



École doctorale 209 : Sciences physiques et de l'ingénieur

THESIS

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presented by

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Confinement and driving effects on continuous and discrete model interfaces

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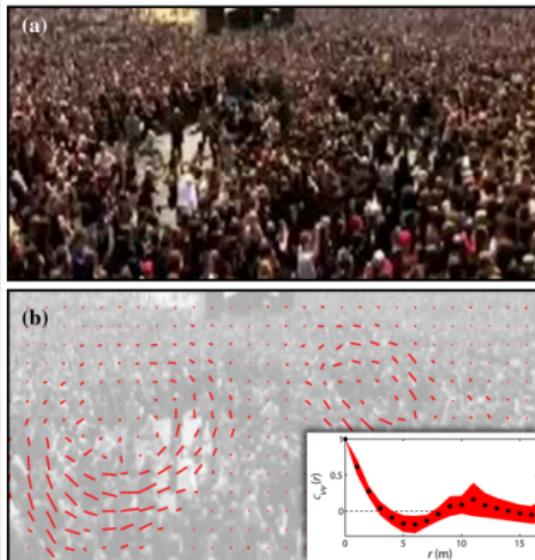
Université de Bordeaux, Laboratoire Onde Matière d'Aquitaine, 351 Cours de la Libération, Talence, France

Content

- 1 Statistical description of physical systems
- 2 Interface definition
- 3 Confinement forces
- 4 Out-of-equilibrium steady-states
- 5 Conclusion and Perspectives

Statistical systems

Collective behavior from a large number of degrees of freedom

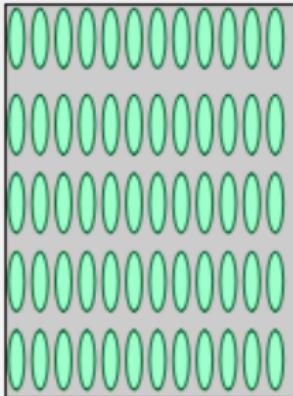


*Collective Motion of Humans in Mosh and Circle Pits at Heavy Metal Concerts
[Silverberg et al. 2013]*

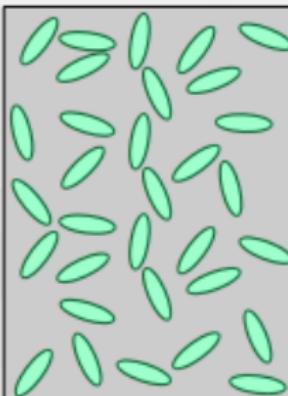
Order parameter : mean people's density (conserved)

Statistical systems

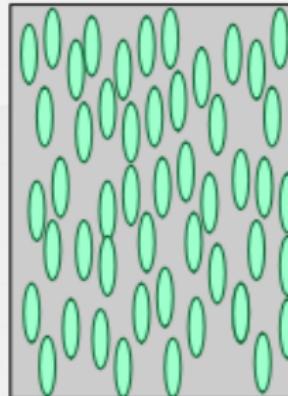
Collective behavior from a large number of degrees of freedom



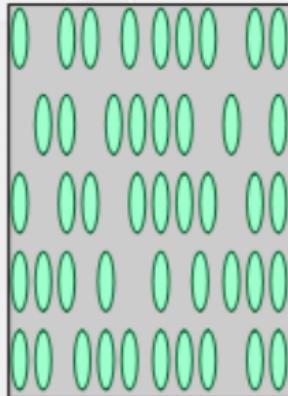
Solid phase:
orientation and
periodicity



Liquid phase:
no orientation
or periodicity



**Nematic
phase:**
orientation, no
periodicity



**Smectic
phase:**
orientation with
some periodicity

Schematics of liquid crystals [Chem.libretext.org]

Order parameter : mean liquid crystal's orientation (non-conserved)

Statistical field theory

Continuous field $\phi(\mathbf{x}, t)$: density, magnetization, orientation... [Hohenberg et Halperin 1977 (18), Bray 1994 (22)]

Total order parameter : $\Phi(t) = \int d\mathbf{x} \phi(\mathbf{x}, t)$

Brownian field dynamics

$$\frac{\partial \phi(\mathbf{x})}{\partial t} = -L \frac{\delta H}{\delta \phi(\mathbf{x})} + \eta(\mathbf{x}, t), \quad \langle \eta(\mathbf{x}, t) \eta(\mathbf{x}', t') \rangle = \delta(t - t') \Gamma(\mathbf{x}, \mathbf{x}') \quad (1)$$

$$p(\phi) = \exp(-\beta H[\phi]), \quad \Gamma(\mathbf{x}, \mathbf{x}') = 2T L(\mathbf{x}, \mathbf{x}') \quad (2)$$

Grand Canonical ensemble : model A

$$\Phi(t) \neq cte$$

$$L(\mathbf{x}, \mathbf{x}') = \alpha \delta(\mathbf{x} - \mathbf{x}'),$$

$$\frac{\partial \phi(\mathbf{x})}{\partial t} = -\alpha \frac{\delta H}{\delta \phi(\mathbf{x})} + \eta(\mathbf{x}, t) \quad (3)$$

Discrete : Glauber dynamics

Canonical ensemble : model B

$$\Phi(t) = cte$$

$$L(\mathbf{x} - \mathbf{x}') = -D \nabla^2 \delta(\mathbf{x} - \mathbf{x}')$$

$$\frac{\partial \phi(\mathbf{x})}{\partial t} = \nabla \cdot [D \nabla \frac{\delta H}{\delta \phi(\mathbf{x})} + \eta(\mathbf{x}, t)] \quad (4)$$

Discrete : Kawasaki dynamics

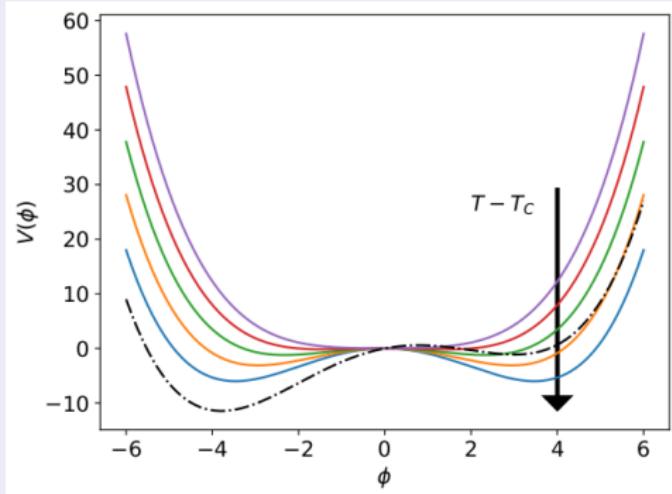
Phase separation

Ginzburg-Landau Hamiltonian [Landau et Lifschitz 1990 (1)]

$$H[\phi] = \int d\mathbf{x} \quad \underbrace{\frac{\kappa}{2} [\nabla \phi]^2}_{\text{cost of changing } \phi} + \underbrace{V(\phi)}_{\text{phase separating potential}} \quad (5)$$

ϕ^4 potential

$$V(\phi) = \frac{1}{2}(T - T_C)\phi^2 + \frac{\lambda}{4!}\phi^4 \quad (6)$$



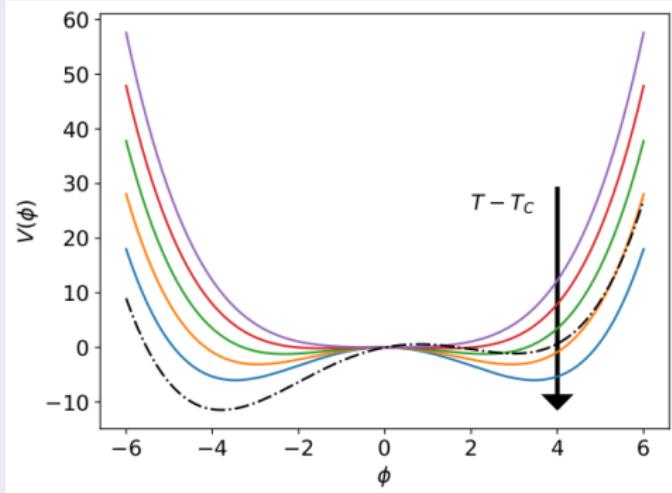
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ϕ^4 potential

$$V(\phi) = \frac{1}{2}(T - T_C)\phi^2 + \frac{\lambda}{4!}\phi^4 + B\phi \quad (7)$$



Interface between two coexisting phases

Mean-field equilibrium system (dynamic independent)

$$\cancel{\frac{\partial \phi(\mathbf{x})}{\partial t}} = -L \frac{\delta H}{\delta \phi(\mathbf{x})} + \eta(\mathbf{x}, t) \implies \frac{\delta H}{\delta \phi(\mathbf{x})} = 0 \quad (8)$$

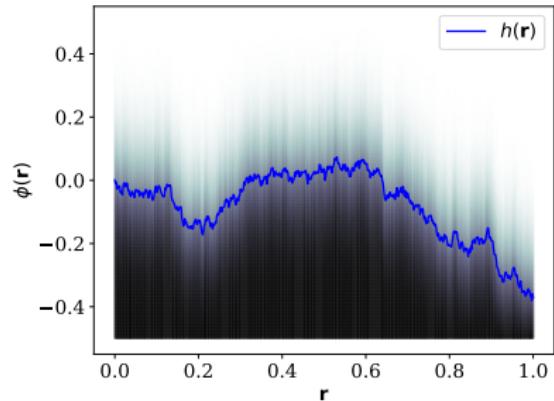
ϕ^4 mean-field kink solution ($h = 0$)

$$\phi_K(z) = \tanh\left(\frac{z}{\xi_\perp}\right) \quad (9)$$

Interface SFT approximation

$$\phi(\mathbf{x}, t) = f(z - h(\mathbf{r}, t)) \quad (10)$$

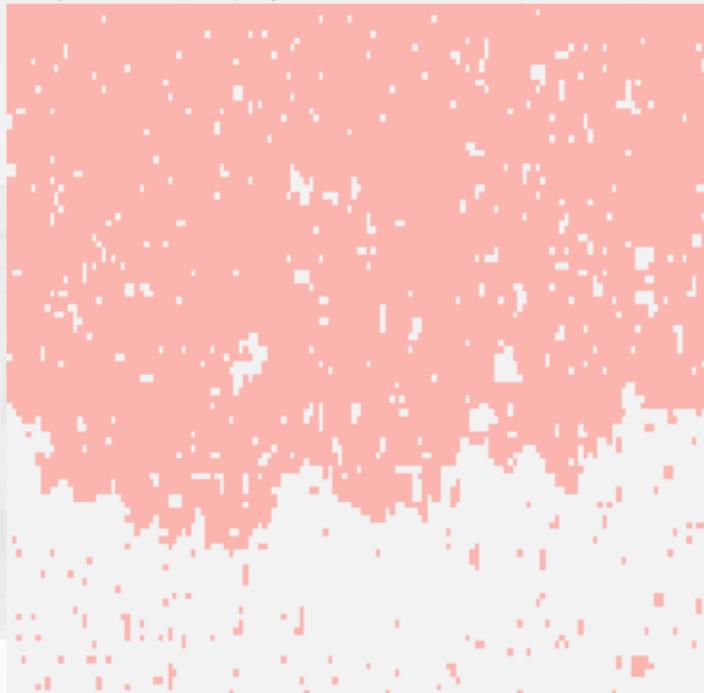
$$\phi_K(z) = f(z) \quad (11)$$



Interface schematics

Interface examples

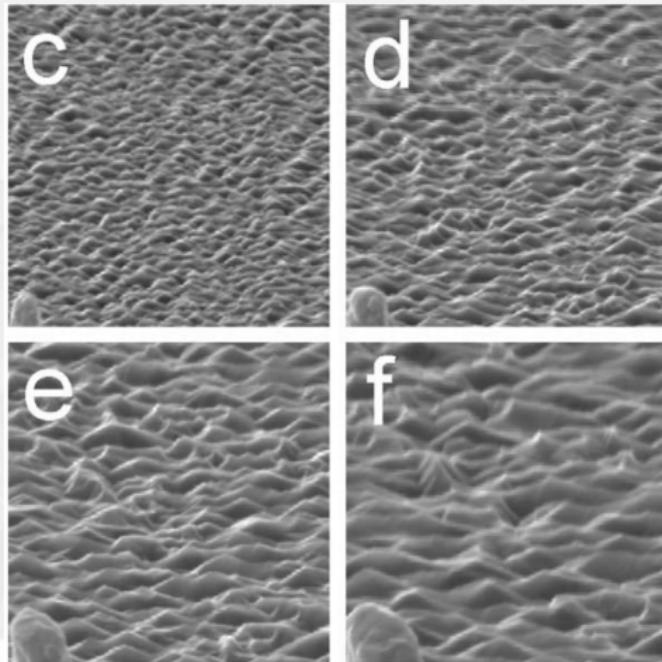
Equilibrium (boundary conditions), grand-canonical (discrete model A - Glauber)



2D Ising Monte Carlo simulation, $T = 0.85T_C$

Interface examples

Out-of-equilibrium (initial conditions) surface growth, grand-canonical (model A)



SEM movie showing a gallium arsenide film grown on silicon [Finnie et al. 2000]

Interface examples

Equilibrium, canonical (model B)



Water-oil interface

Interface examples

Out-of-equilibrium (initial conditions), canonical (model B)



Pigment concentration in cocktails [Cocktailmag.fr]

Surface tension

Definition by the free energy [Abrahams et Reed 76 (46)]

$$\sigma = f_{interface} - f_{homogeneous}[E \cdot L^{-2}] \quad (12)$$

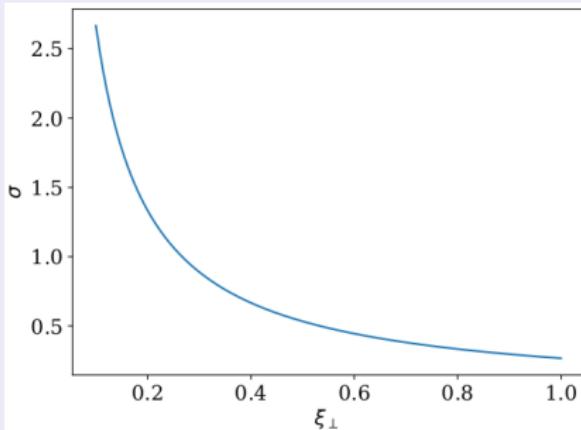
Cahn-Hilliard estimate
[Cahn et Hilliard 58 (25)]

$$\sigma = \int dz \kappa \left(\frac{d\phi_K(z)}{dz} \right)^2 \quad (13)$$

Limits

- $\xi_{\perp} \rightarrow 0$: sharp interface
- $\xi_{\perp} \rightarrow \infty$: ultra-low surface tension, critical systems

Surface tension with respect to interface width ξ_{\perp}



Confinement forces [chapter 3]

Excess free energy and Casimir force [Gambassi 09 (3)]

$$F(t, h, L) = L'^2 \left(L f_{bulk} + \beta^{-1} f_{ex} \right) \quad (14)$$

$$f_{casimir} = -\beta^{-1} \frac{\partial f_{ex}}{\partial L} \quad (15)$$

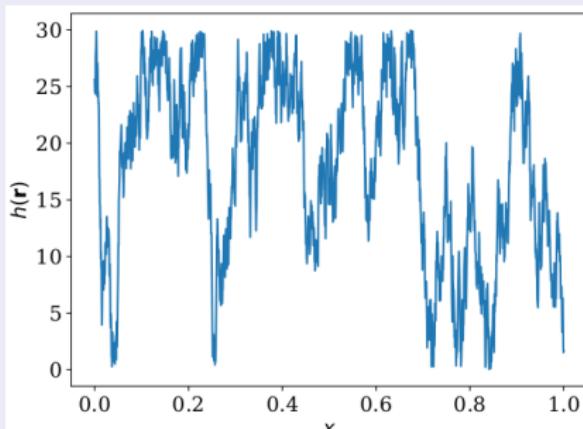
1D Confined elastic line $0 < h(\mathbf{r}, t) < L$

$$f = \frac{T^2 \pi^2}{2\sigma L^2} \quad (16)$$

Finite-size effects surface tension
[Privman 1988 (16)]

$$\sigma(L) \simeq \sigma_{bulk} + \frac{T a}{L} \quad (17)$$

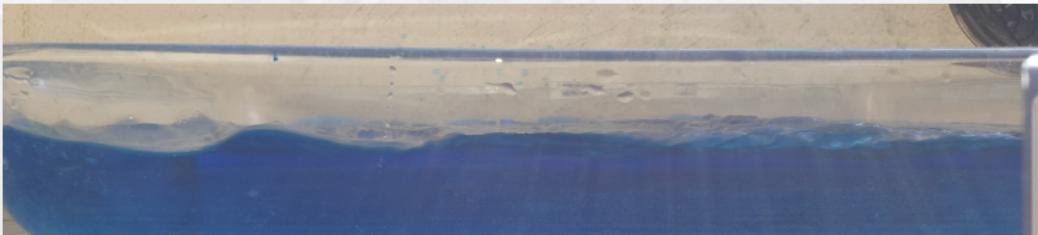
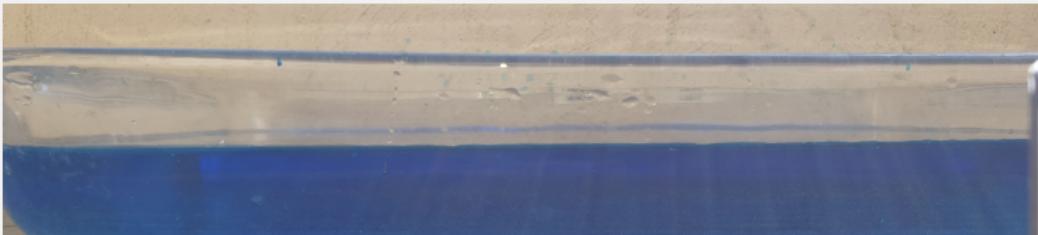
$$f_c = \frac{T \pi^2}{2 a L} \quad (18)$$



Confined interface for $L_Y = 30$ schematics

How do out-of-equilibrium steady-states affect interfaces ?

Driving at the interface



Home-made wind generated waves (from a hair dryer)

The Solid-On-Solid model

Solid-On-Solid model

Lattice model with interface height h_i

$$H = J \sum_{i=0}^{L'} |h_i - h_{i+1}| + \mu \sum_{i=0}^{L'} \frac{h_i + h_{i+1}}{2} \quad (19)$$

Metropolis algorithm

- Glauber

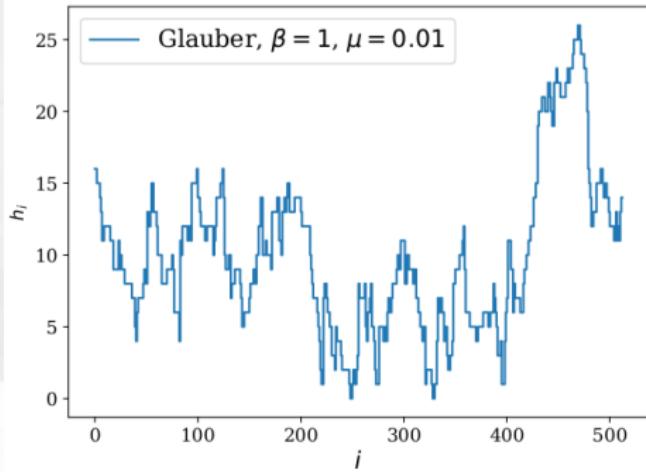
$$\{h_i\} \rightarrow \{h_i \pm 1\} \quad (20)$$

- Kawasaki ($\sum h_i = cte$)

$$\{h_i, h_{i\pm 1}\} \rightarrow \{h_i - 1, h_{i\pm 1} + 1\} \quad (21)$$

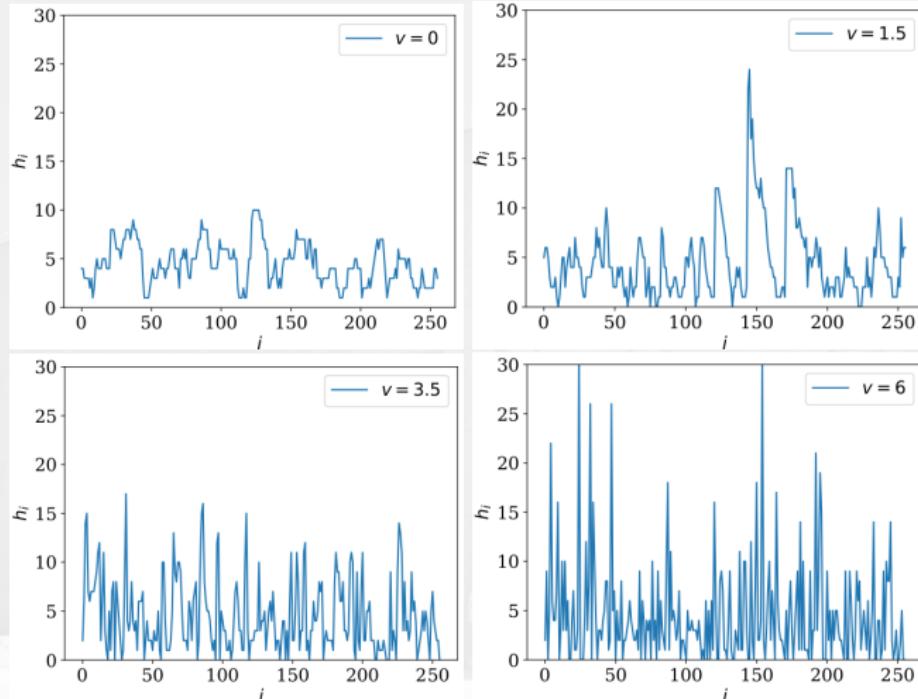
- New configuration with probability

$$A(C \rightarrow C') = \exp(-\beta \Delta H) \quad (22)$$



Driving at the interface

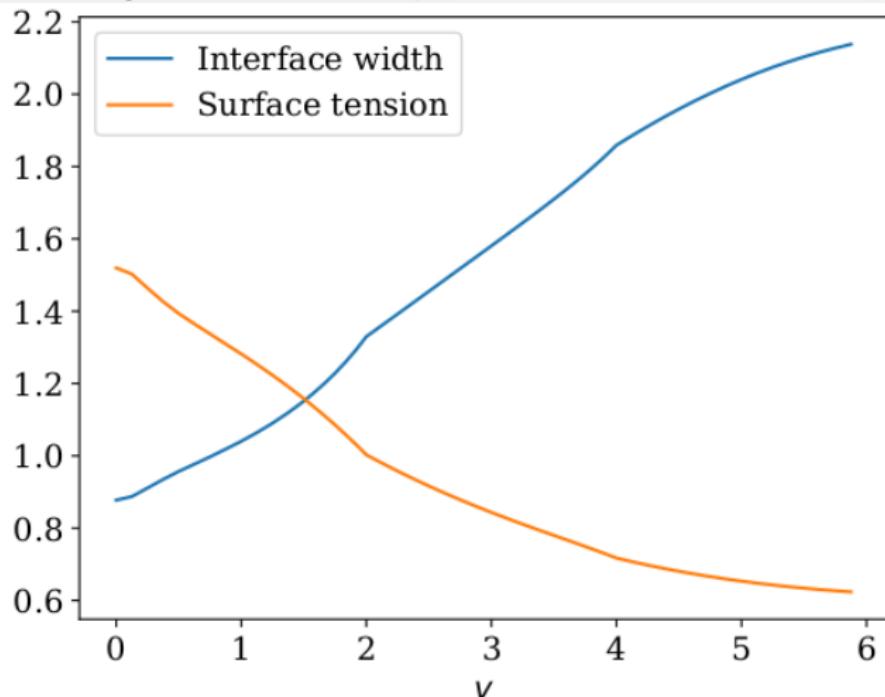
Driving : $\Delta E_d = \Delta E_{eq} \pm v$ in Kawasaki dynamics



$$\beta = 1, L_Y = 200, \frac{1}{L'} \sum h_i = 4.51$$

Driving at the interface

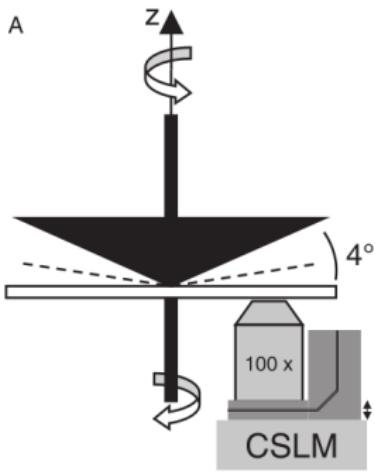
Driving : $\Delta E_d = \Delta E_{eq} \pm v$ in Kawasaki dynamics



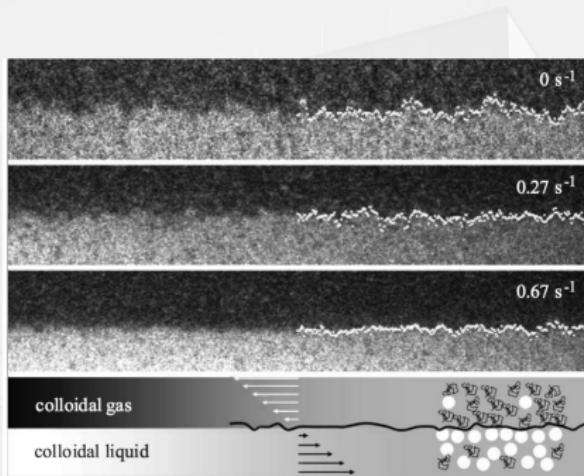
Monte Carlo driving of SOS interface at $\beta = 1$ and $\frac{1}{L'} \sum h_i = 4.51$

What happens if we shear not only the interface, but the whole system ?

PMMA polymers in polystyrene solvent under shear [Derks et al. 2006]

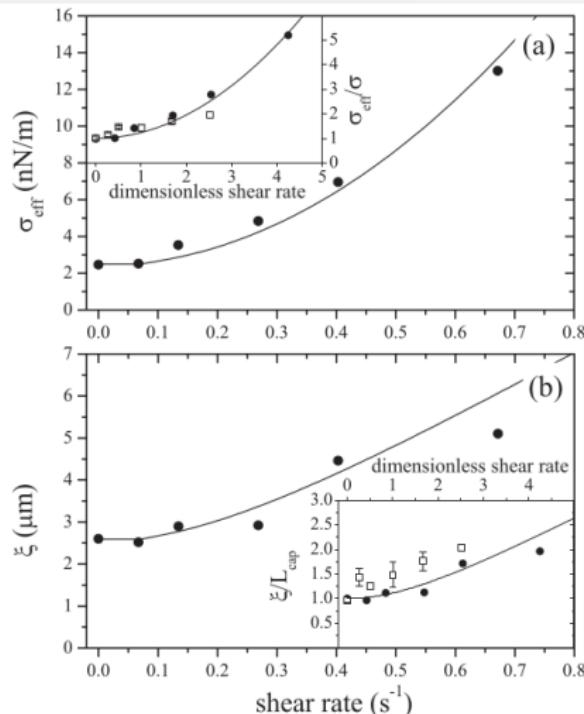


Experimental setup
[Derks et al. 2004]



Interface snapshots under shear
[Derks et al. 2006]

PMMA polymers in polystyrene solvent under shear [Derks et al. 2006]



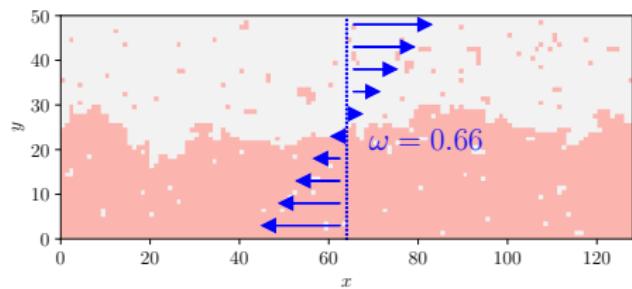
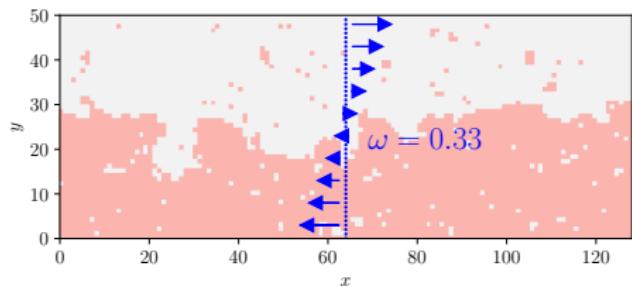
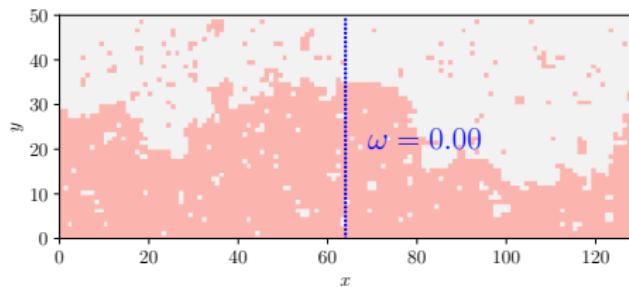
Effective interfacial tension and correlation length along the interface

Phenomenological model

Modes slower than shear rate no longer contribute to the entropy of the interface

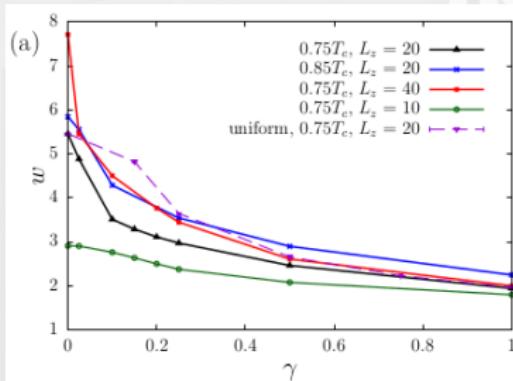
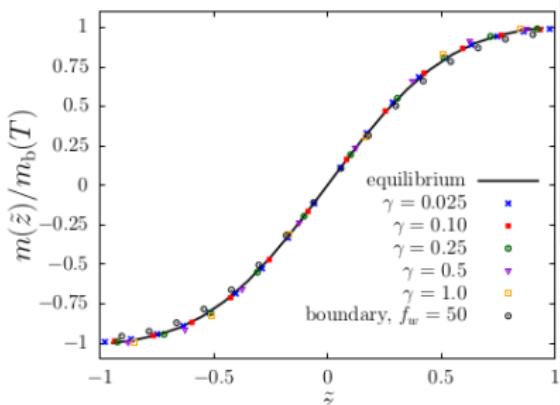
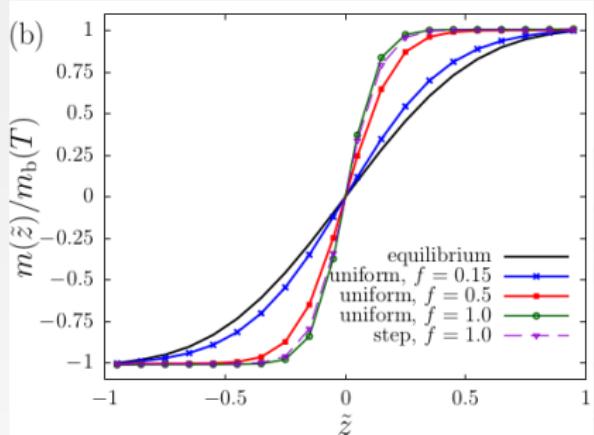
$$\sigma_{eff}(\dot{\gamma}) = \sigma + \frac{3k_B T}{4\pi} \frac{\dot{\gamma}\tau_{cap}}{L_{cap}^2} \sqrt{(\dot{\gamma}\tau_{cap})^2 - 1} \quad (23)$$

2D sheared or driven Ising model [T.H.R. Smith 2010 (71)]



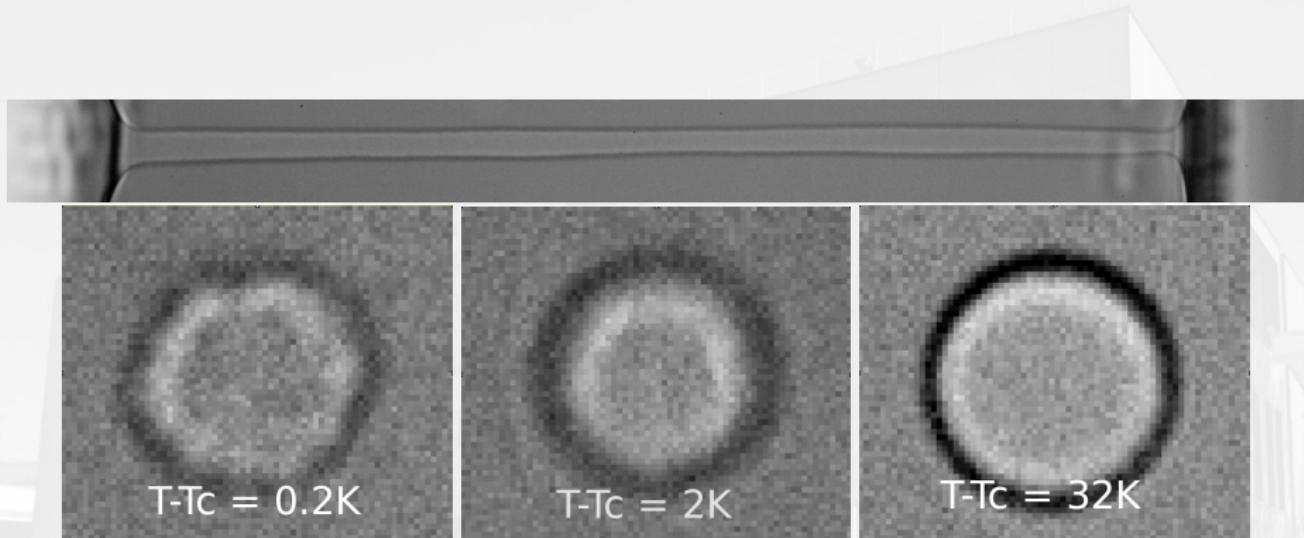
Snapshots of 2D Ising driven systems for $T = 0.9T_C$

2D sheared or driven Ising model [T.H.R. Smith 2010 (71)]



Magnetisation profiles, rescaled magnetisation profiles, interfacial width with respect to shear for different L_Y

Binary mixture under laser radiation pressure [Delville et al. 08 (J. Opt. A)]



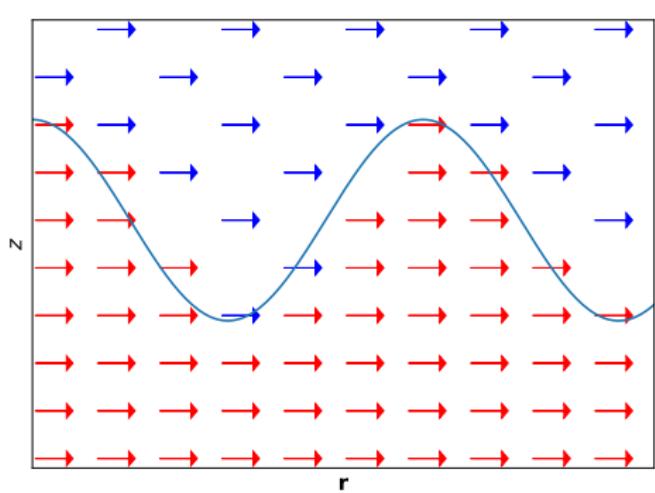
Pictures from R. Saiseau

Quaternary liquid mixture made of toluene, sodium dodecyl sulfate (SDS), n-butanol and water gives 2 separate micellar phases

Imposed hydrodynamic flow

Advecting the field $\psi(\mathbf{x}, t)$ with a flow $\mathbf{v}(\mathbf{x})$ gives

$$\frac{\partial \psi(\mathbf{x}, t)}{\partial t} + \nabla \cdot (\mathbf{v}\psi(\mathbf{x}, t)) = D\nabla^2 \frac{\delta H}{\delta \psi(\mathbf{x})} + \sqrt{2DT} \nabla \cdot \boldsymbol{\eta}_1(\mathbf{x}, t) \quad (24)$$



Uniform advecting flow $\mathbf{v}(\mathbf{x}, t) = v \mathbf{e}_x$ in the **sharp interface approximation**, galilean invariance $\mathbf{x} \rightarrow \mathbf{x} + vt$

The effect of driving on model C interfaces [Dean, Gersberg, Holdsworth 2020 (17)]

ψ : colloid field under model B dynamics

ϕ : passive solvent under model A dynamics

$$H[\psi, \phi] = H_1[\psi] + H_2[\psi, \phi] \quad (25)$$

$$H_1[\psi] = \int d\mathbf{x} \left[\frac{\kappa}{2} [\nabla \psi(\mathbf{x})]^2 + V(\psi(\mathbf{x})) - gz\psi(\mathbf{x}) \right] \quad (26)$$

$$H_2[\psi, \phi] = \int d\mathbf{x} \frac{\lambda}{2} (1 - \psi(\mathbf{x}) - \phi(\mathbf{x}))^2 \quad (27)$$

κ : interface energy

V : phase separating potential

g : gravitational term introducing finite size correlations

λ : coupling parameter

Model C dynamics

Equations

$$\frac{\partial \psi(\mathbf{x}, t)}{\partial t} + \mathbf{v} \cdot \nabla \psi(\mathbf{x}, t) = D \nabla^2 \frac{\delta H}{\delta \psi(\mathbf{x})} + \sqrt{2DT} \nabla \cdot \boldsymbol{\eta}_1(\mathbf{x}, t) \quad (28)$$

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = -\alpha \frac{\delta H}{\delta \phi(\mathbf{x})} + \sqrt{2\alpha T} \eta_2(\mathbf{x}, t) \quad (29)$$

are coupled by H_2 , with a closed form on ψ

$$\underbrace{\frac{\partial \psi(\mathbf{x}, t)}{\partial t}}_{\text{evolution}} - \underbrace{\lambda D \nabla^2 \int_{-\infty}^t dt' \exp(-\alpha \lambda (t - t')) \frac{\partial \psi(\mathbf{x}, t')}{\partial t}}_{\text{coupling term}} + \underbrace{\mathbf{v} \cdot \nabla \psi(\mathbf{x}, t)}_{\text{advection}} = \underbrace{D \nabla^2 \mu(\mathbf{x}, t')}_{\text{model B}} + \underbrace{\zeta(\mathbf{x}, t)}_{\text{thermal noise}} \quad (30)$$

where

$$\mu(\mathbf{x}, t) = \frac{\delta H_1}{\delta \psi(\mathbf{x}, t)} \quad (31)$$

and

$$\tilde{\zeta}(\mathbf{x}, \omega) = \frac{\sqrt{2\alpha T} D \lambda}{i\omega + \alpha \lambda} \nabla^2 \tilde{\eta}_2(\mathbf{x}, \omega) + \sqrt{2DT} \nabla \cdot \tilde{\boldsymbol{\eta}}_1(\mathbf{x}, \omega). \quad (32)$$

Model C interface dynamics

Interface approximation $\psi(\mathbf{x}, t) = f(z - h(\mathbf{r}, t))$ using method of Bray et al. 2001 (9,29)] at first order in h

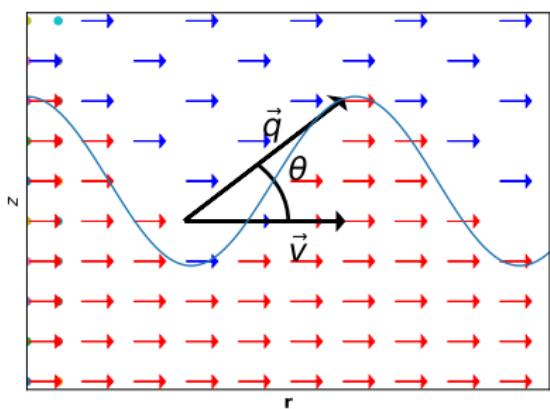
$$\begin{aligned} \Delta\psi^2 \int d\mathbf{r} G(0, \mathbf{r} - \mathbf{r}') & \left[\frac{\partial h(\mathbf{r}, t)}{\partial t} + \mathbf{v} \cdot \nabla h(\mathbf{r}, t) \right] = \sigma [\nabla^2 h(\mathbf{r}, t) - m^2 h(\mathbf{r}, t)] + \xi(\mathbf{r}, t) \\ & + \frac{\sigma\lambda D}{\kappa} \int_{-\infty}^t dt' \exp(-\alpha\lambda(t - t')) \frac{\partial h(\mathbf{r}, t')}{\partial t'} \end{aligned} \quad (33)$$

where $G = -\nabla^{-2}$, $\xi(\mathbf{r}, t) = \int_{-\infty}^{\infty} dz f'(z - h(\mathbf{r}, t)) \nabla^{-2} \zeta(\mathbf{x}, t)$, $m^2 = \Delta\psi g / \sigma$

Model C interface correlation function

Correlation function

$$\tilde{C}_s(\mathbf{q}) = T \frac{(2D\sigma q(\kappa[q^2 + m^2] + \lambda) + \alpha\kappa\lambda\Delta\psi^2)^2 + \kappa^2\Delta\psi^4(\mathbf{q} \cdot \mathbf{v})^2}{\sigma[q^2 + m^2](2Dq\sigma(\kappa[q^2 + m^2] + \lambda) + \alpha\kappa\lambda\Delta\psi^2)^2 + \kappa(\kappa\sigma[q^2 + m^2] + \lambda\sigma)\Delta\psi^4(\mathbf{q} \cdot \mathbf{v})^2} \quad (34)$$



No driving $v \rightarrow 0$

$$\tilde{C}_s(\mathbf{q}) = \frac{T}{\sigma[q^2 + m^2]} \quad (35)$$

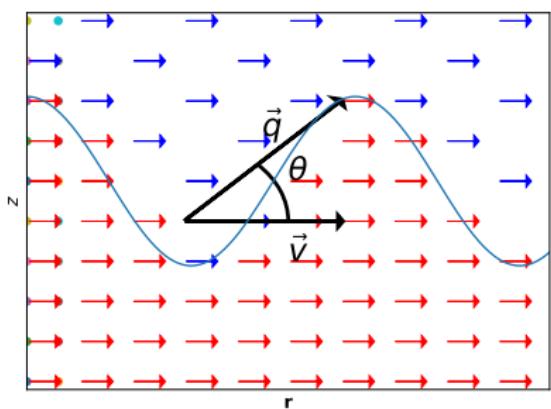
Infinite driving $v \rightarrow \infty$

$$\tilde{C}_s(\mathbf{q}) = \frac{T}{\sigma[q^2 + m^2 + \frac{\lambda}{\kappa}]} \quad (36)$$

Model C interface correlation function

Correlation function

$$\tilde{C}_s(\mathbf{q}) = T \frac{(2D\sigma q(\kappa[q^2 + m^2] + \lambda) + \alpha\kappa\lambda\Delta\psi^2)^2 + \kappa^2\Delta\psi^4(\mathbf{q} \cdot \mathbf{v})^2}{\sigma[q^2 + m^2](2Dq\sigma(\kappa[q^2 + m^2] + \lambda) + \alpha\kappa\lambda\Delta\psi^2)^2 + \kappa(\kappa\sigma[q^2 + m^2] + \lambda\sigma)\Delta\psi^4(\mathbf{q} \cdot \mathbf{v})^2} \quad (34)$$



Small \mathbf{q} approximation

- Angle-dependent surface tension

$$\sigma_s(\theta) = \sigma \left(1 + \frac{\mathbf{v}^2 \cos^2(\theta)}{v_0^2} \right) \quad (37)$$

- Angle-dependent correlation length

$$\xi_s = \xi_{eq} \sqrt{1 + \frac{\mathbf{v}^2 \cos^2(\theta)}{v_0^2}} \quad (38)$$

- Intrinsic velocity

$$v_0 = \sqrt{\alpha^2 \lambda \kappa} \quad (39)$$

Conclusion

Chapter 3 : Equilibrium Interface models and their finite size effects

- General method to compute free energy and probability distribution functions of continuous gaussian interfaces with path integral method
- Casimir-type effect have an interesting manifestation in interface physics
- Generalization the Lopes Cardozo-Jacquin-Holdsworth method to compute free energy in numerical Monte Carlo lattice systems for any type of external potentials, useful for Kawasaki dynamics
- Exact diagonalization of the finite Solid-On-Solid transfer matrix

Chapter 4 : Beyond Solid-On-Solid : the Particles-Over-Particles model

- New model generated from SOS with entropic term
- Multi-particles formulation allow for particles coupling with different temperatures or thermodynamical ensembles (model C) and different hydrodynamical flows (which gives us the idea for model C' paper)
- Numerical Monte Carlo issues : corner case of Metropolis algorithm

Conclusion

Chapter 5 : Driven interfaces

- Similarities between shearing and driving
- Steady-state out-of-equilibrium driving needs a coupling between two fields due to Galilean invariance (model C)
- Increase of the effective surface tension in the direction of driving and also an increase in the correlation length of the height fluctuations with respect to a non-driven equilibrium interface
- Uniform driving leads to effective equilibrium statistics
- Driving at the interface in SOS model does increase interface width, as in wind generated waves

Perspectives

- Thanks to the generalized free energy computation method, study the difference between thermodynamical ensembles on finite-size critical systems
- Get deeper on the relationship between critical and interface systems
- Solve POP's numerical problems. Study coupled systems as presented model C through it
- Better understand the difference between driving at interface and bulk driving
- Do out-of-equilibrium confined interfaces have different physics than equilibrium confined ones ?