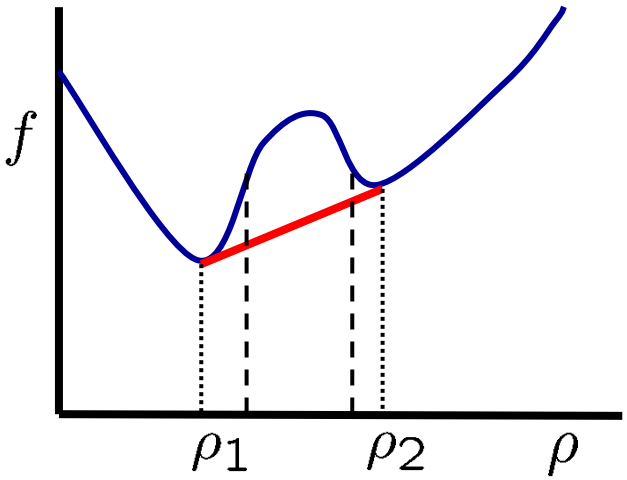
ABPs: The Story So Far

J Stenhammar et al, PRL 111, 145702 (2013)

How can gradient terms change the common tangent construction?

$$\beta f(\rho) = \rho(\ln \rho - 1) + \int_0^\rho \ln v(s) ds$$





Minimal Model

R Wittkowski et al, in review

Free energy density

$$\mathcal{F} = \int d^d\mathbf{x} \left(-\frac{\phi^2}{2} + \frac{\phi^4}{4} + \frac{\nabla\phi^2}{2} \right)$$

Equilibrium chemical potential

$$\mu_0 = -\phi + \phi^3 - \frac{\nabla^2\phi}{2}$$

Add generic leading-order DB violation

$$\mu = \mu_0 + \lambda(\nabla\phi)^2$$

[For previous ABP model $\lambda \propto -d\kappa(\rho)/d\rho$ = const.]

Minimal Model

R Wittkowski et al, in review

Free energy density

$$\mathcal{F} = \int d^d\mathbf{x} \left(-\frac{\phi^2}{2} + \frac{\phi^4}{4} + \frac{\nabla\phi^2}{2} \right)$$

Equilibrium chemical potential

$$\mu_0 = -\phi + \phi^3 - \frac{\nabla^2\phi}{2}$$

Add generic leading-order DB violation

$$\mu = \mu_0 + \lambda(\nabla\phi)^2$$

Now proceed as usual

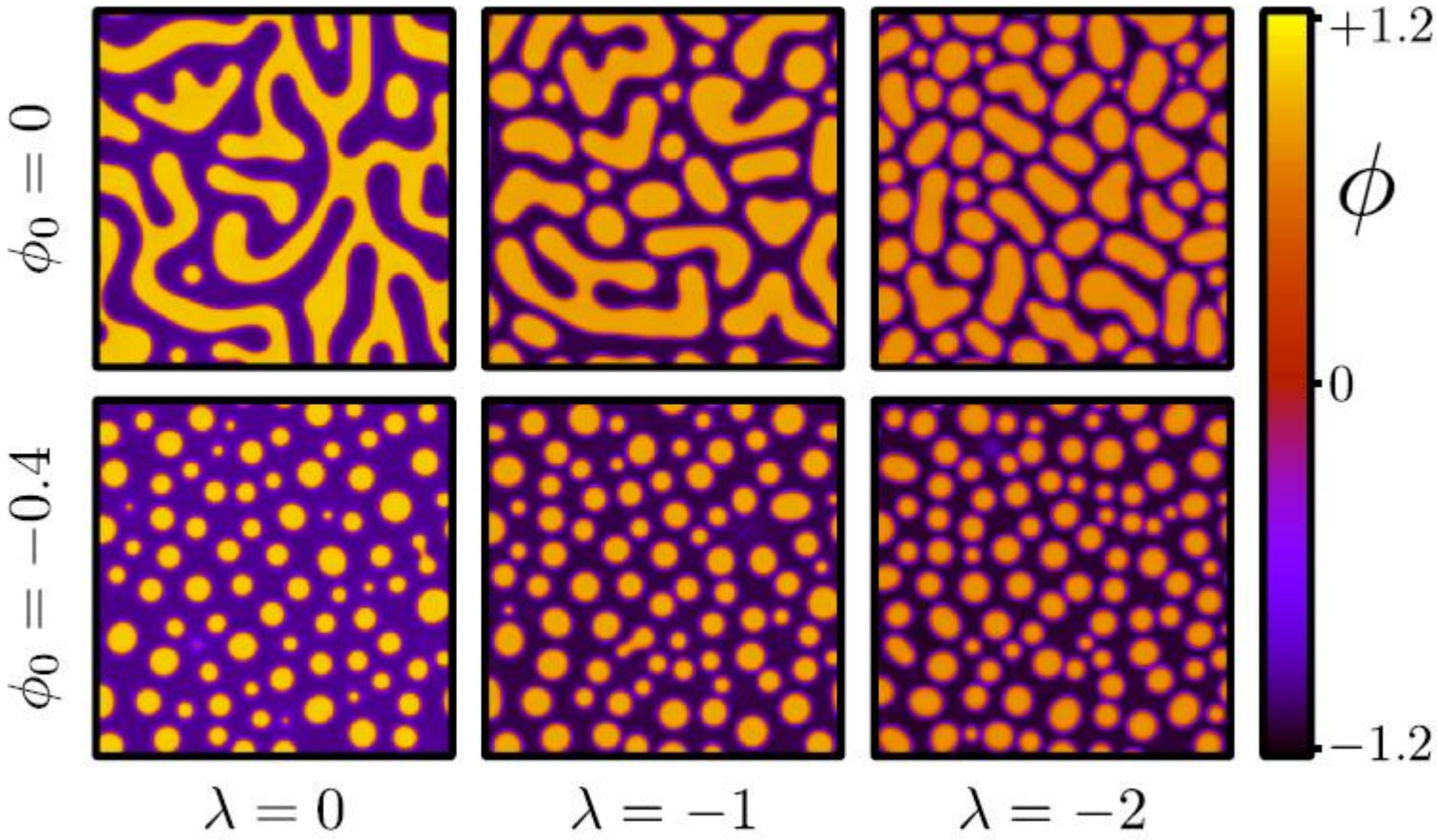
$$\mathbf{J} = -\nabla\mu \ \ (+\ \text{noise})$$

$$\dot{\phi} = -\nabla.\mathbf{J}$$

Active Model B

Active Model B: L(t)

R Wittkowski et al, in review



λ causes asymmetry

little else altered

Active Model B: L(t)

R Wittkowski et al, in review

$\lambda = 0$:

exponent 1/3

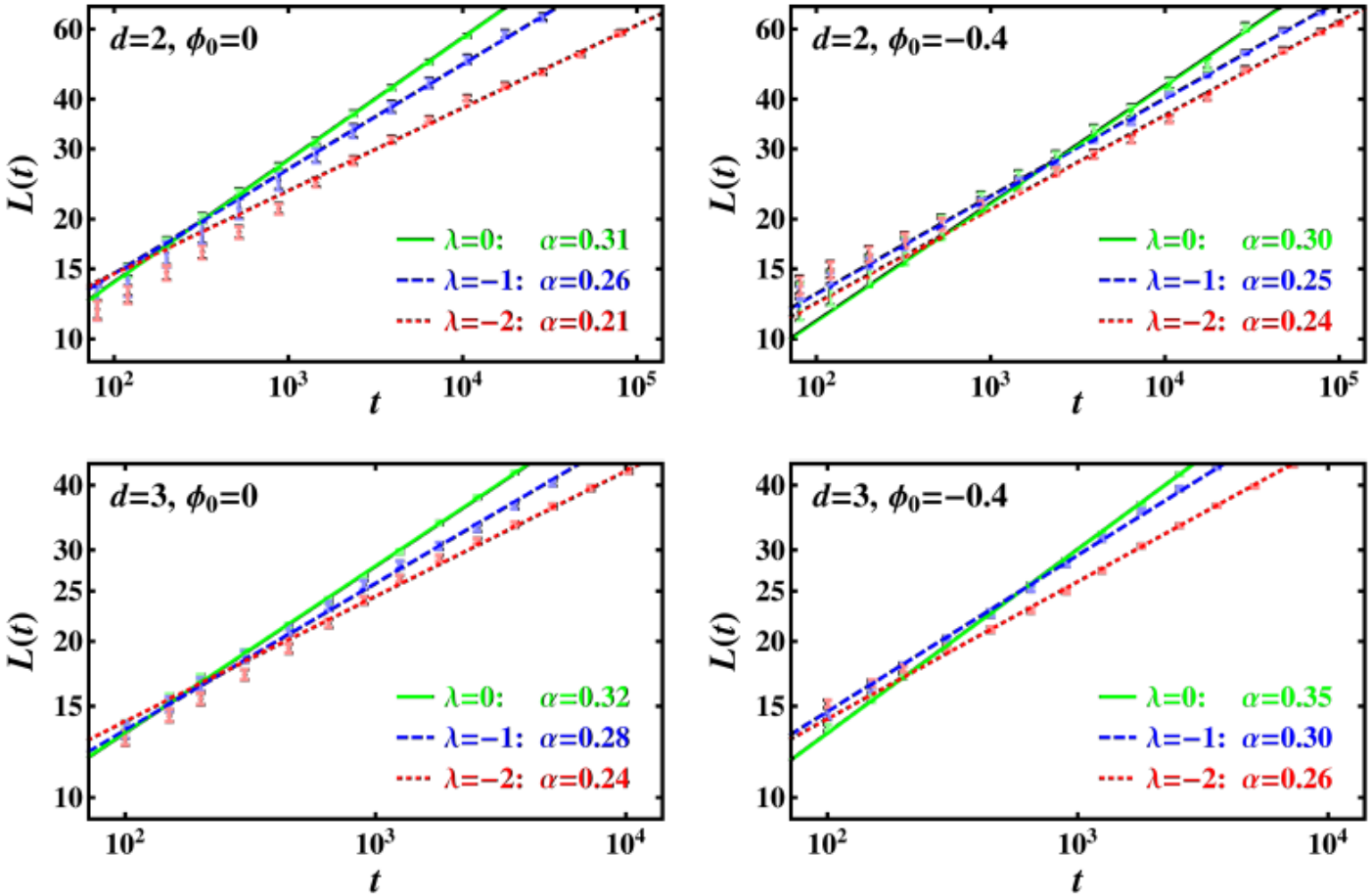
(standard B)

finite λ :

0.25-0.28

kinetics:

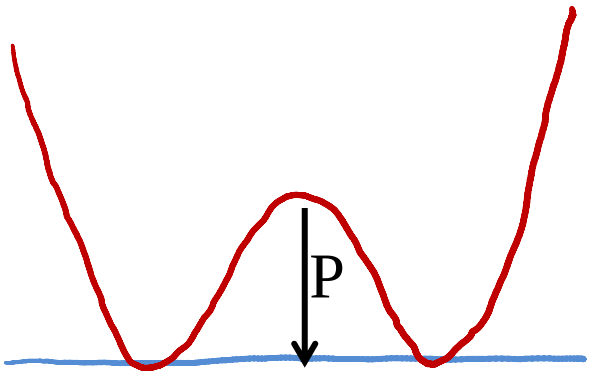
no special features



Active Model B: Phase coexistence

R Wittkowski et al, in review

$\lambda = 0$: equilibrium common tangent



$$f = -\frac{\phi^2}{2} + \frac{\phi^4}{4}$$

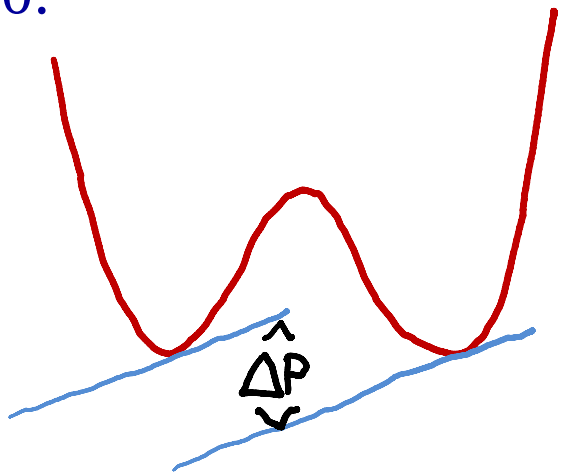
1. equal chemical potential (= slope $df/d\phi$)
2. equal pressure (= intercept, $\mu\phi - f$)

Result: $\mu = 0; \phi = \pm 1$

Active Model B: Phase coexistence

R Wittkowski et al, in review

$\lambda \neq 0$:



"uncommon tangent" construction

$$f = -\frac{\phi^2}{2} + \frac{\phi^4}{4}$$

$J \sim \nabla\mu = 0 \Rightarrow \mu$ = uniform = μ_0 in bulk phases

$\Rightarrow$ common slope retained

But pressures not equal: $\mu_0 \neq 0$

Active Model B: Phase coexistence

R Wittkowski et al, in review

Explicit calculation of offset:

seek 1D profile $\phi(z)$ connecting bulk phases of $\mu \neq 0$

$J = 0 \Rightarrow$

$$-\phi + \phi^3 - \phi'' + \lambda(\phi')^2 = \mu$$

[nonlinear eigenvalue problem for μ]

$\phi(z) \Leftrightarrow x(t)$ for Newtonian particle in inverted potential

$$U(x) = \mu x + \frac{x^2}{2} - \frac{x^4}{4}$$

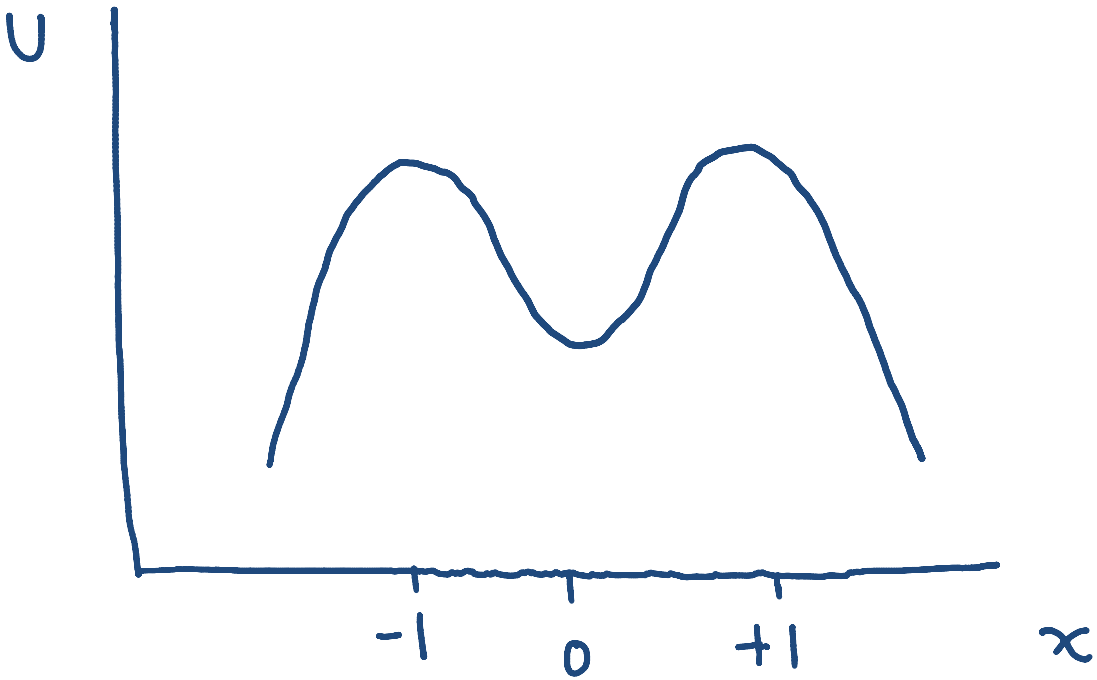
$$\ddot{x} = -U'(x) + \lambda \dot{x}^2$$

$\lambda \Leftrightarrow$ velocity dependent force

Active Model B: Phase coexistence

R Wittkowski et al, in review

Explicit calculation of offset $$\ddot{x} = -U'(x) + \lambda \dot{x}^2$$

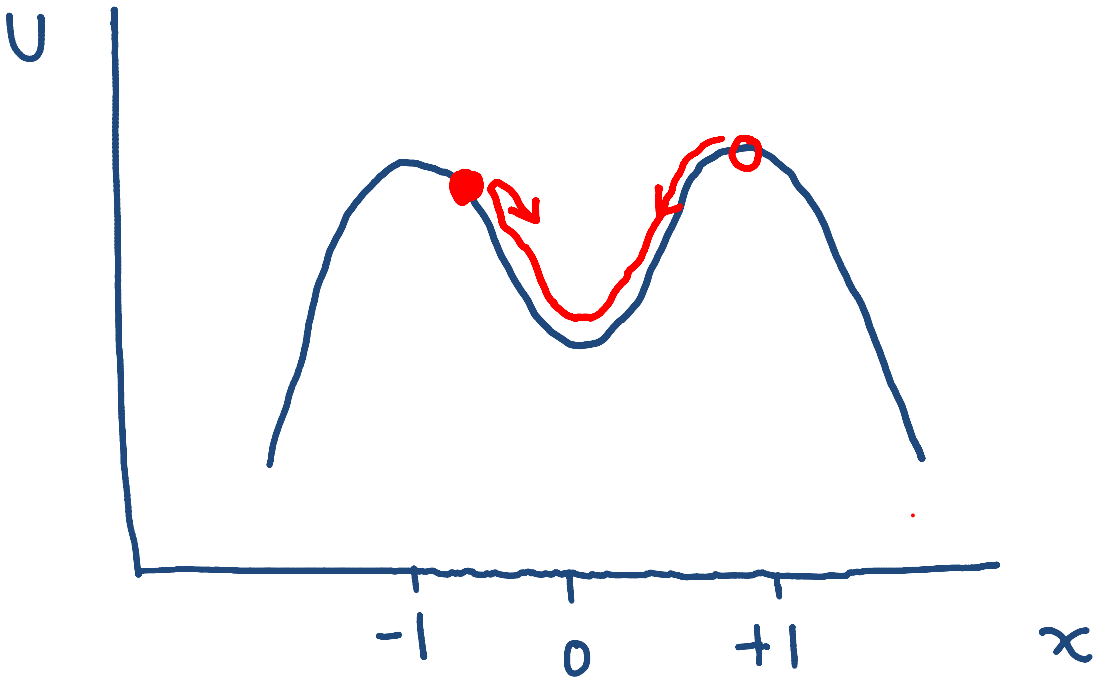


$\mu = 0$:

Active Model B: Phase coexistence

R Wittkowski et al, in review

Explicit calculation of offset $$\ddot{x} = -U'(x) + \lambda \dot{x}^2$$

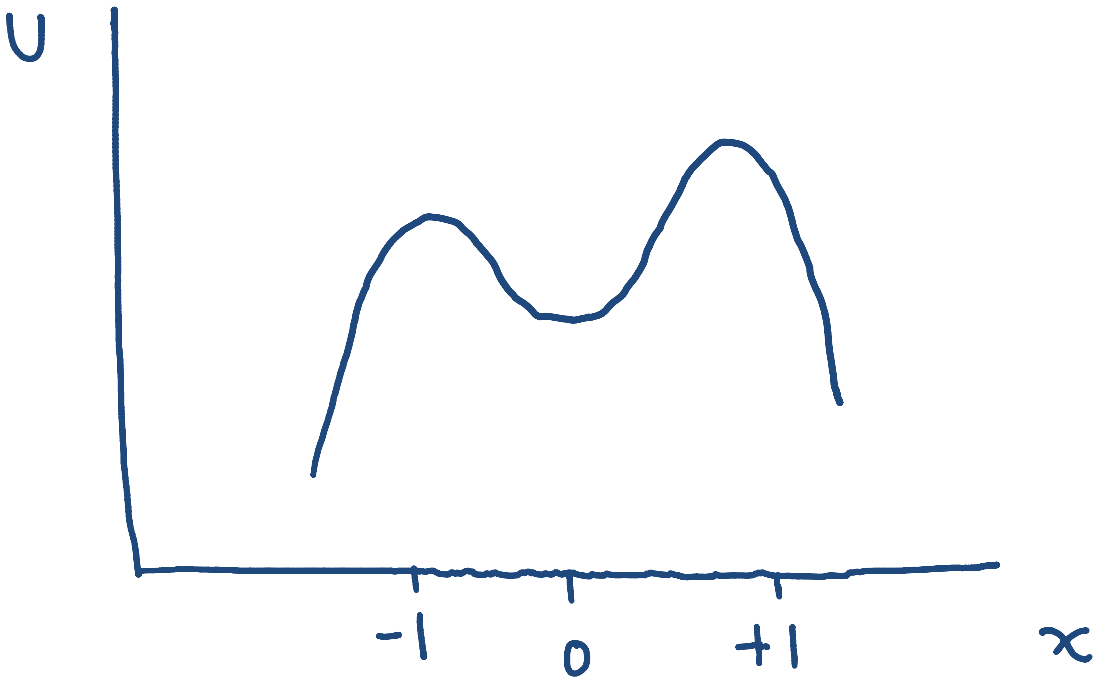


$\mu = 0$: all solutions oscillatory $\Rightarrow$ microphase separation

Active Model B: Phase coexistence

R Wittkowski et al, in review

Explicit calculation of offset $$\ddot{x} = -U'(x) + \lambda \dot{x}^2$$

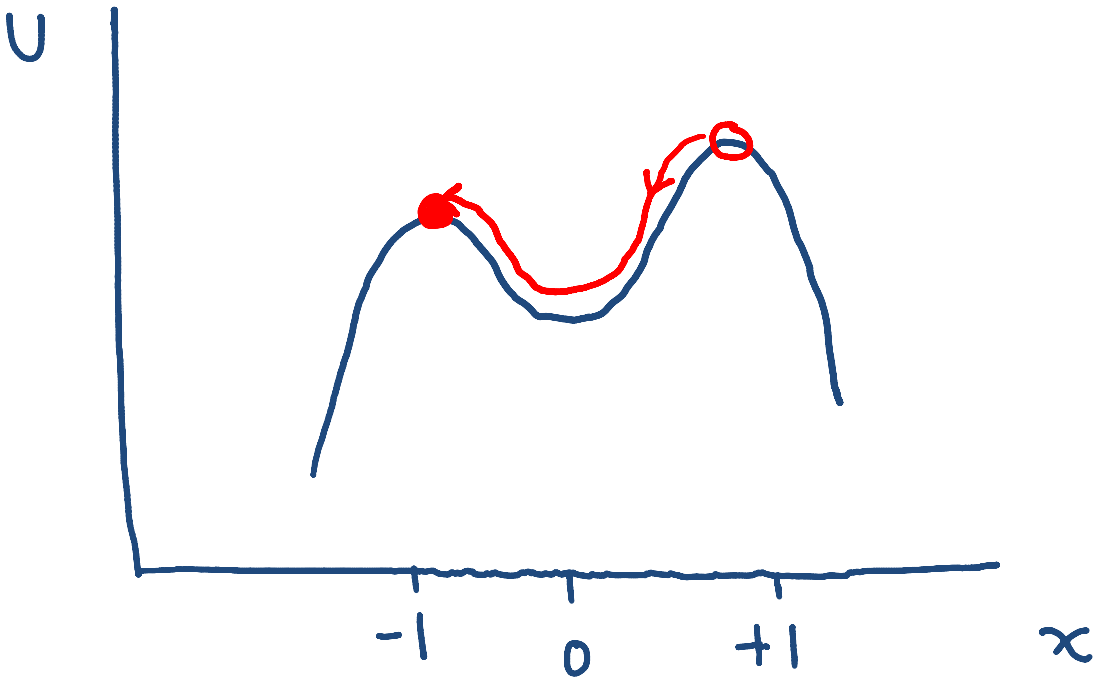


For eigenvalue $\mu(\lambda)$:

Active Model B: Phase coexistence

R Wittkowski et al, in review

Explicit calculation of offset $$\ddot{x} = -U'(x) + \lambda \dot{x}^2$$

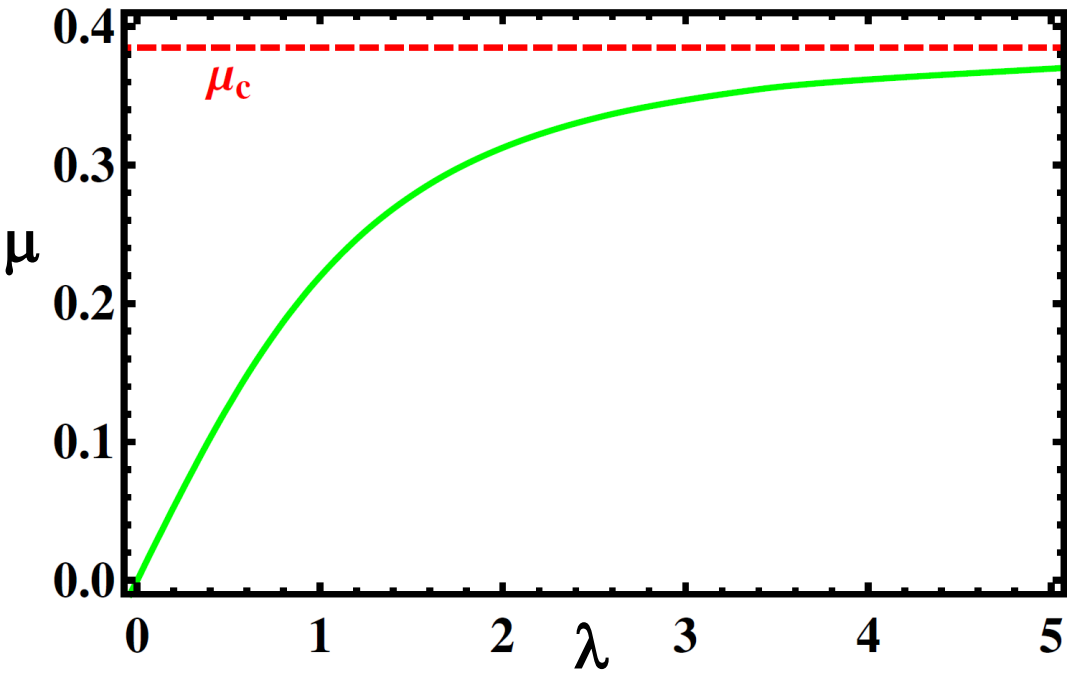


For eigenvalue $\mu(\lambda)$: planar interface between bulk phases

Active Model B: Phase coexistence

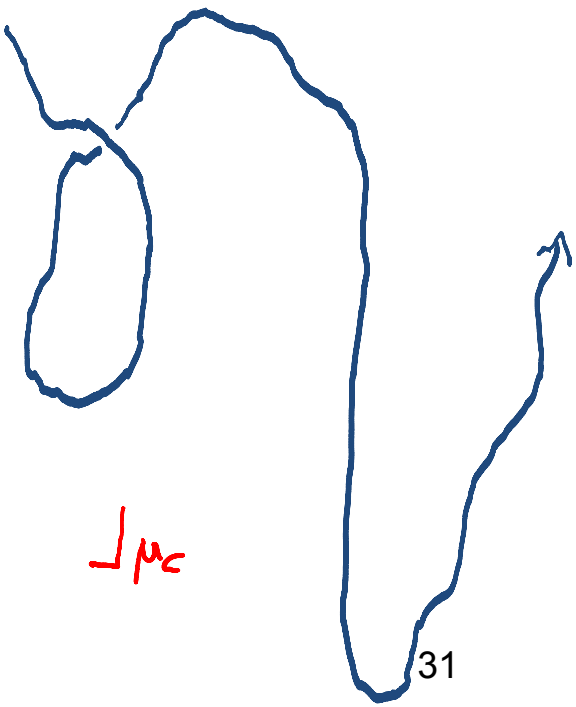
R Wittkowski et al, in review

Explicit calculation of offset



Flat interface solution always exists

Pressure jump ΔP_λ saturates at large λ



Active pressure vs Laplace pressure

R Wittkowski et al, in review

For $\lambda << 1$: active pressure jump across flat interface

$$\Delta P_\lambda = \frac{8}{15}\lambda$$

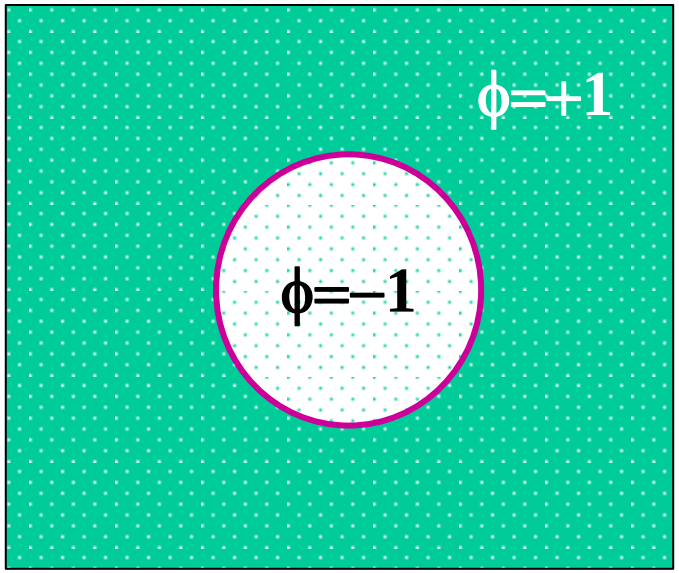
Passive droplet, radius R: Laplace pressure

$$\Delta P_L = (d-1)\frac{\sigma}{R} = (d-1)\frac{2\sqrt{2}}{3R}$$

Explicit calculation gives $\mu = 0$ solution when these balance

$$R^* = \frac{5(d-1)}{2\sqrt{2}\lambda}$$

Active pressure is "thermodynamically real" like Laplace pressure (within mapping)



Stable Droplet Phases?

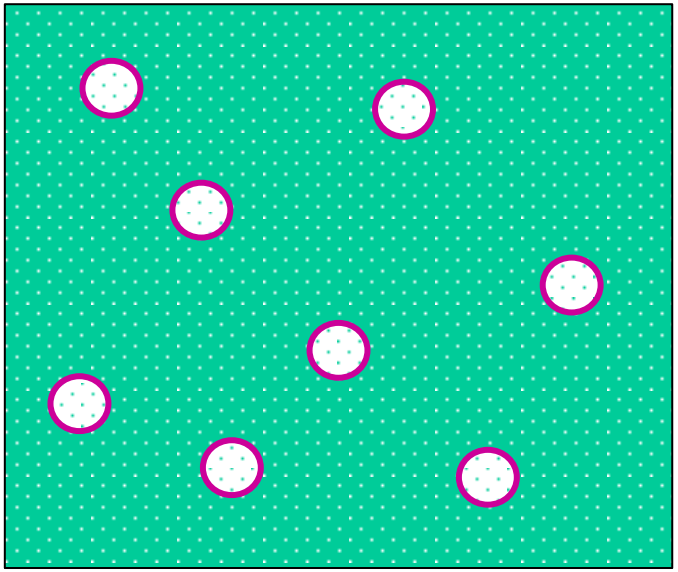
R Wittkowski et al, in review

Experiments sometimes see stable clusters/droplets

Palacci et al Science 339, 936 (2013), Theurkauff et al PRL 108, 268303 (2012)

Schwarz-Linek et al PNAS 109, 4052 (2012)

Q: Can we get a stable phase of R* droplets?



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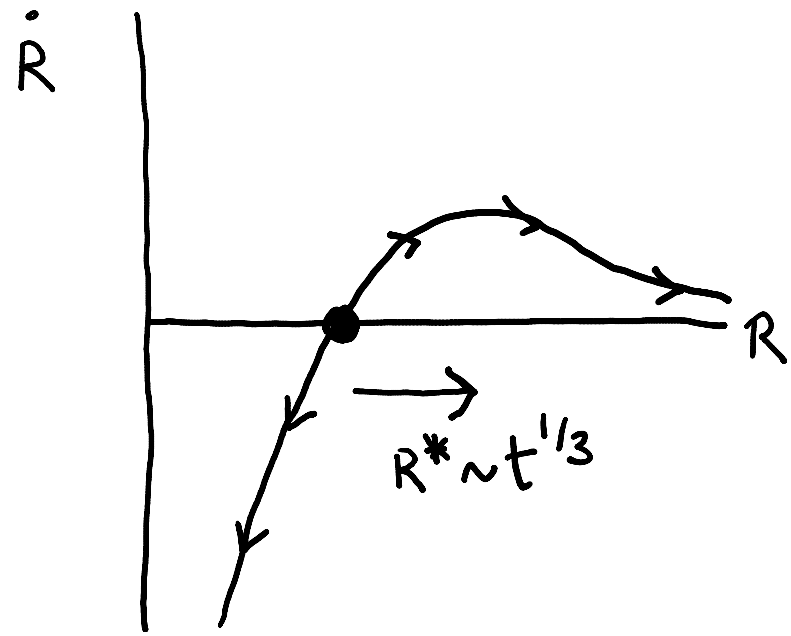
Q: Can we get a stable phase of R* droplets?

A: No!



R > R*: growth
R < R*: shrinkage

Ostwald ripening as in passive case

All droplet phases unstable

Active Model B: Summary

R Wittkowski et al, in review

Phase separation kinetics ≈ as with DB

no new kinetic universality class (?)

no arrest into cluster phase

Uncommon tangent construction

'active Laplace pressure'

planar interface solution always exists

Antecedents:

shear banding, driven surface coarsening models

PD Olmsted, Rheol. Acta 47, 283 (2008)

SJ Watson and SA Norris, Phys. Rev. Lett. 96, 176103 (2006).

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