

## École doctorale 209 : Sciences physiques et de l'ingénieur

THESIS

to obtain a PhD from

Université de Bordeaux

Spécialité doctorale “Laser, Matière, Nanosciences”

presented by

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on July 16th 2020

# Confinement and driving effects on continuous and discrete model interfaces

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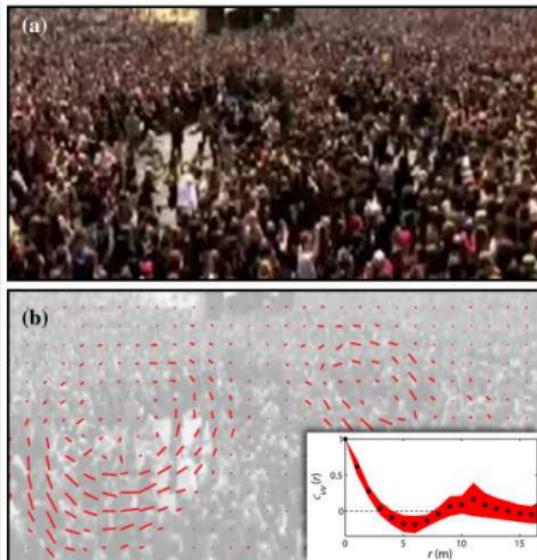
Université de Bordeaux, Laboratoire Onde Matière d'Aquitaine, 351 Cours de la Libération, Talence, France

# Content

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

# Statistical systems

Collective behavior from a large number of degrees of freedom

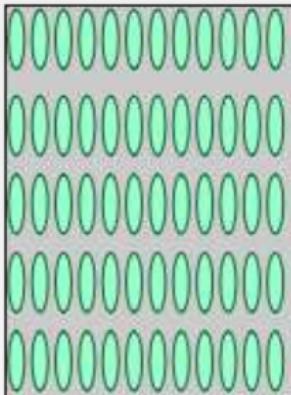


*Collective Motion of Humans in Mosh and Circle Pits at Heavy Metal Concerts  
[Silverberg et al. 2013]*

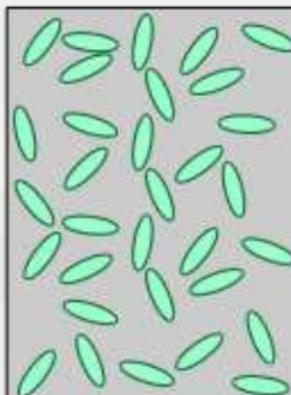
Order parameter : mean people's density (conserved)

# Statistical systems

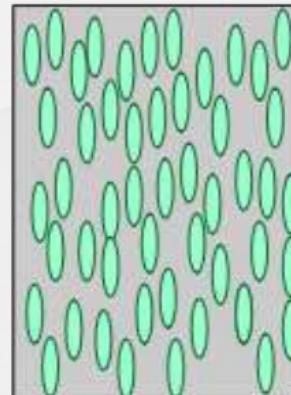
Collective behavior from a large number of degrees of freedom



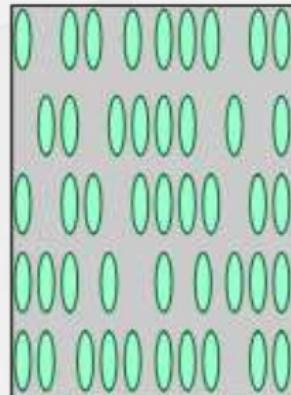
**Solid phase:**  
orientation and  
periodicity



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

## Field dynamics

$$\frac{\partial \phi(\mathbf{x})}{\partial t} = -L \frac{\delta H}{\delta \phi(\mathbf{x})} + \eta(\mathbf{x}, t) \quad (1)$$

$$\langle \eta(\mathbf{x}, t) \eta(\mathbf{x}', t') \rangle = \delta(t - t') \Gamma(\mathbf{x}, \mathbf{x}') , \quad \Gamma(\mathbf{x}, \mathbf{x}') = 2T L(\mathbf{x}, \mathbf{x}') \quad (2)$$

### 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

$$\Phi(t) = cte$$

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

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

Discrete : **Kawasaki** dynamics

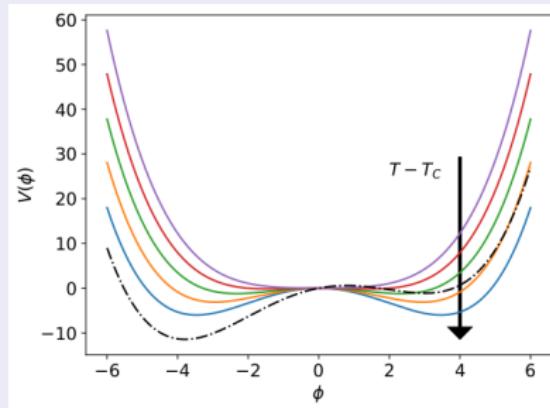
# Phase separation

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

$$H[\phi] = \int d\mathbf{x} \frac{\kappa}{2} [\nabla \phi]^2 + V(\phi) \quad (5)$$

$\phi^4$  potential

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



# Interface between two coexisting phases

Mean-field equilibrium system

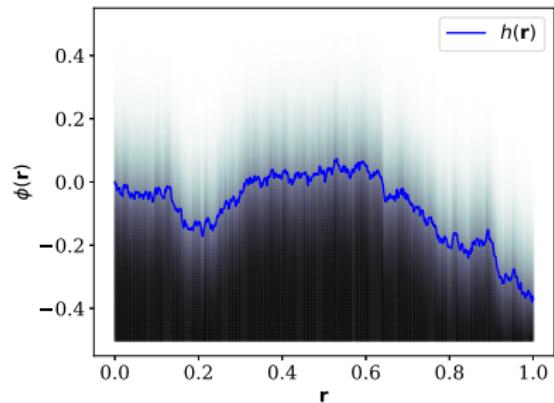
$$\cancel{\frac{\partial \phi(\mathbf{x})}{\partial t}} = -L \frac{\delta H}{\delta \phi(\mathbf{x})} + \eta(\mathbf{x}, t) \implies \frac{\delta H}{\delta \phi(\mathbf{x})} = 0 \quad (7)$$

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

$$\phi_K(z) = \tanh\left(\frac{z}{w}\right) \quad (8)$$

Interface SFT approximation along  $z$

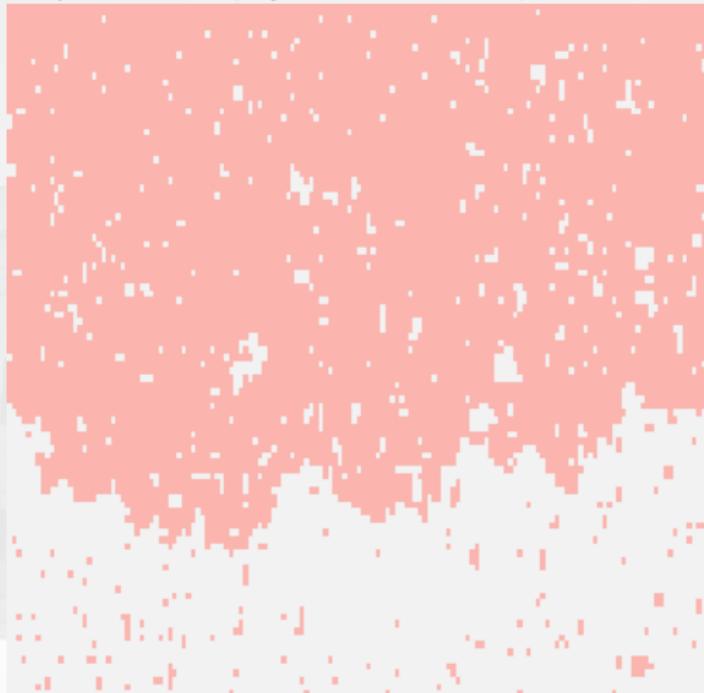
$$\phi(\mathbf{x}, t) = f(z - h(\mathbf{r}, t)) \quad (9)$$



Interface schematics

## Interface examples

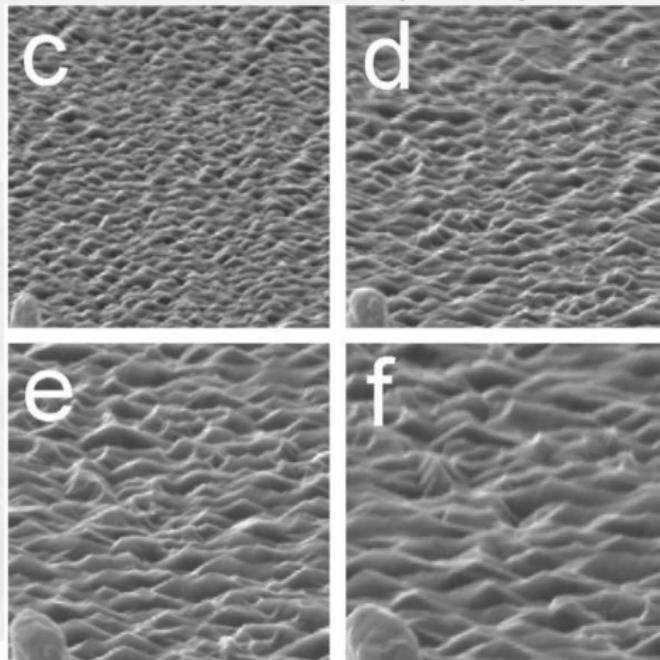
Equilibrium (boundary conditions), grand-canonical (discrete model A - Glauber)



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]

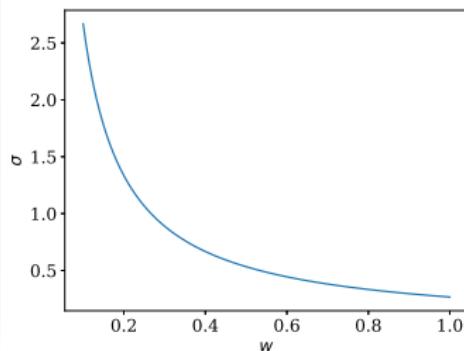
# Surface tension

## Free energy

$$\sigma = f_{interface} - f_{homogeneous}[E \cdot L^{-2}] \quad (10)$$

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

$$\sigma = \int dz \kappa \left( \frac{d\phi_K(z)}{dz} \right)^2 \quad (11)$$



Surface tension with respect to interface width  $w$

# Confinement forces

## Excess free energy [Gambassi 09 (3)]

$$p(t, h, L) = -\frac{1}{L^2} \frac{\partial F}{\partial L} = -f_{bulk} - \beta^{-1} \frac{\partial f_{ex}}{\partial L} \quad (12)$$

## Confined elastic line

Interface is confined :  $0 < h(\mathbf{r}, t) < L$

Free energy

$$f = \frac{T^2 \pi^2}{2\sigma L^2} \quad (13)$$

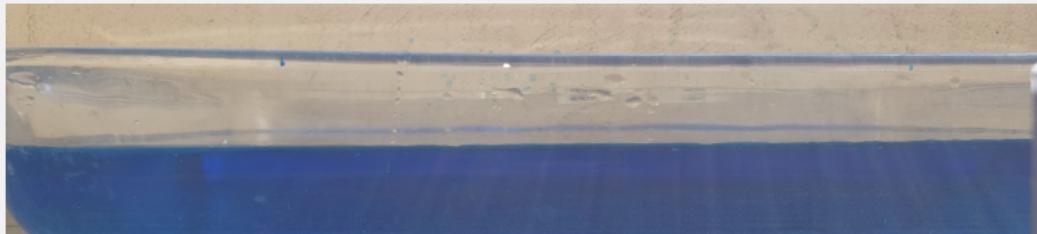
Supposing finite-size effects on surface tension [Privman 1988 (16)]

$$(\sigma(L) \simeq \sigma_{bulk} + \frac{T a}{L}), \text{ for } \sigma_{bulk} \rightarrow 0$$

$$f_c = \frac{T \pi^2}{2 a L}, \quad \text{excess free energy in Casimir form} \quad (14)$$

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

# Shearing at the interface



Wind generated waves (from a hair dryer)

# The Solid-On-Solid model

## Solid-On-Solid model

Lattice model with interface height  $h_i$

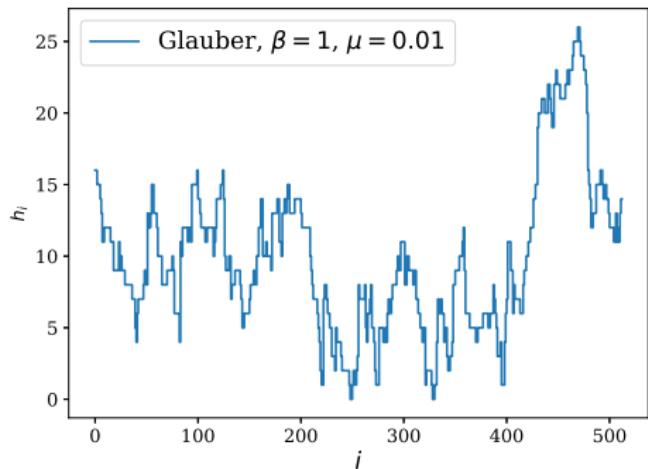
$$H = J \sum_{i=0}^{L'} |h_i - h_{i+1}| + B \frac{V(h_i) + V(h_{i+1})}{2} \quad (15)$$

## Kawasaki driving algorithm

- Generate new configuration

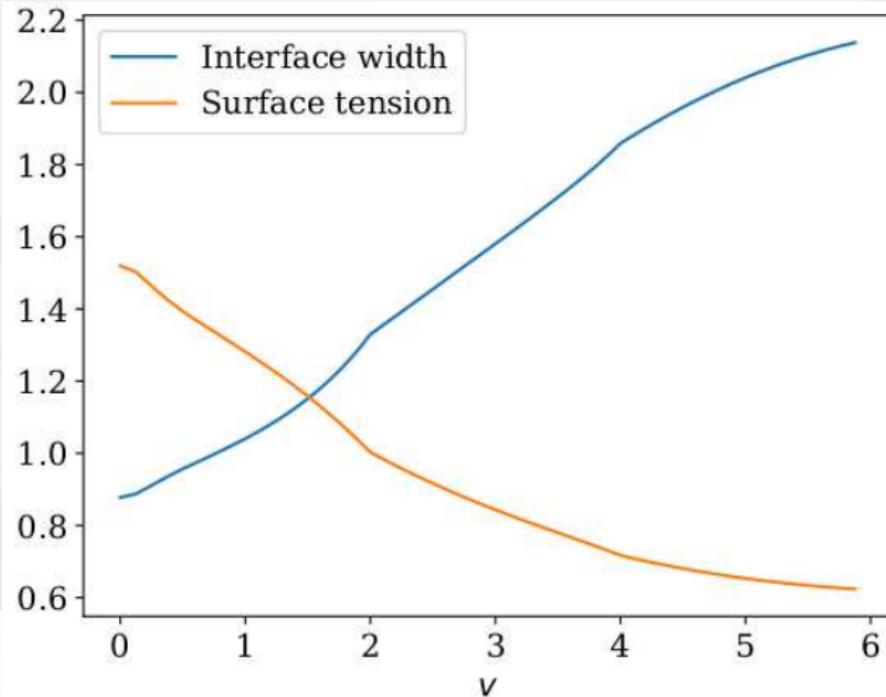
$$\begin{aligned} C &= h_0, \dots, h_i, \dots, h_L' \rightarrow \\ C' &= h_0, \dots, h_i - 1, h_{i+1} + 1, \dots, h_L' \end{aligned} \quad (16)$$

- Accepte new configuration with rate  $A(C \rightarrow C') = \exp(-\Delta E_{eq})$



# Driving at the interface

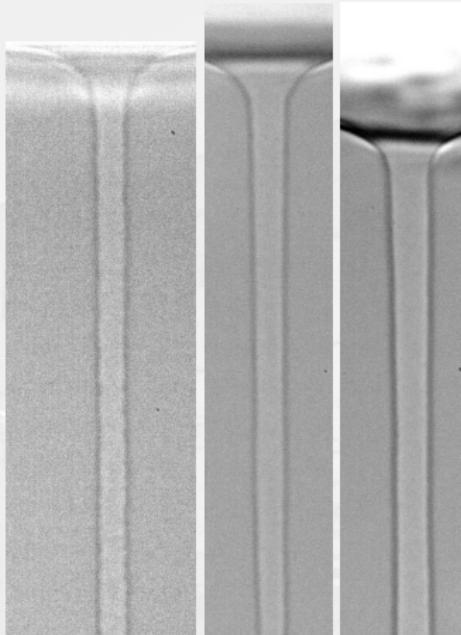
Driving :  $\Delta E_d = \Delta E_{eq} \pm v$  in Kawasaki dynamics



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 ?

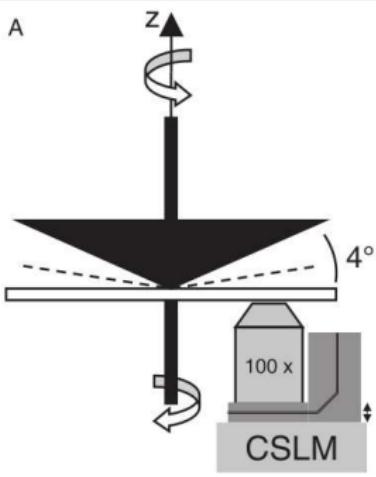
# Binary mixture under laser radiation pressure



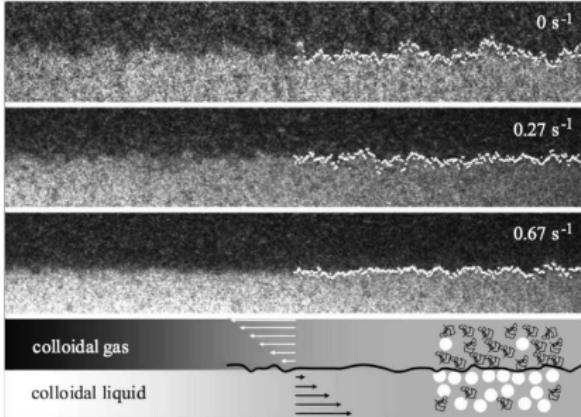
$T - T_C = 1K$  (a),  $T - T_C = 4K$  (b),  $T - T_C = 10K$  (c) [R. Saiseau, Delville et al. 08 (J. Opt. A)]

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

# PMMA polymers in polystyrene solvent under shear

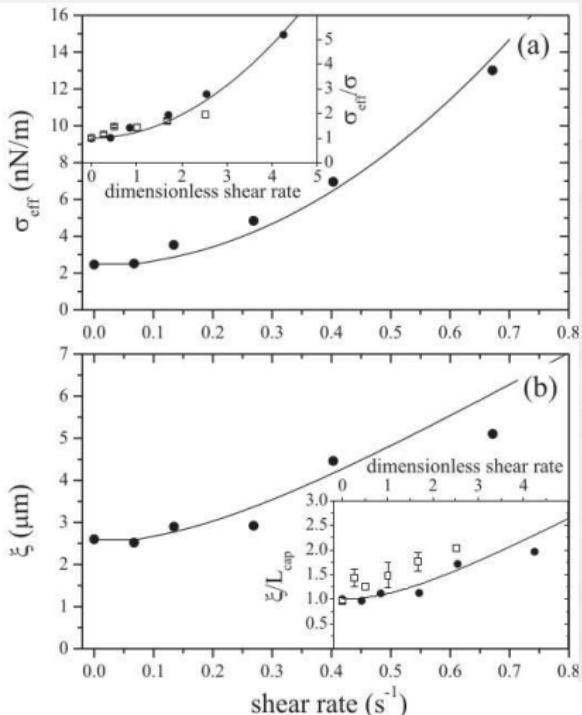


Experimental setup  
[Derk et al. 2004]



Interface snapshots under shear  
[Derk et al. 2006]

# PMMA polymers in polystyrene solvent under shear

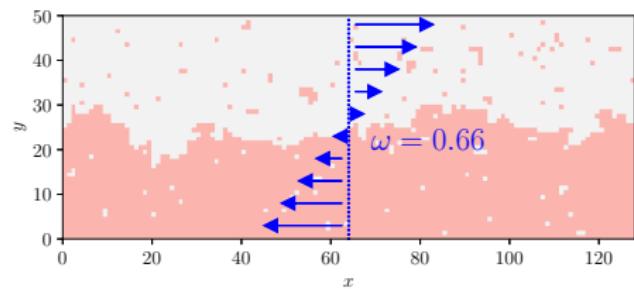
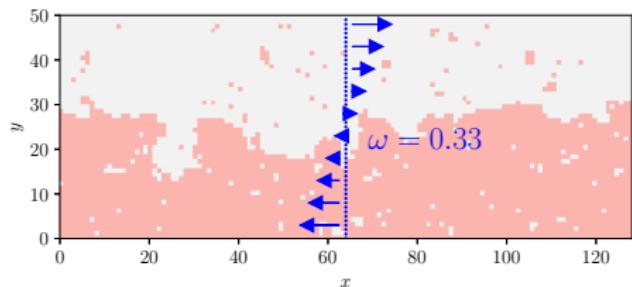
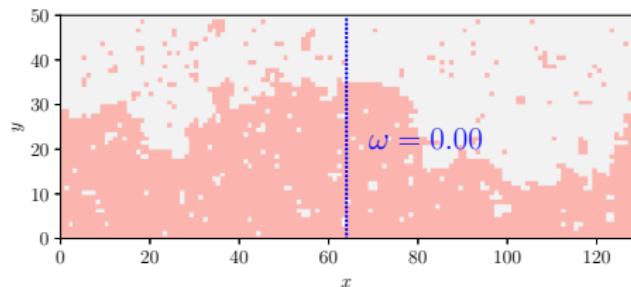


Assuming that slow modes, while still present, no longer contribute to the entropy of the interface, effective surface tension becomes

$$\sigma_{eff}(\dot{\gamma}) = \sigma + \frac{3k_B T}{4\pi} \frac{\dot{\gamma}\tau_{cap}}{L_{cap}^2} \sqrt{(\dot{\gamma}\tau_{cap})^2 - 1} \quad (17)$$

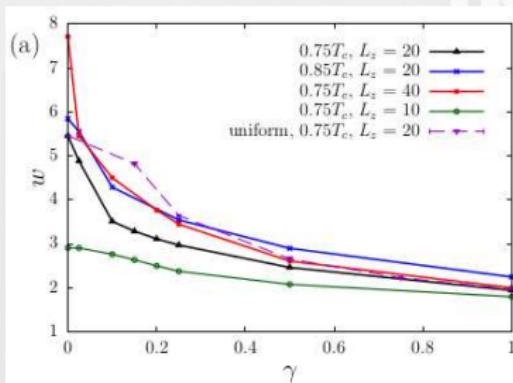
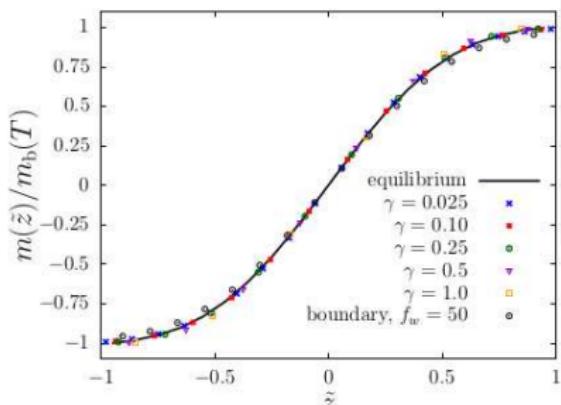
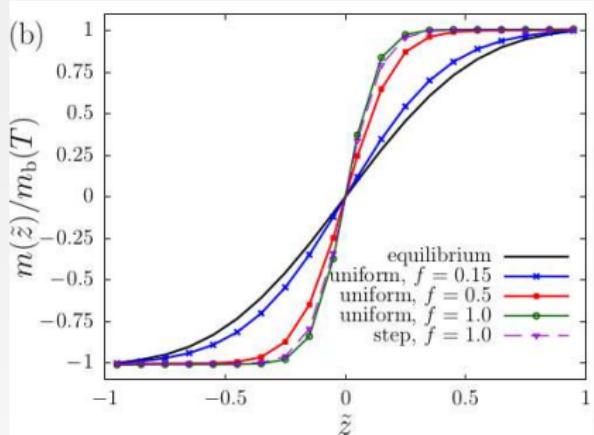
Effective interfacial tension and correlation length along the interface

## 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)]

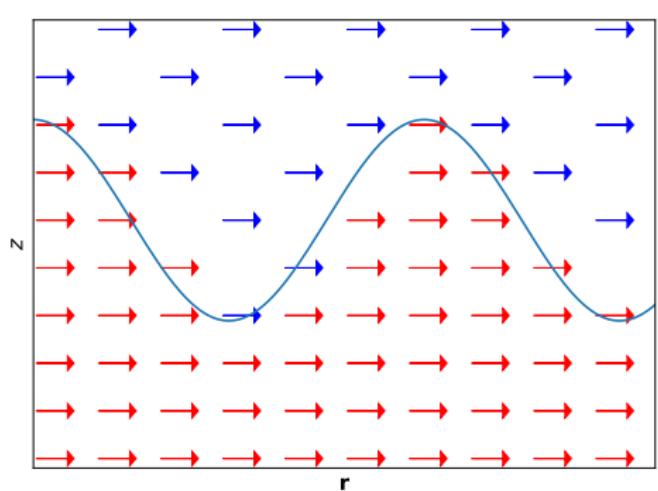


Magnetisation profiles, rescaled magnetisation profiles, interfacial width with respect to shear for different  $L_Y$

# Imposed hydrodynamic flow

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

$$\frac{\partial \psi(\mathbf{x}, t)}{\partial t} + \nabla \cdot (\mathbf{v}\psi(\mathbf{x}, t)) = D\nabla^2 \frac{\delta H}{\delta \psi(\mathbf{x})} + \sqrt{2DT} \nabla \cdot \boldsymbol{\eta}_1(\mathbf{x}, t) \quad (18)$$



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)]

$\psi$  : colloid field under model B dynamics

$\phi$  : passive solvent under model A dynamics

$$H[\psi, \phi] = H_1[\psi] + H_2[\psi, \phi] \quad (19)$$

$$H_1[\psi] = \int d\mathbf{x} \left[ \frac{\kappa}{2} [\nabla \psi(\mathbf{x})]^2 + V(\psi(\mathbf{x})) - gz\psi(\mathbf{x}) \right] \quad (20)$$

$$H_2[\psi, \phi] = \int d\mathbf{x} \frac{\lambda}{2} (1 - \psi(\mathbf{x}) - \phi(\mathbf{x}))^2 \quad (21)$$

$\kappa$  : interface energy

$V$  : phase separating potential

$g$  : gravitational term introducing finite size correlations

$\lambda$  : coupling parameter

## Model C dynamics

Equations

$$\frac{\partial \psi(\mathbf{x}, t)}{\partial t} + \mathbf{v} \cdot \nabla \psi(\mathbf{x}, t) = D \nabla^2 \frac{\delta H}{\delta \psi(\mathbf{x})} + \sqrt{2DT} \nabla \cdot \boldsymbol{\eta}_1(\mathbf{x}, t) \quad (22)$$

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = -\alpha \frac{\delta H}{\delta \phi(\mathbf{x})} + \sqrt{2\alpha T} \eta_2(\mathbf{x}, t) \quad (23)$$

are coupled by  $H_2$ , with a closed form on  $\psi$

$$\underbrace{\frac{\partial \psi(\mathbf{x}, t)}{\partial t}}_{\text{evolution}} - \underbrace{\lambda D \nabla^2 \int_{-\infty}^t dt' \exp(-\alpha \lambda (t - t')) \frac{\partial \psi(\mathbf{x}, t')}{\partial t}}_{\text{coupling term}} + \underbrace{\mathbf{v} \cdot \nabla \psi(\mathbf{x}, t)}_{\text{advection}} = \underbrace{D \nabla^2 \mu(\mathbf{x}, t')}_{\text{model B}} + \underbrace{\zeta(\mathbf{x}, t)}_{\text{thermal noise}} \quad (24)$$

where

$$\mu(\mathbf{x}, t) = \frac{\delta H_1}{\delta \psi(\mathbf{x}, t)} \quad (25)$$

and

$$\zeta(\mathbf{x}, \omega) = \frac{\sqrt{2\alpha T} D \lambda}{i\omega + \alpha \lambda} \nabla^2 \tilde{\eta}_2(\mathbf{x}, \omega) + \sqrt{2DT} \nabla \cdot \tilde{\boldsymbol{\eta}}_1(\mathbf{x}, \omega). \quad (26)$$

## 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  $h$

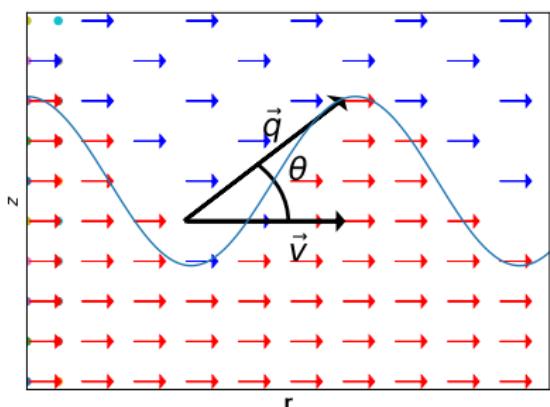
$$\begin{aligned} \Delta\psi^2 \int d\mathbf{r} G(0, \mathbf{r} - \mathbf{r}') & \left[ \frac{\partial h(\mathbf{r}, t)}{\partial t} + \mathbf{v} \cdot \nabla h(\mathbf{r}, t) \right] = \sigma [\nabla^2 h(\mathbf{r}, t) - m^2 h(\mathbf{r}, t)] + \xi(\mathbf{r}, t) \\ & + \frac{\sigma \lambda D}{\kappa} \int_{-\infty}^t dt' \exp(-\alpha \lambda (t - t')) \frac{\partial h(\mathbf{r}, t')}{\partial t'} \end{aligned} \quad (27)$$

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

The correlation function is

$$\tilde{C}_s(\mathbf{q}) = T \frac{(2D\sigma q(\kappa[q^2 + m^2] + \lambda) + \alpha\kappa\lambda\Delta\psi^2)^2 + \kappa^2\Delta\psi^4(\mathbf{q} \cdot \mathbf{v})^2}{\sigma[q^2 + m^2](2Dq\sigma(\kappa[q^2 + m^2] + \lambda) + \alpha\kappa\lambda\Delta\psi^2)^2 + \kappa(\kappa\sigma[q^2 + m^2] + \lambda\sigma)\Delta\psi^4(\mathbf{q} \cdot \mathbf{v})^2} \quad (28)$$



For  $\mathbf{q}$  small,  
Angle-dependent surface tension

$$\sigma_s(\theta) = \sigma \left( 1 + \frac{\mathbf{v}^2 \cos^2(\theta)}{v_0^2} \right) \quad (29)$$

with the intrinsic velocity  $v_0 = \sqrt{\alpha^2 \lambda \kappa}$   
Angle-dependent correlation length

$$\xi_s = \xi_{eq} \sqrt{1 + \frac{\mathbf{v}^2 \cos^2(\theta)}{v_0^2}} \quad (30)$$

# Conclusion

## Confined interfaces

- Relation between critical and interface systems

## Sheared Model C

- Uniform driving on the dynamics of the interface is presented in a two phase system
- Model C was used to generate a non-equilibrium state
- 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
- Qualitative agreement with experimental sheared PMMA colloids [Derk et al. 2006] and numerical 2D sheared Ising [T.H.R. Smith 2010]

## Sheared SOS

- Shearing does increase interface width, as in waves

# Perspective

- Get deeper on the relation between critical and interface systems
- Get a theory of wind generated waves and see the difference with model C driving
- Do out-of-equilibrium confined interfaces have different physics than equilibrium confined ones ?
- We developed a new model (Particles-Over-Particles) which can have new physics but have some technical issues
- Use the new developed formalism for interfaces under more general external fields