Three problems not too far from equilibrium: from passive to active systems

LARGE DEVIATION THEORY IN STATISTICAL PHYSICS: RECENT ADVANCES AND FUTURE CHALLENGES

ICTS, 11 September 2017, Bangalore

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Outline

Part I

- Weak-noise Large Deviations (Freidlin-Wentzell theory)
- Perturbative calculation of quasi-potential
- Diffusing particles interacting by mean-field forces

[F. Bouchet, K. Gawedzki, CN, J. Stat. Phys., 163, 2016]

Part II

- Active Ornstein-Uhlenbeck particles

[E. Fodor, CN, ME Cates, J Tailleur, P Visco, F van Wijland, PRL, 2016]

Part III

- Incomplete phase separation in Active Matter

[E Tjhung, CN, ME Cates, in preparation]

Collaborators

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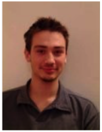
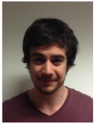


J. Tailleur (Paris)

Van Wijland (Paris)



E. Fodor (Cambridge)

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- EPSRC Programme Grant EP/J007404
- LabEx PALM (ANR-10-LABX-0039-PALM)

Weak-noise, Quasi-Potential

$$\dot{x} = K(x) + \sqrt{2T}\,\eta_t \qquad T \ll 1$$

$$\left\langle \eta_t^i \, \eta_{t'}^j \right\rangle = Q(x_t)\delta_{i,j}\delta(t-t')$$

Quasi-Potential $\mathcal{F}$

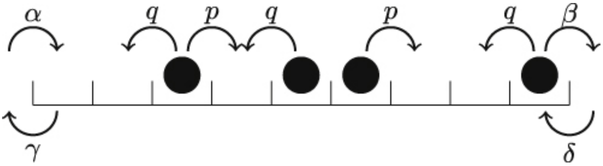
For $T \to 0$, P_∞ satisfy a LDP

$$P_\infty(x) \asymp \exp\left(-\frac{\mathcal{F}(x)}{T}\right) \qquad \mathcal{F}(x) = -\lim_{T\to 0} T \log P_\infty(x)$$

Macroscopic Fluctuation Theory

Macroscopic description of several stochastic lattice gases [SEP, WASEP, KMP, ...]

WASEP: $q - p \sim E/N$



$$\partial_t \phi = \nabla \left(E\sigma(\phi) - D(\phi)\nabla\phi + \sqrt{\frac{\sigma(\phi)}{N}}\,\eta \right) \qquad \langle \eta\eta \rangle = \delta(x-y)\delta(t-s)$$

- ϕ : particle density
- $D(\phi)$: Diffusivity $\qquad \sigma(\phi)$: Mobility

$$P[\phi(x)] \asymp \exp\left(-\frac{\mathcal{F}[\phi(x)]}{N} \right)$$

Instanton dynamics

$$\mathcal{A}[x_t] = \frac{1}{4}\int_0^T [\dot{x}_t - K(x_t)] \cdot Q(x_t)^{-1} \cdot [\dot{x}_t - K(x_t)]\, dt$$

$$F(x) = \min_{\{\hat{x}_t \,|\, \hat{x}(-\infty)=x_0\,,\, \hat{x}(0)=x\}} \mathcal{A}[\hat{x}_t]$$

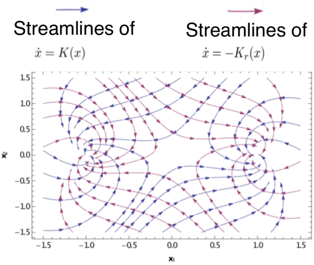
Adjoint or instanton dynamics

Minimum of $\mathcal{A}$ realised on solutions of

$$\dot{x} = K_r(x)$$

$$K_r \equiv K + 2Q \cdot \nabla \mathcal{F}$$

$K = K_r$ iff equilibrium



Perturbative computation of quasi-potential

$$\dot{x} = K_\lambda(x) + \sqrt{2T}\,\eta_t^\lambda \qquad \lambda : \text{external parameter}$$

$$\left\langle \eta_t^i \, \eta_{t'}^j \right\rangle = Q_\lambda(x_t)\delta_{i,j}\delta(t - t')$$

Suppose we know $\mathcal{F}_0$ for $\lambda = 0$

Can we calculate $\mathcal{F}_\lambda$ perturbatively in λ?

- In literature
  - first order theories
  - specific cases treated
  - finite-dimensional systems

[Graham & Schenzle (1983); Graham & Tel (1984); Gang & Haken (1989), Jauslin (1986), Maier & Stein (1993), ...]

Existence, convergence and remarks

$$\mathcal{F}_\lambda(x) = \sum_{n=0}^{\infty} \lambda^n \mathcal{F}^{(n)}(x) \qquad \text{, analogously for } K_\lambda \text{and } Q_\lambda$$

$$F^{(n)}(y) = \int_{-\infty}^{0} S^{(n)}[\ldots](y_r(t;y))\,dt \qquad \forall n \qquad (1)$$

$$\dot{y} = K_r^{(0)}(y) \qquad K_r^{(0)} \equiv K^{(0)} + 2\,Q^{(0)} \cdot \nabla \mathcal{F}^{(0)}$$

$S^{(n)}[\ldots](x)$ explicit functional of $\mathcal{F}^{(i)}$, $K^{(i)}$, $Q^{(i)}$, $i < n$

- Existence: easy for $n = 1$ (Fredholm), true but tricky for $n > 1$
- Convergence: finite radius of convergence if K_λ, Q_λ analytic
- 'Usefulness': only the solution of the unperturbed instanton dynamics $\dot{y}_t = K_r^{(0)}$ needed to compute $\mathcal{F}^{(n)}$, $\forall n$

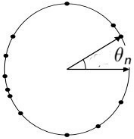
Mean-field interacting diffusions

Mean-field scaling (the $1/N$)!

$$\dot{\theta}_n = b(\theta_n)\, dt - \frac{J}{N} \sum_{m=1}^{N} \nabla U(\theta_n - \theta_m) + \sqrt{2T}\, \eta_n(t)$$

Ku-Shi model (1986,1988)

- $b(\theta) = f - h \sin\theta$
- $\nabla U(\theta) = \sin\theta$

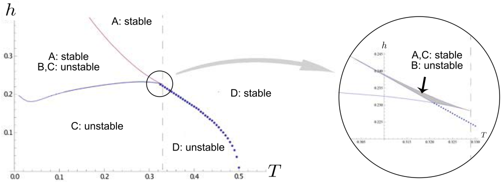


- f: non-equilibrium driving
- h: external 'magnetic' field

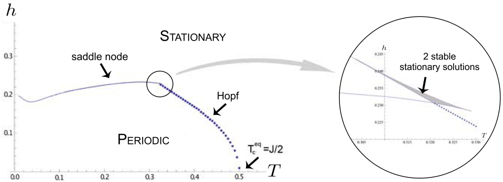
[Kuramoto & Shinomoto (1986,1988), Giacomin et al. (20xx)]

Simplified version of Kuramoto model (no disorder on f)

Typical behavior ($N \to \infty$, stationary)



Stationary states and their stability obtained analytically



Dean equation

- Empirical density $\phi_N(t,\theta) = \frac{1}{N}\sum_{n=1}^{N}\delta(\theta-\theta_n(t))$

$$\partial_t \phi_N = \nabla\cdot\left\{ -\phi_N b + J\phi_N \nabla(U\star\phi_N) + T\nabla\phi_N + \sqrt{\frac{2T\phi_N}{N}}\,\eta\right\}$$

Looking at smooth solutions $\phi \Longrightarrow$ rigorous results

- For $N\to\infty$, no noise (McKean, Vlasov, mean-field)
  [McKean 1967, Snitzman 1991, Meleard 1996]

- $N \gg 1$: weak noise large deviations
  [Dawson-Gartner 1987]

!Noise is weak because coupling is weak!

[Dean, 1995]

Perturbative calculation of QP

$$\dot{\theta}_n = f - h\sin\theta_n\, dt - \frac{J}{N}\sum_{m=1}^{N}\sin(\theta_n - \theta_m) + \sqrt{2T}\,\eta_n(t)$$

Perturbative calculations close to

- $J = 0$ (free particles dynamics): from Sanov theorem

$$F_0[\rho] = \int d\theta\,\phi(\theta)\log\frac{\phi(\theta)}{\phi_0(\theta)} - \phi(\theta) + \phi_0(\theta)$$

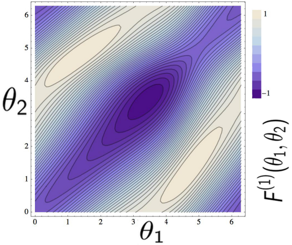
ϕ_0: stationary solution of mean-field equation

- $h = 0$; Taylor expansion close to the attractor...

Explicit computation at first order

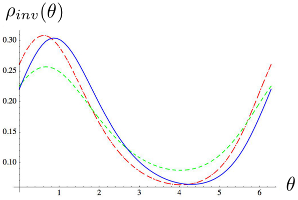
f=0.2, T=0.3, h=0.5

$$F[\phi] \simeq F_0[\phi] + J \int d\theta_1 d\theta_2 \; \phi(\theta_1)\phi(\theta_2) \; F^{(1)}(\theta_1,\theta_2) + \mathcal{O}(J^2)$$



Typical states ρ_{inv} for $J = 0.3$:

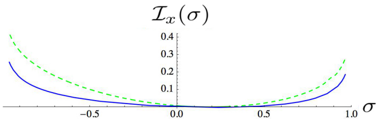
- unperturbed
- exact
- perturbative at $O(J)$

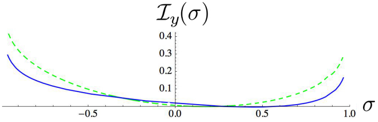


- The calculation can be generalised at any order without increasing the computational complexity

Fluctuations of the magnetization

f=0.2, T=0.3, h=0.5, J=0.3





Green: unperturbed syst.

Blue: perturbed syst.

$$m_x = \sum_n \cos\theta_n \qquad P(m_x = \sigma) \asymp \exp\left(-\frac{I_x(\sigma)}{N}\right)$$

$$m_y = \sum_n \cos\theta_n \qquad P(m_y = \sigma) \asymp \exp\left(-\frac{I_y(\sigma)}{N}\right)$$

Comparison of I_x, I_y with particles-based simulations?

Cesare Nardini

Introduction

Part I

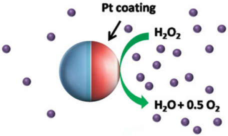
Part II

Part III

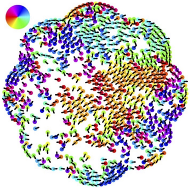
Part II - Active systems

Objects able to transform some ‘fuel’ into motion

- Bacteria, algae



- Autophoretic colloids



- Anysotropic (and shaken) granular matter
- ...

Phase Separation

Fully established in simulations of minimal models

[Seminal work: Tailleur & Cates, PRL 2008; Ann. Rev. Cond. Mat. 2015]

Particles with purely repulsive interactions (e.g., hard-core)

[Speck et al., PRL 2014, EPL 2013; Fily et al, PRL 2012, Stenhammar et al, PRL 2014]

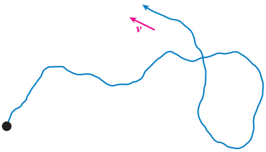
Video and simulation by J. Stenhammar

A minimal framework: AOUPs

Active Ornstein-Uhlenbeck Particles

$$\dot{r}_i = -\nabla_i U + v_i$$

$$\langle \mathbf{u}_i(t)\mathbf{u}_j(0)\rangle = \delta_{ij}\frac{T}{\tau}e^{-t/\tau}\mathbf{1}$$



- $\mathbf{u}_i$: Gaussian random variables
- typical velocity $\langle u_i^2\rangle \sim T/\tau$
- U : interaction potential

$\tau = 0$: equilibrium

- $\langle \mathbf{u}_i(t)\mathbf{u}_i(0)\rangle = T\mathbf{1}\,\delta(t)$
- $P_{ss} \propto \exp(-U/T)$

$\tau \neq 0$: active

- non-Boltzmann-Gibbs P_{ss}

Stationary measure (τ small)

- velocities $p_i = \sqrt{\tau}\, \dot{r}_i$
- Stationary measure perturbatively in $\tau \to 0$

$$P_\infty \propto \quad \exp\Big\{ -\frac{U + p_i^2/2}{T} - \frac{\tau}{2T}\Big[(\nabla_i U)^2 + (p_i \cdot \nabla_i)^2 U - 3T \nabla_i^2 U \Big] + \tau^{3/2} \Big[\frac{1}{6T} (p_i \cdot \nabla_i)^3 U - \frac{1}{2} (p_i \cdot \nabla_i) \nabla_j^2 U \Big] + \mathcal{O}(\tau^2) \Big\}$$

- not only $\mathcal{F}$ but also $\mathcal{O}(T^0)$ corrections
- $\tau \to 0$ and $T \to 0$ commute
- Non-Boltzmann already at order $\mathcal{O}(\tau)$
- Time-reversible at order τ: $\quad S = \frac{\sqrt{\tau}}{2T} \langle (p_i \cdot \nabla_i)^3 U \rangle \sim \mathcal{O}(\tau^2)$

[E. Fodor, CN, M. Cates, J. Tailleur, F. va Wijland, P. Visco, PRL 2016; Graham 1989]

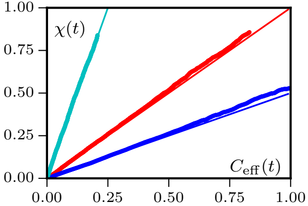
Effective Fluctuation-Dissipation Theorem (τ small)

$$\dot{r}_i = -\nabla_i U + v_i \quad \longrightarrow \quad \dot{r}_i = -\nabla_i U + v_i + f_i$$

$$R_{ij}(t-s) = -\frac{1}{T}\frac{\mathrm{d}}{\mathrm{d}t} C_{ij}^{eff}(t-s)$$

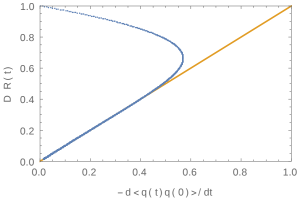
$$C_{ij}^{eff}(t) = \langle r_i(t) r_j(s)\rangle + \tau \langle p_i(t) p_j(s)\rangle + \mathcal{O}(\tau^{3/2})$$

Effective FDT



$N = 720,\ \tau = 0.01,\ A = 20,\ T = 2, 1, 0.25$

Equilibrium FDT



Part III - Incomplete phase separation in active matter

M.E. Cates
(Cambridge)

E. Tjhung
(Cambridge)

E Tjhung, CN, ME Cates, Incomplete phase separation in active systems, in preparation

Phase Separation

Fully established in simulations of minimal models

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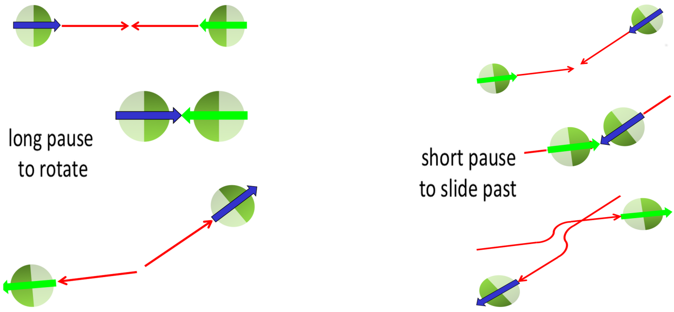
[Speck et al., PRL 2014, EPL 2013; Fily et al, PRL 2012, Stenhammar et al, PRL 2014]

Video and simulation by J. Stenhammar

Caused by breakdown of time-reversal symmetry

... not because fuel is transformed into motion ...

... but because of interactions!



Density dependent speed $v(\phi)$

Interactions encoded in $v(\phi)\downarrow$ when density $\phi\uparrow$

$$\dot{\mathbf{r}}_i = v(\phi(\mathbf{r}_i))\mathbf{u}_i + \sqrt{2T}\xi_i \qquad \dot{\mathbf{u}}_i = -\frac{\mathbf{u}_i}{\tau} + \frac{\sqrt{2}}{\tau}\eta_i$$

$\tau \to 0$ limit and coarse graining (Dean equation)...

Surprise! ... Effective equilibrium with free energy

$$\mathcal{F} = \int d\mathbf{r}\; f(\phi(\mathbf{r})) \qquad f(\phi) = \phi(\log\phi - 1) + \frac{1}{2}\int^{\phi} \log(\tau v^2(y) + T)dy$$

[Tailleur & Cates, PRL 2008; Ann. Rev. Cond. Mat. 2015]

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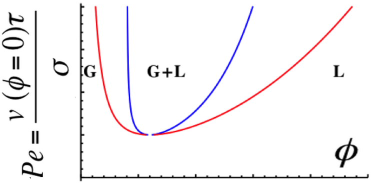
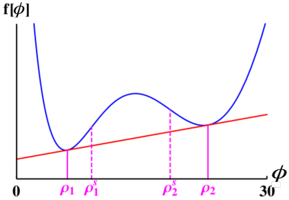




[Tailleur & Cates, PRL 2008; Ann. Rev. Cond. Mat. 2015]

Part III - Incomplete Phase Separation

Photo-activated colloids (experiment)

[J. Palacci et al., Science, 2013]

Repulsive particles (simulations WCA pot)

[J. Stenhammar et al, Soft Matter, 2014]

[Buttinoni et al, PRL 2013; J Schwarz-Linek et al, PNAS 2012; I Theurkauff et al, PRL 2012; ...]

Active Field Theories

$$\dot{\phi} = -\nabla \cdot (\mathbf{J} + \eta) \qquad \mathbf{J} = -\nabla \mu + \zeta(\nabla^2 \phi)\nabla\phi$$

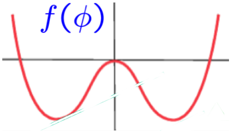
$$\mu(\mathbf{r}) = \frac{\delta \mathcal{F}}{\partial \phi(\mathbf{r})} + \lambda |\nabla \phi|^2 \qquad \mathcal{F} = \int d\mathbf{r} \left[f(\phi) + k|\nabla\phi|^2 \right]$$

$$\langle \eta(\mathbf{r}, t)\eta(\mathbf{r}', t'))\rangle = 2D\,\mathbf{1}\,\delta(\mathbf{r} - \mathbf{r}')\delta(t - t')$$

Minimal modifications of Model B allowing breakdown of Time-Reversal-Symmetry

Lowest order in gradient expansion:

- chemical potential does not derive from a free energy (λ)
- current is not curl-free (ζ)



Active field theories from explicit coarse graining

$$\dot{\mathbf{r}}_i = v(\phi(\mathbf{r}_i))\mathbf{u}_i - \nabla_i \sum_j U(\mathbf{r}_i - \mathbf{r}_j) + \sqrt{2T}\eta_i$$

$$\dot{\mathbf{u}}_i = -\frac{\mathbf{u}_i}{\tau} + \frac{\sqrt{2}}{\tau}\eta_i$$

- Similar in spirit to liquid-state-theory
- Hard-core $\Longrightarrow v(\phi)$
- Tails of the interactions $\Longrightarrow U$

- QS particles + excluded volume

Sign of ζ

U repulsive $\Longrightarrow \zeta > 0$ $\quad$ U attractive $\Longrightarrow \zeta < 0$

Active field theories from explicit coarse graining

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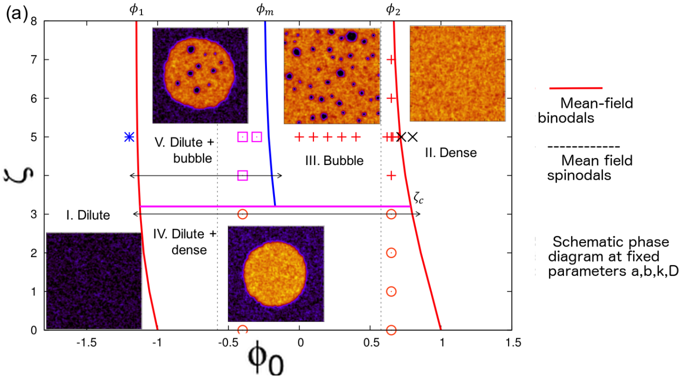
Sign of ζ

U repulsive $\Longrightarrow \zeta > 0$ $\qquad$ U attractive $\Longrightarrow \zeta < 0$

Phase diagram ($\zeta > 0, d = 2$)

$$\dot{\phi} = -\nabla \cdot (\mathbf{J} + \eta) \qquad \mathbf{J} = -\nabla\mu + \zeta(\nabla^2\phi)\nabla\phi \qquad \mu = -a\phi + b\phi^3 - k\nabla^2\phi$$



- average density $\phi_0 = \int d\mathbf{r}\phi$
- $\zeta = 0$: Model B
- noise amplitude: $D = 0.1$
- $a = 1, b = 1, k = 1$

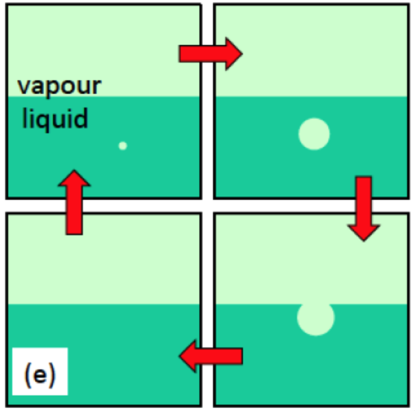
[E. Tjhung, CN, M. Cates, in preparation]

Bubbly phase separation ($\zeta > 0$)

Obvious TRS breakdown in the steady state

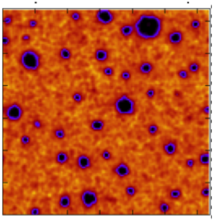
- Bubbles are created by nucleation
- They are destroyed by ejection or merging with others

Bubbles violate Time-Reversal-Symmetry: Circulating phase-space current

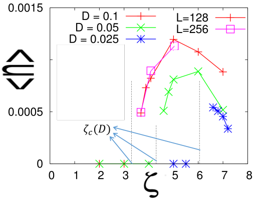


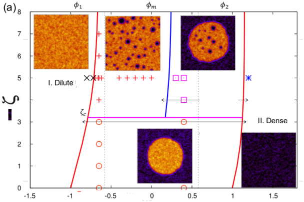
Cluster phase ($\zeta < 0$, low density)

The model is symmetric under $(\zeta, \phi) \to (-\zeta, -\phi)$



$\zeta < 0$:
dense droplets in a dilute environment at low ϕ_0

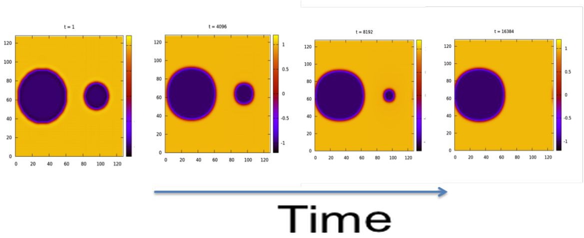




$D = 0.1$

Ostwald Ripening (OR), equilibrium - I

Bubbles/Clusters of different size seem to coexist...



Real-life application of Ostwald Ripening

Mean-field phenomena (no noise $D = 0$)

OR, equilibrium - II

Mean-field argument (no noise $D = 0$)

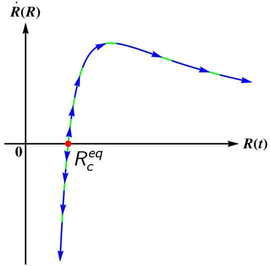
- Quasi-static diffusion of the droplet
- supersaturated environment ($\phi_\infty = \phi_{binodal} - \epsilon$)
- R: droplet radius, $\sigma \equiv \int_{interface} \phi'^2$: surface tension
- Laplace pressure $P \propto \sigma/R$

$$\dot{R} \propto \frac{\sigma\alpha}{R}\left(\frac{1}{R_c^{\zeta=0}} - \frac{1}{R}\right) + \mathcal{O}\left(\frac{1}{R^3}\right)$$

$$\alpha = k/\Delta\phi^2$$

$$\Delta\phi = \text{density difference}$$

$$R_c^{\zeta=0} = \sigma/\epsilon$$



$R \sim t^{1/3}$ at large times $\tau_{coarsening}^{\zeta=0} \sim R(0)^3/\alpha$

Exponentially suppressed OR

- $\zeta \neq 0$ causes a strong slow-down of Ostwald Ripening

$$\dot{R} \propto \frac{\sigma \alpha e^{-\zeta \Delta\phi / k}}{R} \left(\frac{1}{R_c} - \frac{1}{R} \right) + \mathcal{O}\left(\frac{1}{R^3} \right)$$

- Still, $R \sim t^{1/3}$ at large times (but exponentially large in ζ / k !)

$$t_{coarsening} \sim t_{coarsening}^{\zeta=0} \; e^{\zeta \Delta\phi / k}$$

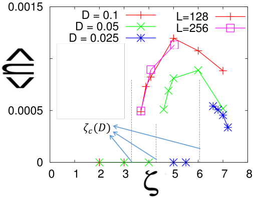
- Small clusters can be nucleated (when $D \neq 0$)

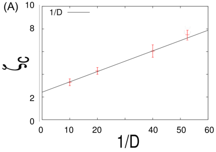
$$R_c = R_c^{\zeta=0} e^{-\zeta \Delta\phi / k}$$

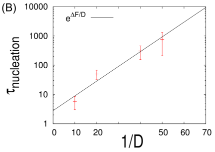
A rare-event activated transition

Transition to cluster/bubble phase takes place when $\tau_{Nucleation} \sim \tau_{coarsening}$

- $\zeta_c = \zeta_c(D) \uparrow$ when $D \downarrow$
- Well defined average density of clusters $\langle n \rangle$







Assuming $\tau_{Nucleation} \sim e^{-A/D}$

$$\Longrightarrow \zeta_c \sim 1/D$$

Thank you!

- F. Bouchet, K. Gawedzki, CN, J. Stat. Phys., 163, 2016
- E. Fodor, CN, ME Cates, J Tailleur, P Visco, F van Wijland, PRL, 2016
- E Tjhung, CN, ME Cates, in preparation