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# Out of equilibrium dynamics of complex systems

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# Plan of the 1st Lecture

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1. Equilibrium vs. out of equilibrium classical systems
2. How can a classical system stay far from equilibrium ?

From single-particle to many-body

Diffusion

Phase-separation & domain growth

Quenched randomness & glasses

Driven systems

Active matter

3. Plan of the rest of the Course

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# Statistical physics

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## Advantage

**No need to solve the dynamic equations!**

Under the *ergodic hypothesis*, after some *equilibration time*  $t_{\text{eq}}$ , *macroscopic observables* can be, on average, obtained with a *static* calculation, as an average over all configurations in phase space weighted with a probability distribution function  $P(\{\mathbf{p}_i, \mathbf{x}_i\})$

$$\langle A \rangle = \int \prod_i d\mathbf{p}_i d\mathbf{x}_i P(\{\mathbf{p}_i, \mathbf{x}_i\}) A(\{\mathbf{p}_i, \mathbf{x}_i\})$$

$\langle A \rangle$  should coincide with  $\overline{A} \equiv \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_{t_{\text{eq}}}^{t_{\text{eq}} + \tau} dt' A(\{\mathbf{p}_i(t'), \mathbf{x}_i(t')\})$

the *time average* typically measured experimentally

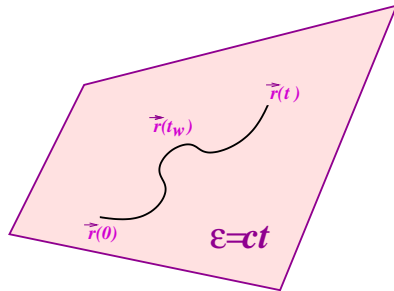
**Ergodicity**

**Boltzmann, late XIX**



# Statistical physics

Recipes for  $P(\{p_i, x_i\})$  according to circumstances



## Microcanonical ensemble

$$P(\{p_i, x_i\}) \propto \delta(\mathcal{H}(\{p_i, x_i\}) - \mathcal{E})$$

Flat probability density

Isolated system

$$\mathcal{E} = \mathcal{H}(\{p_i, x_i\}) = ct$$

$$S_{\mathcal{E}} = k_B \ln g(\mathcal{E})$$

Entropy

$$\beta \equiv \frac{1}{k_B T} = \left. \frac{\partial S_{\mathcal{E}}}{\partial \mathcal{E}} \right|_{\mathcal{E}}$$

Temperature

$$\mathcal{E} = \mathcal{E}_{syst} + \mathcal{E}_{env} + \mathcal{E}_{int}$$

Neglect  $\mathcal{E}_{int}$  (short-range interact.)

$$\mathcal{E}_{syst} \ll \mathcal{E}_{env} \quad \beta = \frac{\partial S_{\mathcal{E}_{env}}}{\partial \mathcal{E}_{env}}$$

$$P(\{p_i, x_i\}) \propto e^{-\beta \mathcal{H}(\{p_i, x_i\})}$$

*Environment*

*Interaction*

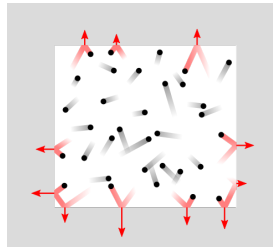
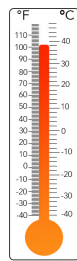
*System*

Canonical ensemble

# Statistical physics

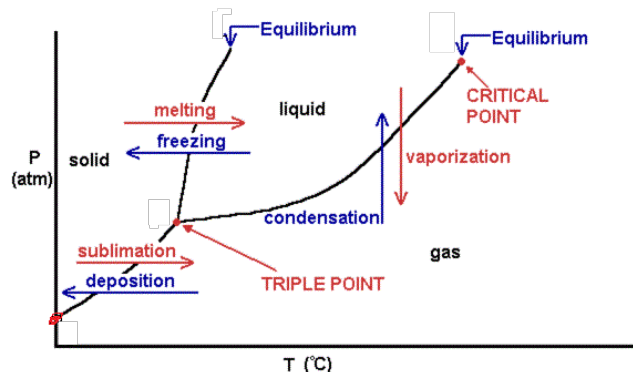
## Accomplishments

- Microscopic definition & derivation of **thermodynamic** concepts  
(**temperature**, **pressure**, *etc.*) and laws (**equations of state**, *etc.*)



$$PV = nRT$$

- Theoretical understanding of **collective effects**  $\Rightarrow$  **phase diagrams**



**Phase transitions** : sharp changes in the macroscopic behavior when an external (e.g. the temperature of the environment) or an internal (e.g. the interaction potential) parameter is changed

- Calculations can be difficult but the **theoretical frame** is set beyond doubt

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# Statistical physics

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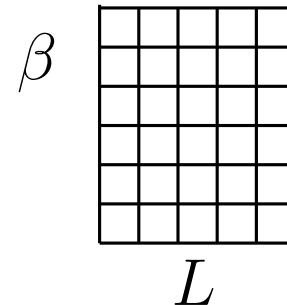
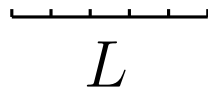
Classical  $\Leftrightarrow$  Quantum

## Partition function correspondence

Quantum  $d$  dimensional  $\equiv$  Classical  $d + 1$  dimensional

$$\mathcal{Z}(\beta) = \text{Tr } e^{-\beta \hat{H}}$$

$$\mathcal{Z}(\beta) = \sum_{\text{conf}} e^{-\beta \mathcal{H}(\text{conf})}$$



$\beta\hbar$ -periodic imaginary time direction

$$\phi(\mathbf{x})$$

$$\phi(\tau, \mathbf{x}) = \phi(\tau + \beta\hbar, \mathbf{x})$$

**Feynman-Hibbs 65, Trotter & Suzuki 76, Matsubara 70s**

Quantum Phase transitions, Quantum Monte Carlo methods, *etc.*

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# Dynamics $\Rightarrow$ Stat Mech

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## Different cases

- Closed & open systems
- Equilibrium & out of equilibrium
  - Long time scales
  - Forces & energy injection
- Individual & collective effects

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# General setting

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## Different cases

- **Closed** & open systems
- Equilibrium & **out of equilibrium**
  - Long time scales
  - Forces & energy injection
- Individual & collective effects

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# Isolated systems

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## Dynamics of a classical isolated system

### Foundations of statistical physics

**Question:** does the dynamics reach a flat distribution over the constant energy surface in phase space ?

Ergodic theory,  $\in$  mathematical physics at present

Dynamics of a (quantum) isolated system :

a problem of current interest, boosted by (cold atom) experiments

**Question:** after a quench, i.e. a rapid variation of a parameter in the system, are at least some local observables described by canonical thermal ones ? When, how, which ?

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# General setting

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## Different cases

- Closed & **open** systems
- **Equilibrium** & out of equilibrium
  - Long time scales
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# Open systems

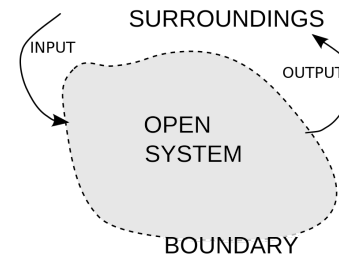
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## Aim

Interest in describing the **statics** and **dynamics** of a **classical** (or quantum) **system** coupled to a **classical** (or quantum) **environment**.

The Hamiltonian of the ensemble is

$$H = H_{syst} + H_{env} + H_{int}$$



The dynamics of all variables are given by **Newton** (or Heisenberg) rules, depending on the variables being classical (or quantum).

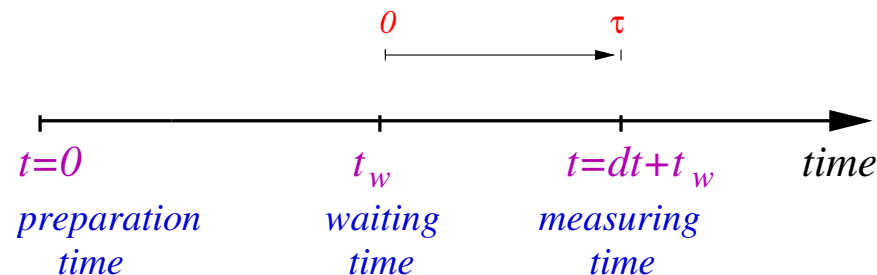
The total energy is conserved,  $\mathcal{E} = \text{ct}$  but each contribution is not, in particular,  $\mathcal{E}_{syst} \neq \text{ct}$ , and we'll take  $e_0 \ll \mathcal{E}_{syst} \ll \mathcal{E}_{env}$ .



# In and out of equilibrium

Take a **mechanical point of view** and call  $\{\zeta_i\}(t)$  the variables  
e.g. the particles' coordinates  $\{x_i(t)\}$  and momenta  $\{p_i(t)\}$

Choose an initial condition  $\{\zeta_i\}(0)$  and let the system evolve.

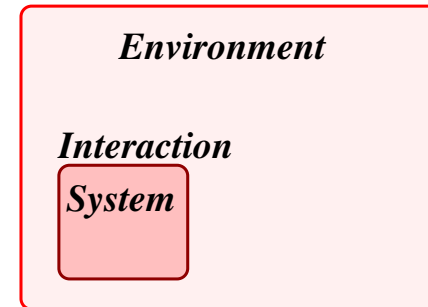


- For  $t_w > t_{eq}$  :  $\{\zeta_i\}(t)$  reach the equilibrium pdf and **thermodynamics** and **statistical mechanics** apply (e.g., **temperature** is a well-defined concept).
- For  $t_w < t_{eq}$  : the system remains out of equilibrium and **thermodynamics** and (Boltzmann) **statistical mechanics** **do not** apply.

# Dynamics in equilibrium

## Conditions

Take an open system coupled to an environment



Necessary :

- The **bath** should be **in equilibrium**

same origin of noise and friction

- Deterministic force

**conservative forces** only,  $\mathbf{F} = -\nabla V$

- Either the initial condition is taken from the equilibrium pdf, or the latter should be reached after an **equilibration time**  $t_{\text{eq}}$  :

$$P_{\text{eq}}(\mathbf{v}, \mathbf{x}) \propto e^{-\beta(\frac{mv^2}{2} + V(\mathbf{x}))}$$

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# Out of equilibrium

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## Three possible reasons

- The equilibration time goes beyond the experimentally accessible times in macroscopic systems in which  $t_{\text{eq}}$  grows with the system size,

$$\lim_{N \gg 1} t_{\text{eq}}(N) \gg t$$

*e.g.*, **critical slowing down, coarsening, glassy physics**

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- Driven systems      Energy injection

$$F_{\text{ext}} \neq -\nabla V(x)$$

*e.g.*, **active matter**

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- Integrability

$$I_{\mu}(\{p_i, x_i\}) = ct, \quad \mu = 1, \dots, N$$

Too many constants of motion inhibit equilibration to the Gibbs ensembles.

*e.g.*, **1d bosonic gases**

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# Macroscopic systems

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Discussion of several macroscopic systems with slow dynamics due to

$$\lim_{N \gg 1} t_{\text{eq}}(N) \gg t$$

Examples :

## Ordering processes

Domain growth, phase separation

## Systems with frustrated interactions

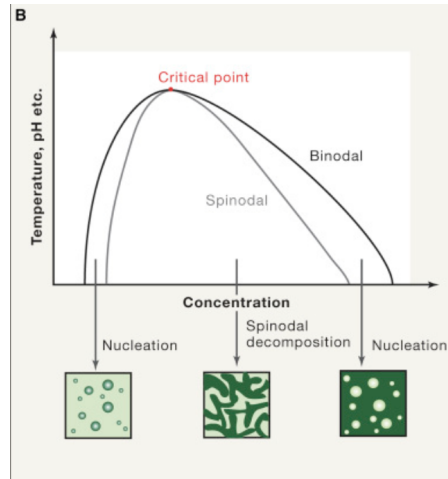
Spin ices

## Systems with quenched disorder

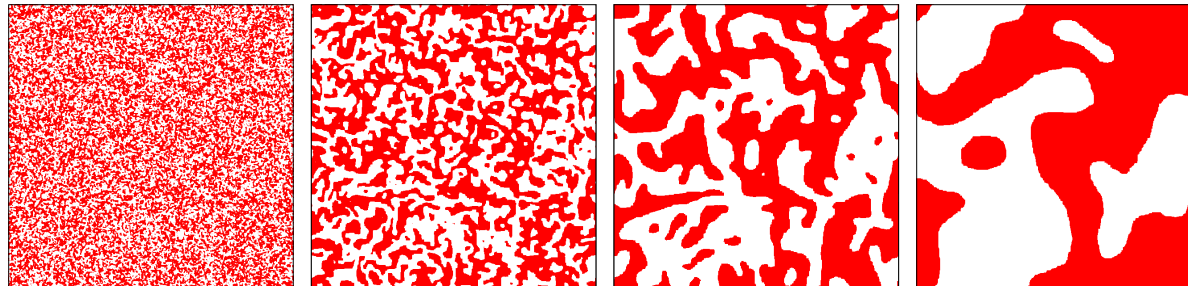
Random ferromagnets, spin-glasses

# Phase separation

Quench below the binodal: remnant interfaces



$t_1 < t_2 < t_3 < t_4 < \dots$

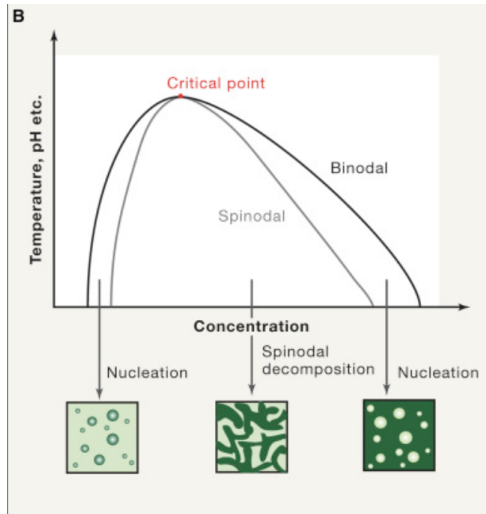


Coarsening process with growing length  $\mathcal{R}(t) \simeq t^{1/z} \implies t_{\text{eq}} \sim L^z$

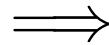
Equilibration time diverges with the system size

# Phase separation

## Quench below the binodal: universality

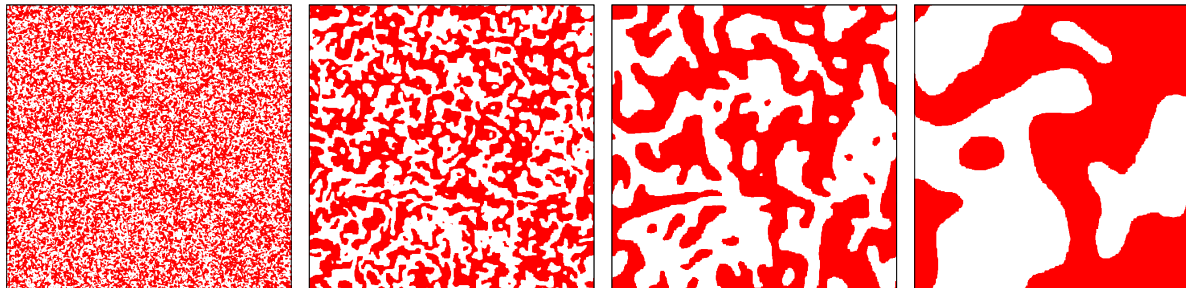


Microscopic details are irrelevant  
but conservation laws and  
dimension of order parameter fix the



**Dynamic universality class**

$t_1 < t_2 < t_3 < t_4 < \dots$



Coarsening process classified according to  $\mathcal{R}(t) \simeq t^{1/z}$



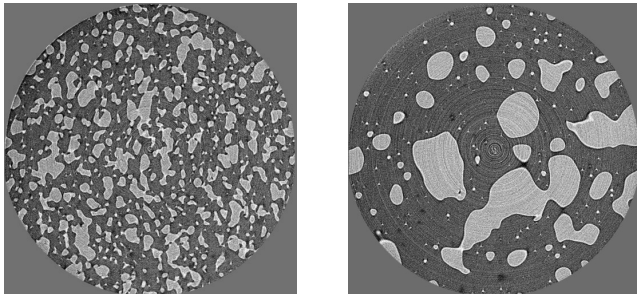
# Phase ordering kinetics

Are these quench dynamics fast processes ? Can we simply forget what happens during the transient,  $t_{eq}$ , and focus on the subsequent *equilibrium* behaviour ?

No !

It turns out that this is a very slow regime. Its duration grows with the size of the system and it diverges in the thermodynamic limit  $N \rightarrow \infty$ .

We understand the mechanisms for relaxation : *interface local curvature driven dynamics and matter diffusion*.



The domains get rounder

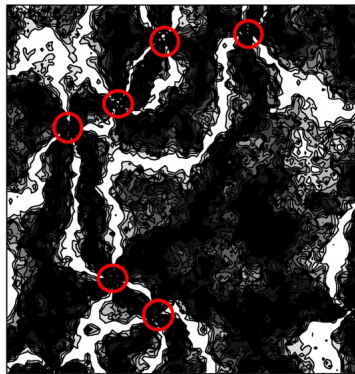
The regions get darker and lighter

# Topological phase transitions

## Vortices in the $2d$ XY model - O(2) field theory

$$\mathcal{H} = -\frac{J}{2} \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j \quad \Longrightarrow \quad \int d^2x \left[ \frac{1}{2} (\nabla \phi(\mathbf{x}))^2 - \frac{r}{2} \phi^2(\mathbf{x}) + \frac{\lambda}{4} \phi^4(\mathbf{x}) \right]$$

Unbinding of vortex pairs  $\rho_v^{\text{free}}(T > T_{KT}) > 0$  **Kosterlitz & Thouless 70s**



After a quench to  $T < T_{KT}$

**Free vortex annihilation**

Schlieren pattern

gray scale

$\sin^2(2\mathbf{s}_i \cdot \hat{e}_x)$

**Jelić & LFC 12**

Growing length scale  $\mathcal{R}(t) \simeq (t / \ln t)^{1/z}$  & free vortex density  $\rho_v^{\text{free}}(t) \sim \mathcal{R}^{-2}(t)$

$$\Longrightarrow \quad t_{\text{eq}} \sim L^z \ln L$$

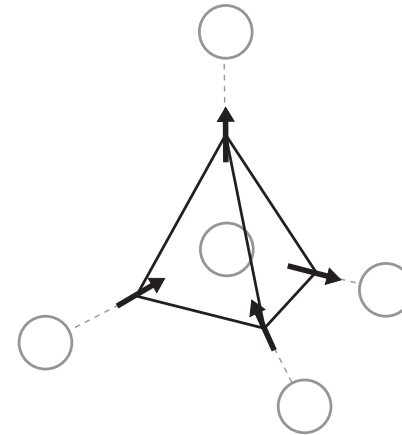
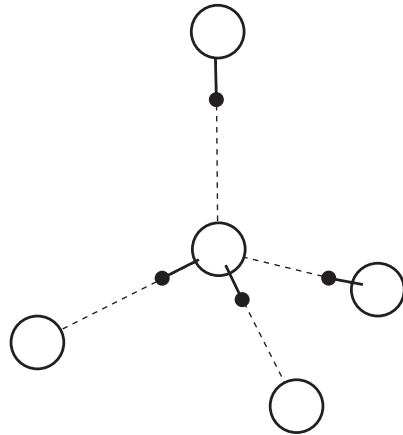
In boson gases, polaritons, *etc.* **Blakie, Capusotto, Davis, Proukakis, Symanska, ...**  
numerics & **Beugnon-Dalibard, ... Popovic et al., ...** experiments. Last 15 years

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# Natural ices

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Single cell unit - tetrahedron - in water-ice and spin-ice



**Water-ice**: coordination four lattice. **Bernal & Fowler 33** rules, two H near and two far away from each O.

**Spin-ice**: four (Ising) spins on each tetrahedron forced to point along the axes that join the centres of two neighbouring units (Ising anisotropy). Local interactions imply the two-in two-out ice rule

e.g.  $\text{Dy}_2 \text{Ti}_2 \text{O}_7$  **Harris, Bramwell, McMorro, Zeiske & Godfrey 97**

# Artificial spin-ice - model

Instead of dipolar interactions, a simpler modelling

Metamaterials

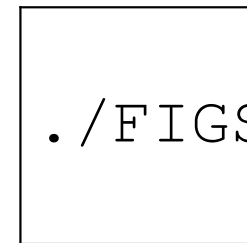
Arrays of nanoscale **Ising magnets**

single domain magnetic islands

placed at the edges of a tiling or

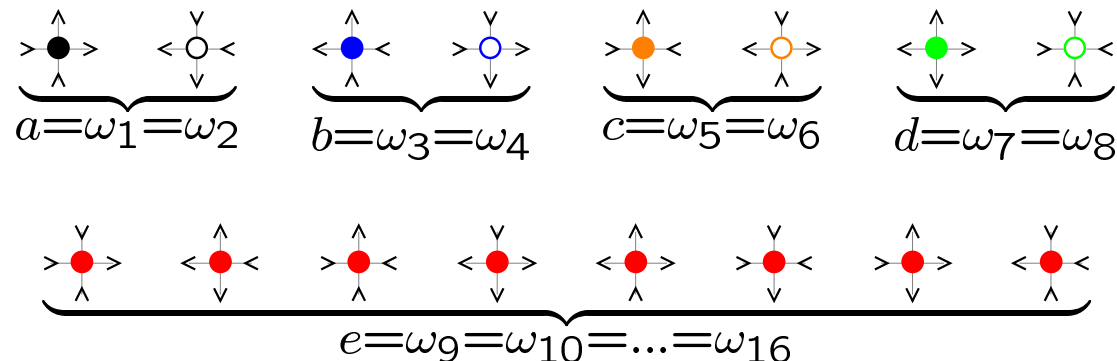
the edges of a **square lattice**

Parameters specified by design



Magnetic force microscopy

Local approx: **2d vertex model with experimentally relevant parameters**



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# Quenched disorder

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**Quenched variables** *are frozen during time-scales over which other variables fluctuate*

## Time scales

$$t_{\text{micro}} \ll t \ll t_q$$

$t_q$  could be the **diffusion** time-scale for magnetic impurities, the magnetic moments of which will fluctuate in a **magnetic system** or the **flipping time** of impurities that create random fields acting on other magnetic variables.

**Weak disorder** (modifies the critical properties but not the phases) vs. **strong disorder** (modifies both)

*E.g.*, **random ferromagnets** ( $J_{ij} > 0$ ) vs. **spin-glasses** ( $J_{ij} \gtrless 0$ )

# Rugged free-energy landscapes

Glassy physics: beyond the  $\lambda\phi^4$  Ginzburg-Landau Questions !

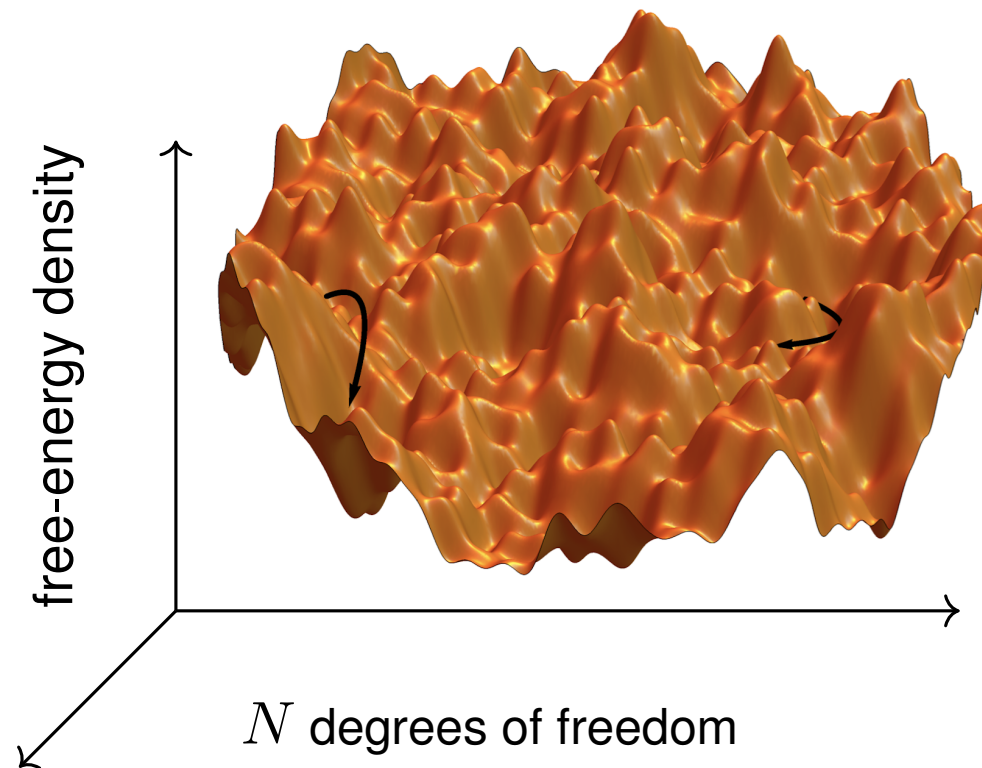


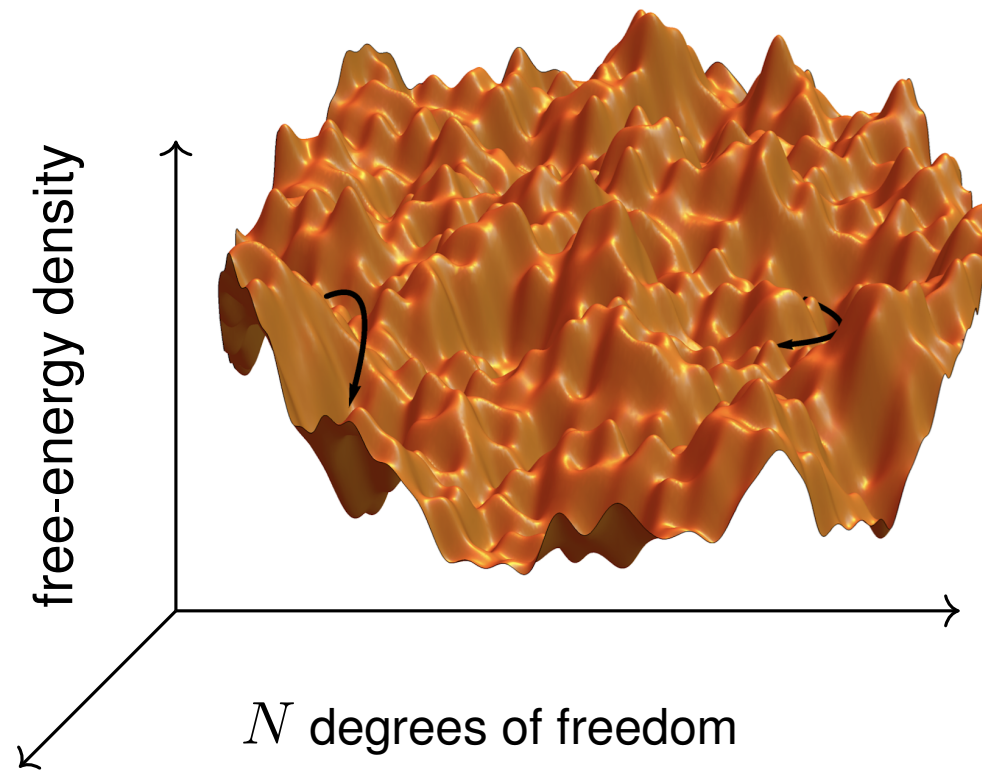
Figure adapted from a picture by C. Cammarota

Topography of the landscape on the  $N$ -dimensional substrate made by the  $N$  order parameters ?

Numerous studies by **theoretical physicists** and **probabilists**

# Rugged free-energy landscapes

Glassy physics: beyond the  $\lambda\phi^4$  Ginzburg-Landau Questions !



How to reach the absolute minimum ?

Thermal activation, surfing over tilted regions, quantum tunneling ?

Optimisation problem Smart algorithms ? Computer sc - applied math

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# Spin-glasses

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Magnetic impurities (spins) randomly placed in an inert host

Quenched random interactions

Interacting via the RKKY potential

$$V(r) \propto \frac{\sin 2\pi k_F r}{r^3}$$

very rapid oscillations (change in sign) and slow power law decay

Standard lore : there is a 2nd order static phase transition at  $T_s$   
separating a paramagnetic from a spin-glass phase.

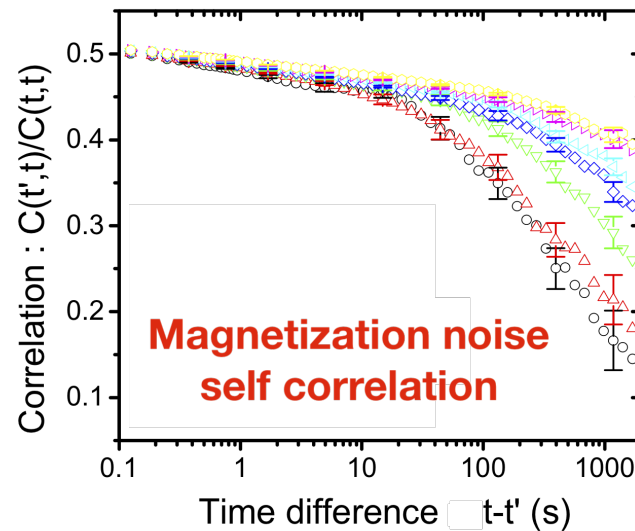
No dynamic precursors above  $T_s$ .

Glassy dynamics below  $T_s$  with aging, memory effects, etc.

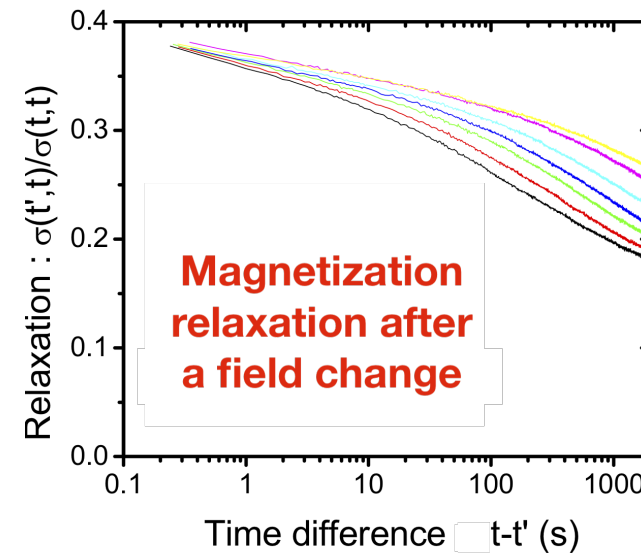


# Rugged free-energy landscapes

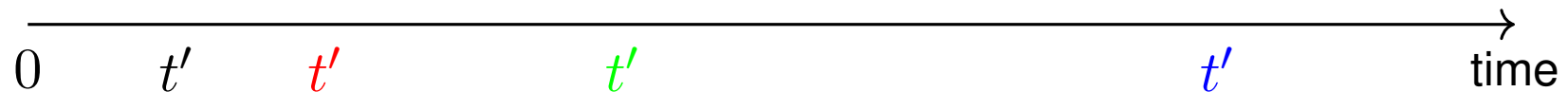
Glassy physics: slow relaxation & loss of stationarity (aging)



Correlation



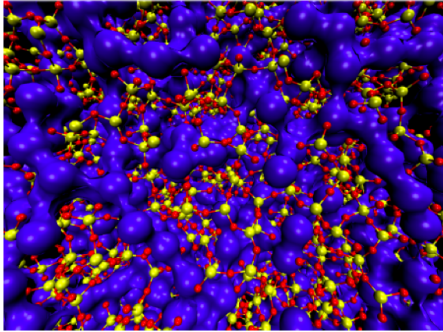
Linear response



Different curves are measured after log-spaced reference times  $t'$  after the quench: **breakdown of stationarity**  $\implies$  far from equilibrium

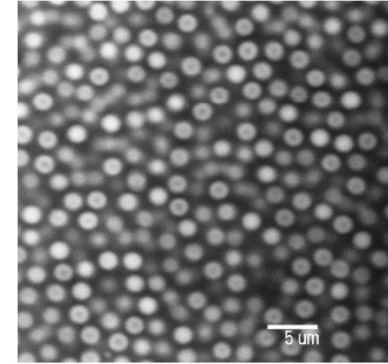
No identifiable growing length  $\mathcal{R}(t)$ : **glassy microscopic mechanisms?**

# What do glasses look like ?



Simulation

Molecular (Sodium Silicate)



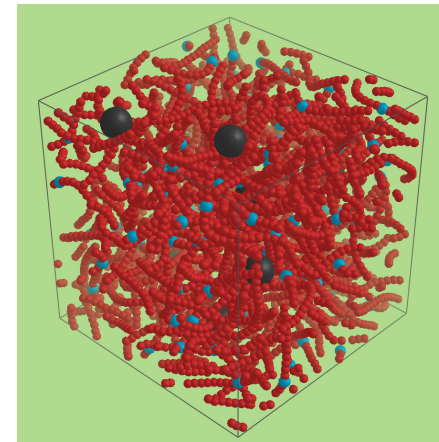
Confocal microscopy

Colloids (e.g.  $d \sim 162$  nm in water)



Experiment

Granular matter



Simulation

Polymer melt

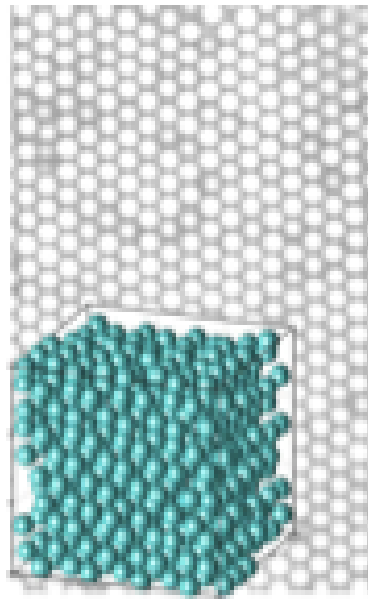
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# Structural Glasses

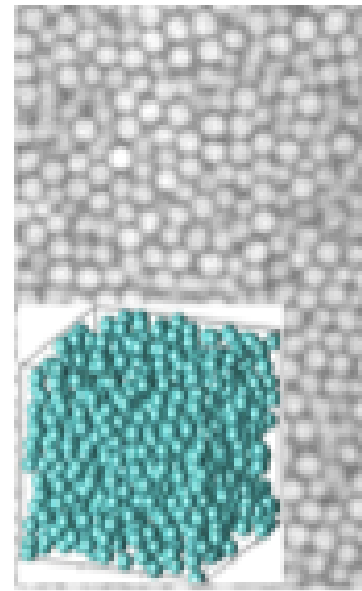
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*e.g.*, colloidal ensembles

Micrometric spheres immersed in a fluid



Crystal



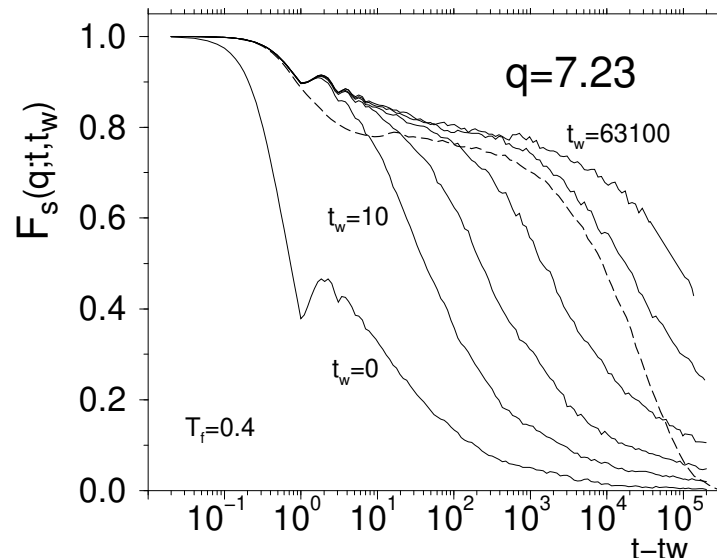
Glass

In the glass: no obvious growth of order, slow dynamics with, however, scaling properties

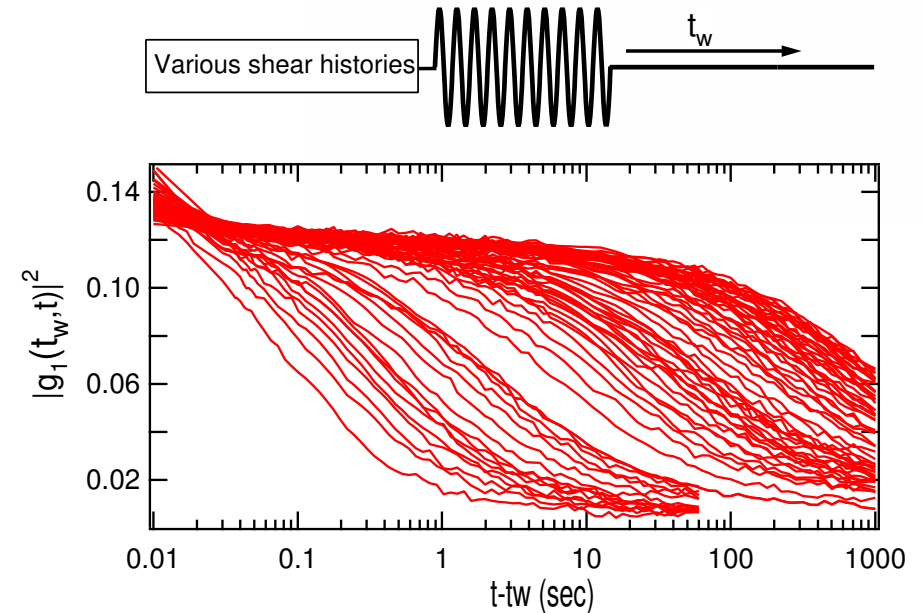
**What drives the slowing down ?**

# Low temp/high densities

## Out of equilibrium relaxation



L-J mixture **J-L Barrat & Kob 99**



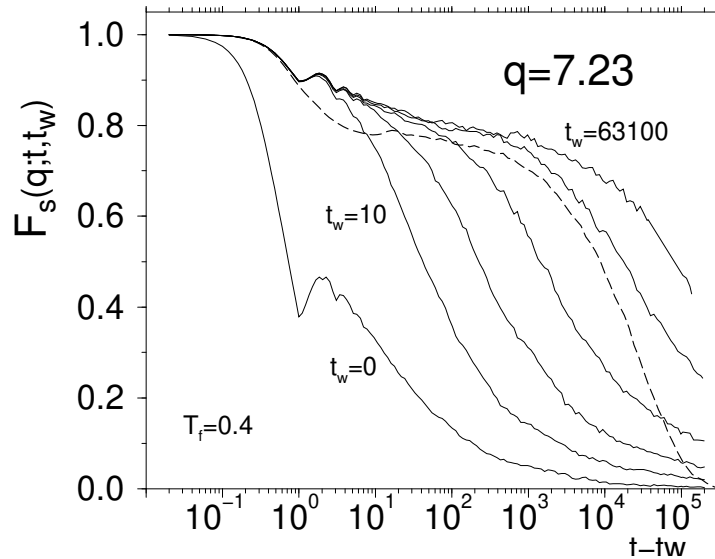
Colloids **Viasnoff & Lequeux 03**

$$t_{\text{micro}} \ll t \ll t_{\text{eq}}$$

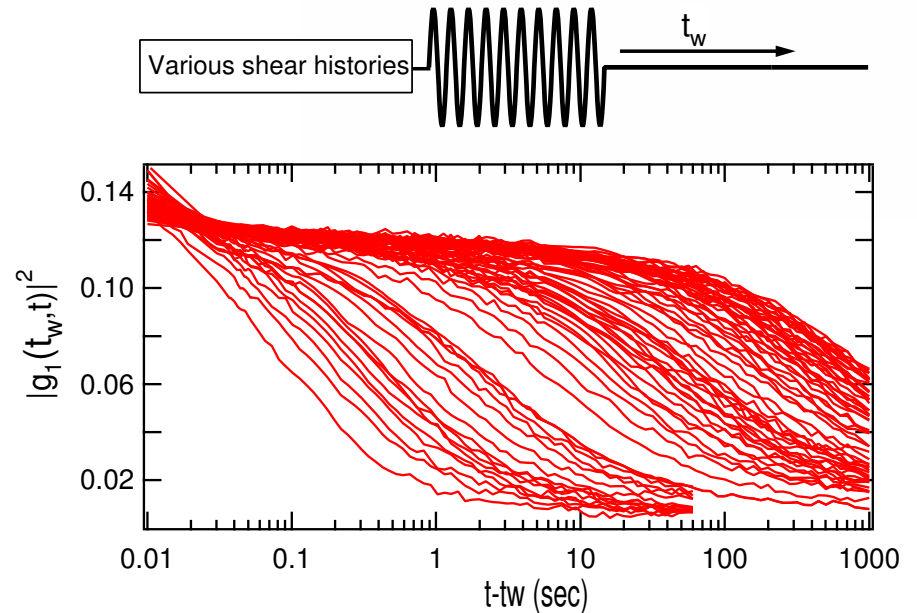
The equilibration time goes beyond the experimentally accessible times  
Similar curves found in all other glasses.

# Low temp/high densities

## Ageing effects



L-J mixture **J-L Barrat & Kob 99**



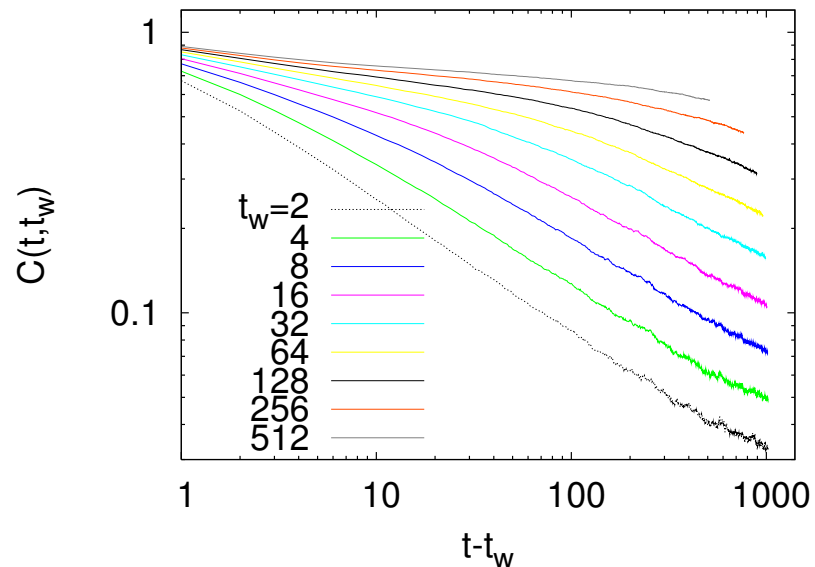
Colloids **Viasnoff & Lequeux 03**

$$t_{micro} \ll t \ll t_{eq}$$

**Ageing** the relaxation is slower for older systems

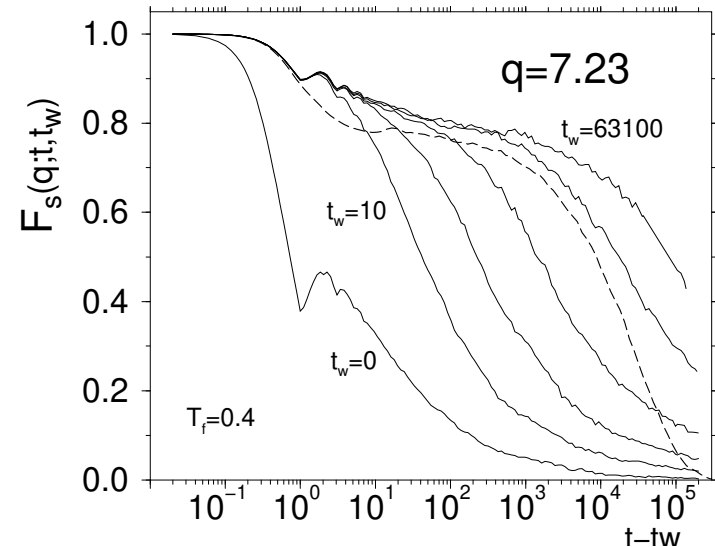
# Ferromagnet vs glass

Not so different as long as correlations are concerned



2d Ising model - spin-spin

**Sicilia *et al.* 07**



Lennard-Jones - density-density

**Kob & Barrat 99**

One correlation can exhibit stationary and non stationary relaxation

in different two-time regimes

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# Long time-scales

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## for relaxation

Systems with **competing interactions** remain **out of equilibrium** and it is not clear

- whether there are phase transitions,
- which is the nature of the putative ordered phases,
- which is the dynamic mechanism.

Examples are :

- systems with quenched disorder,
- systems with geometric frustration,
- glasses of all kinds.

Static and dynamic **mean-field theory** has been developed – both classically and quantum mechanically – and they yield new concepts and predictions.

Extensions of the RG have been proposed and are currently being explored.

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# Out of equilibrium

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## Three possible reasons

- The equilibration time goes beyond the experimentally accessible times in macroscopic systems in which  $t_{\text{eq}}$  grows with the system size,

$$\lim_{N \gg 1} t_{\text{eq}}(N) \gg t$$

*e.g.*, diffusion, critical slowing down, coarsening, glassy physics

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- Driven systems      Energy injection

$$\mathbf{F}_{\text{ext}} \neq -\nabla V(\mathbf{x})$$

*e.g.*, **active matter**

---

- Integrability

$$I_{\mu}(\{\mathbf{p}_i, \mathbf{x}_i\}) = ct, \quad \mu = 1, \dots, N$$

Too many constants of motion inhibit equilibration to the Gibbs ensembles.

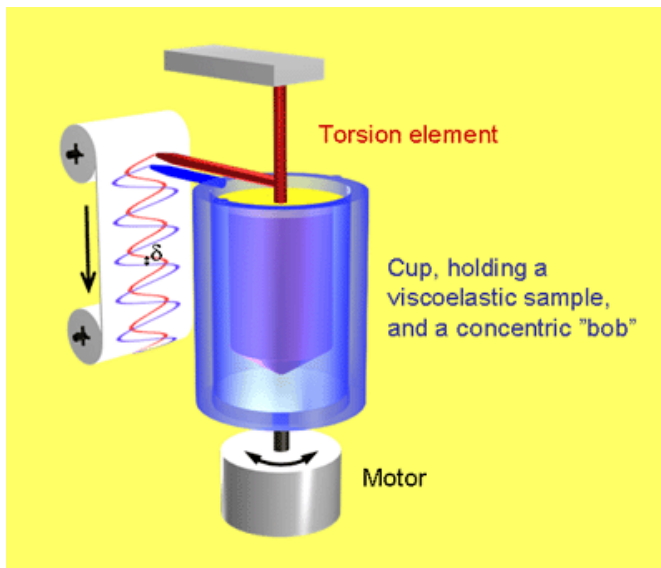
*e.g.*, **1d bosonic gases**

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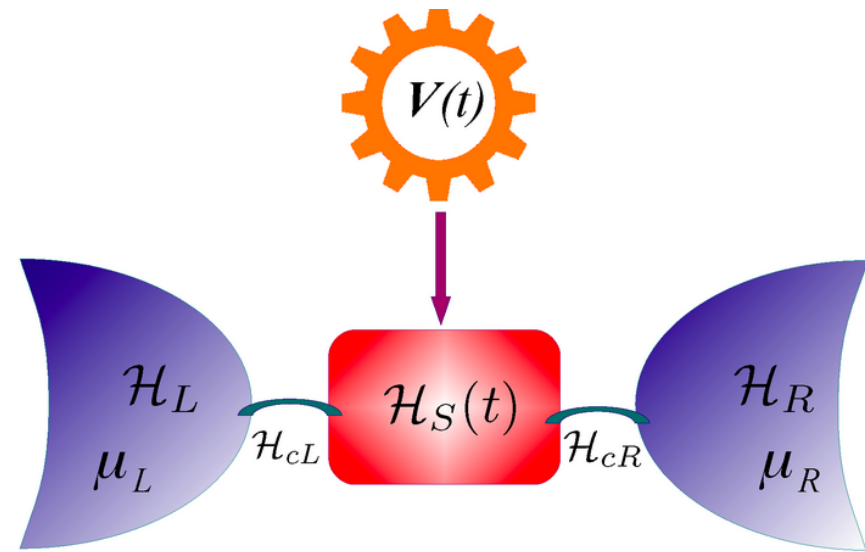


# Energy injection

Traditional: from the borders (outside)



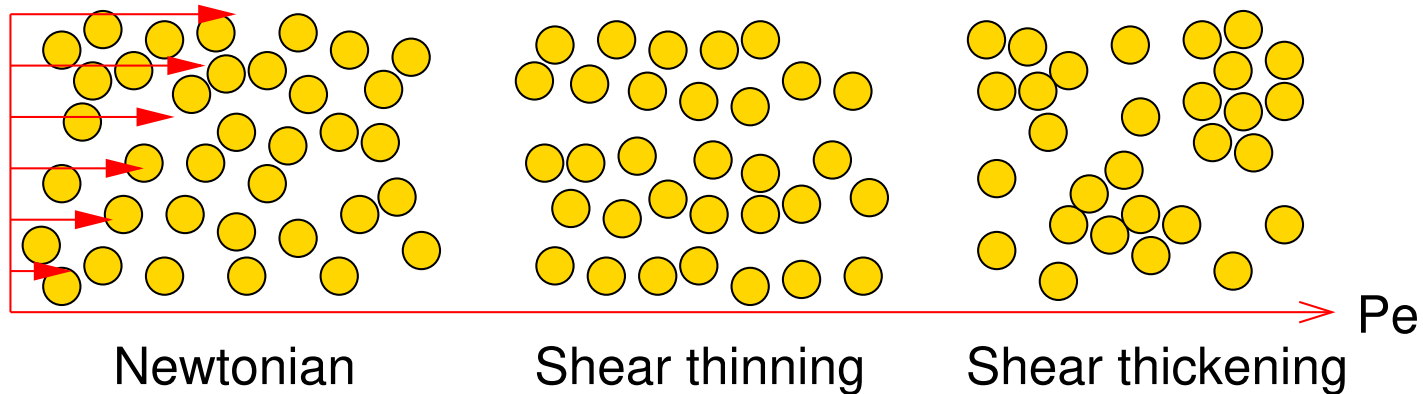
Rheology



Transport

# Drive & transport

## Rheology of complex fluids



Rheology of complex fluids

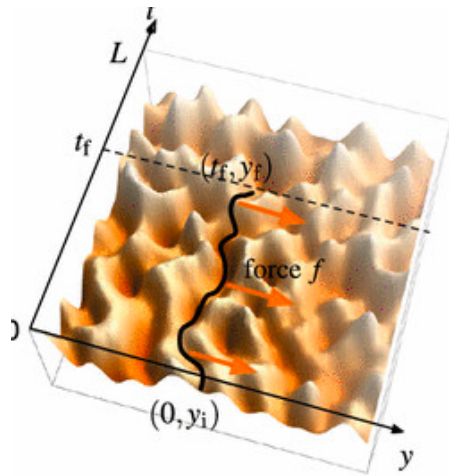
Shear thinning  $\tau_{\text{relax}}$  decreases, e.g. paints

Shear thickening  $\tau_{\text{relax}}$  increases, e.g. cornstarch & water mix

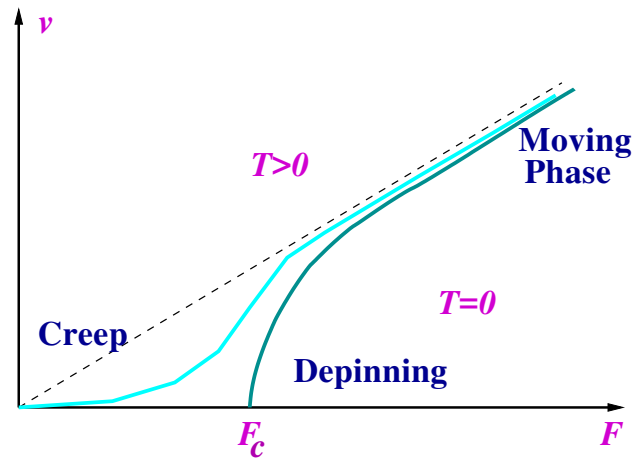
e.g. review **Brader 10**

# Drive & transport

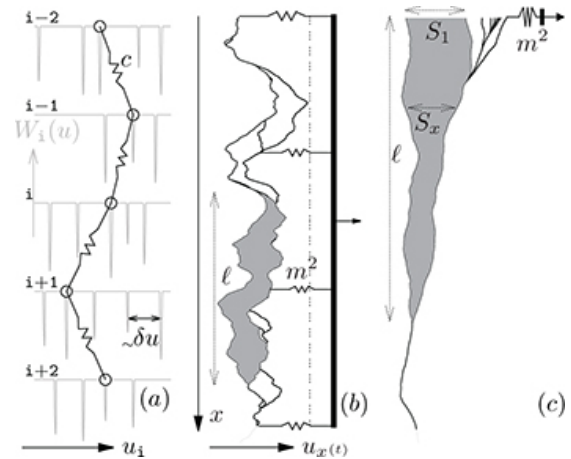
## Driven interface over a disordered background



A line



Depinning & creep



avalanches

e.g. review **Giamarchi et al 05**, connections to earthquakes **Landes 16**

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# Active matter

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## Definition

Active matter is composed of large numbers of active "agents", each of which consumes energy in order to move or to exert mechanical forces.

Due to the energy consumption, these systems are intrinsically out of thermal equilibrium.

Energy injection is done “uniformly” within the samples (and not from the borders).

Coupling to the environment (bath) allows for the dissipation of the injected energy.

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# Natural systems

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## Birds flocking



# Natural systems

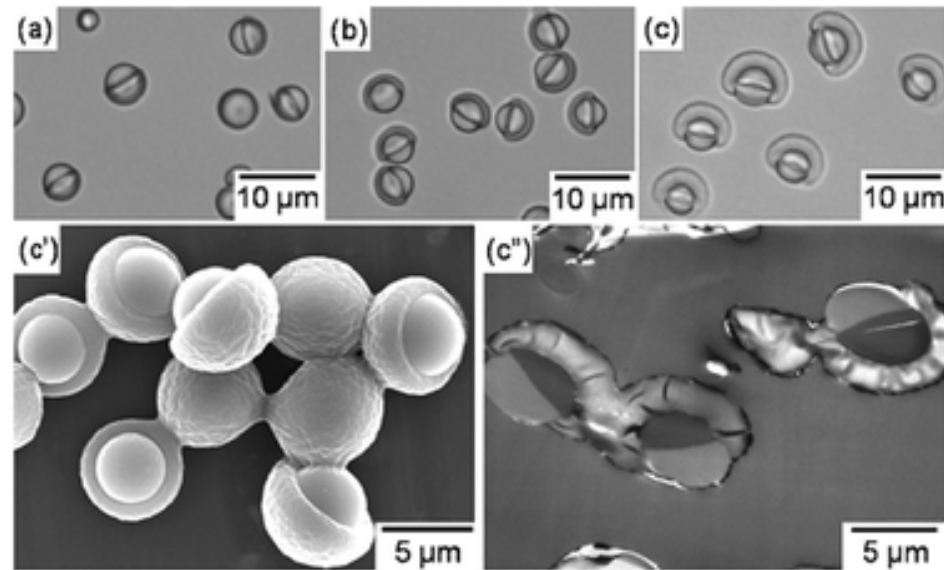
## Bacteria



Escherichia coli - Pictures borrowed from the internet.

# Artificial systems

## Janus particles



Particles with two faces (Janus God)

*e.g.* **Bocquet group** ENS Lyon-Paris, **di Leonardo group** Roma

# Active Brownian particles

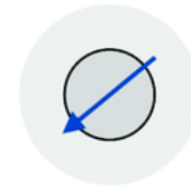
## The standard model – ABPs

Spherical particles with diameter  $\sigma_d$

Environment  $\implies$  Langevin dynamics

Scales  $\implies$  over-damped motion

Self-propulsion  $\implies$  active force  $\mathbf{F}_{\text{act}}$  along  $\mathbf{n}_i = (\cos \theta_i(t), \sin \theta_i(t))$



$$\underbrace{\gamma \dot{\mathbf{r}}_i}_{\text{friction}} = \underbrace{F_{\text{act}} \mathbf{n}_i}_{\text{propulsion}} - \underbrace{\nabla_i \sum_{j(\neq i)} U(r_{ij})}_{\text{inter-particle repulsion}} + \underbrace{\xi_i}_{\text{translational white noise}}$$

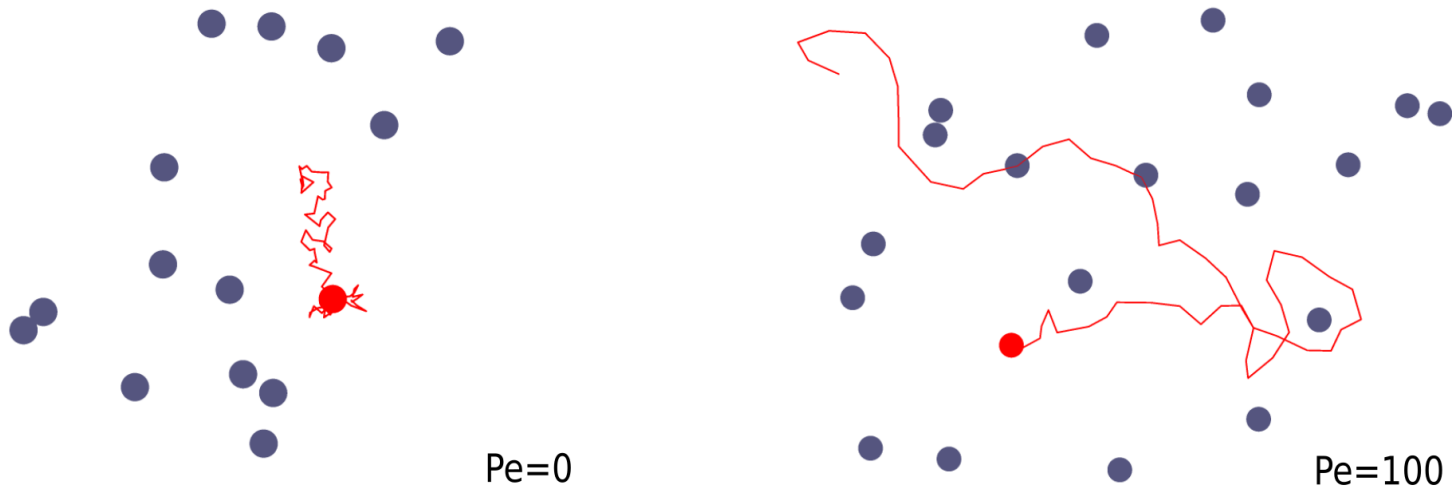
$$\underbrace{\dot{\theta}_i}_{\text{rotational white noise}} = \eta_i$$

$2d$  packing fraction  $\phi = \pi \sigma_d^2 N / (4S)$  Péclet number  $\text{Pe} = F_{\text{act}} \sigma_d / (k_B T)$



# Active Brownian particles

## Typical motion of ABPs in interaction



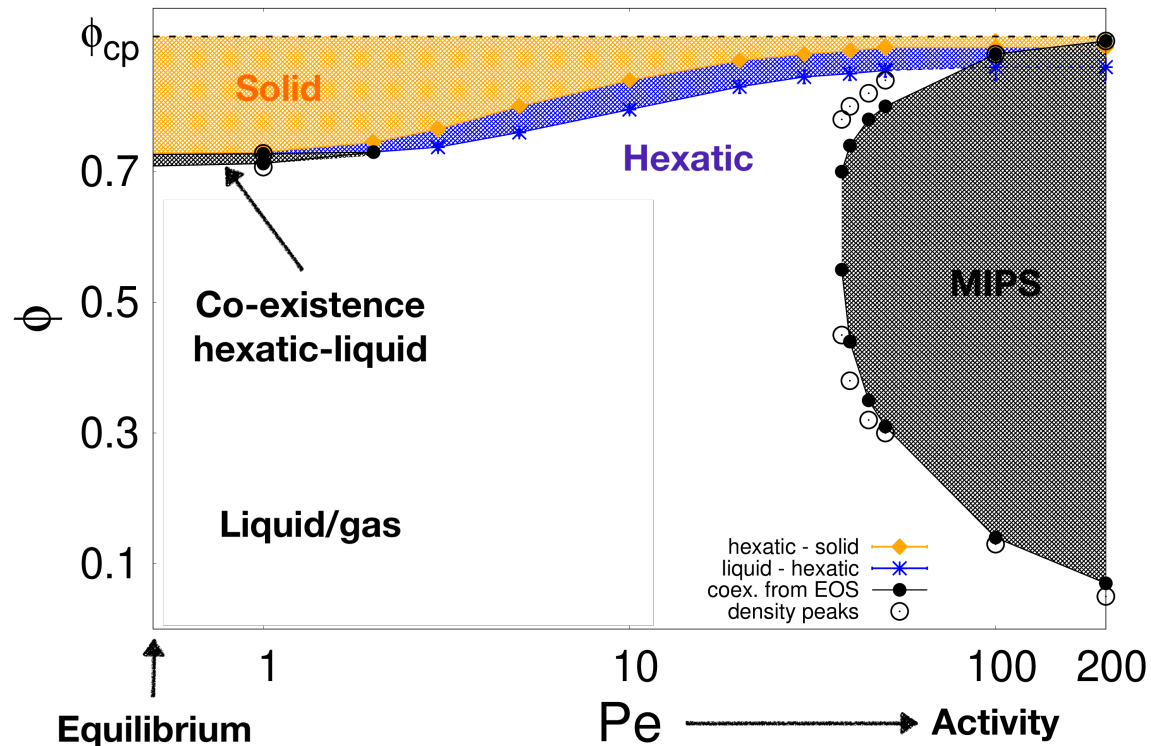
The **activity** induces a **persistent random motion**

Long running periods  $\ell_p \propto \text{Pe } \sigma_d$  and

sudden changes in direction

# Active Brownian particles

Complex out of equilibrium phase diagram



Motility induced  
phase separation  
(MIPS)  
gas & dense  
droplet

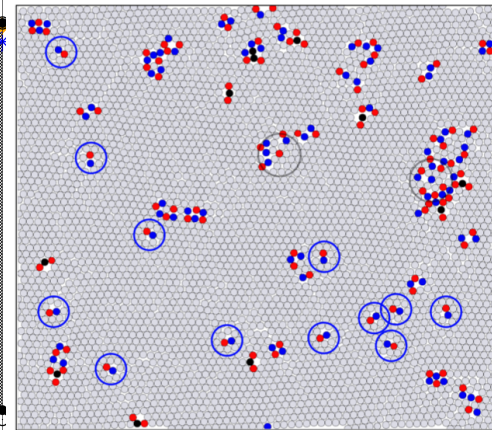
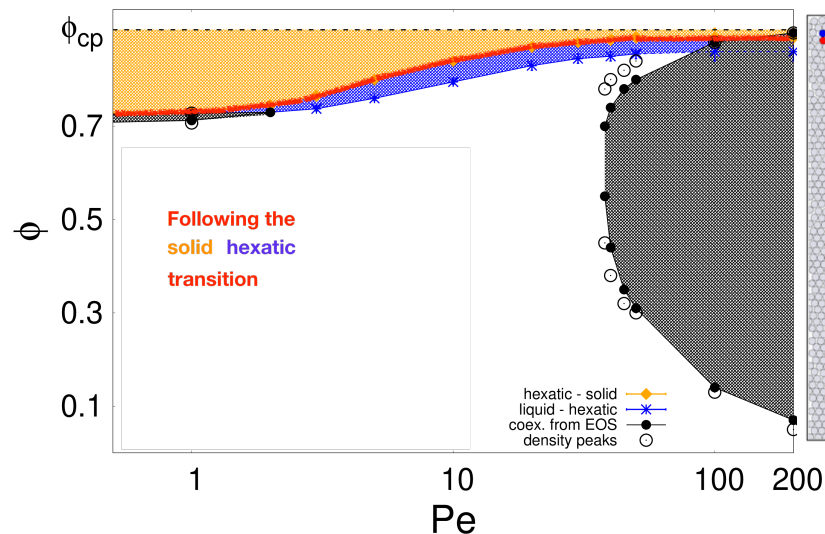
Cates & Tailleur 12

From virial pressure  $P(\phi)$ , translational and orientational correlations  $G_T$  and  $G_6$ , distributions of local density and hexatic order  $\phi_i$  and  $\psi_{6i}$ , at fixed  $k_B T = 0.05$

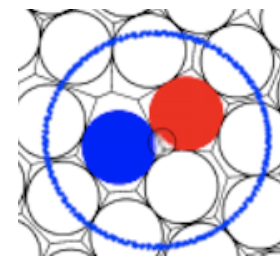
Digregorio, Levis, Suma, LFC, Gonnella & Pagonabarraga 18

# Active Brownian particles

Out of equilibrium phase diagram First question (out of many !)



Free dislocation:  
a 7-5 neighbor



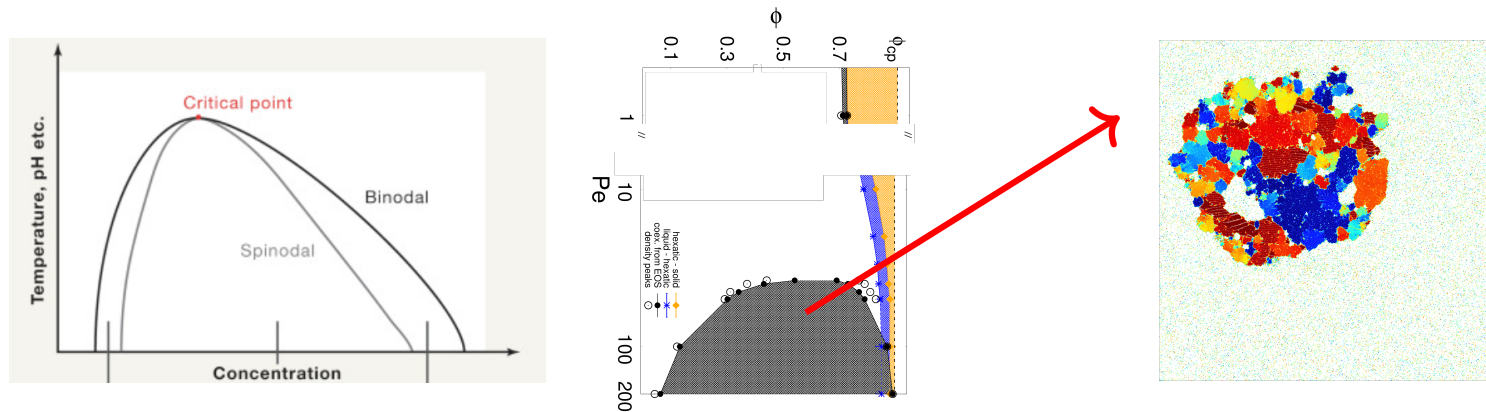
$\neq$  from  $\Delta$  lattice

**Solid** - **Hexatic** transition at  $\phi_{sh}$ , driven by unbinding of dislocation pairs as in Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young universality ?

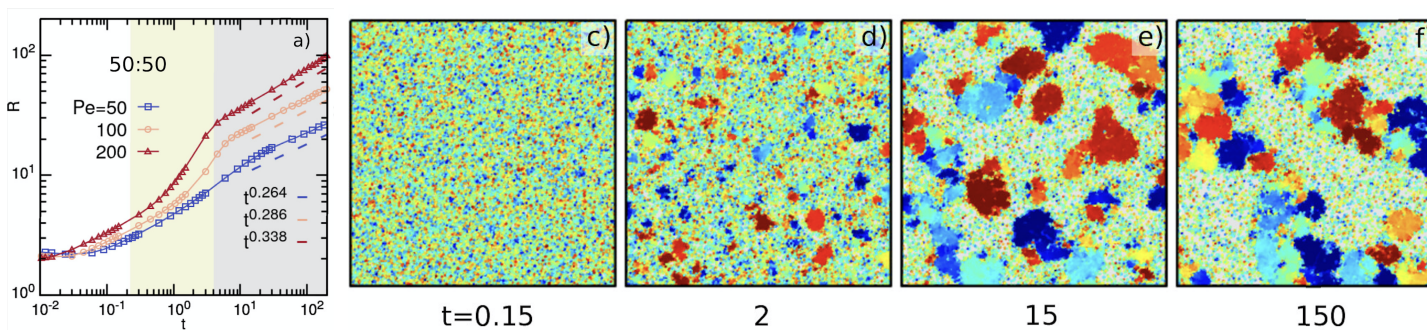
$$\rho_{disloc} \simeq a \exp \left[ -b \left( \frac{\phi_{sh}}{\phi_{sh} - \phi} \right)^\nu \right] \quad \nu \sim 0.37 \quad \forall Pe ?$$

# Active Brownian particles

Out of equilibrium phase diagram So many questions !



Dynamics of formation of the dense phase ? but bubbles, hexatic order, ...



Universality with the Lifshitz-Slyozov law  $\mathcal{R}(t) \simeq t^{1/3}$  ? Geometry ?

Redner *et al* 13, Stenhammar *et al* 14, ... , Caporusso *et al* 20, Caprini *et al* 20, ...

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# Out of equilibrium

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## Three possible reasons

- The equilibration time goes beyond the experimentally accessible times in macroscopic systems in which  $t_{\text{eq}}$  grows with the system size,

$$\lim_{N \gg 1} t_{\text{eq}}(N) \gg t$$

*e.g.*, diffusion, critical slowing down, coarsening, glassy physics

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- Driven systems    Energy injection

$$F_{\text{ext}} \neq -\nabla V(x)$$

*e.g.*, active matter

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- Integrability

$$I_{\mu}(\{p_i, x_i\}) = ct, \quad \mu = 1, \dots, N$$

Too many constants of motion inhibit equilibration to the Gibbs ensembles

*e.g.*, **1d bosonic gases**

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# Questions

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## Does an isolated quantum system reach some kind of equilibrium ?

Boosted by recent interest in

- the dynamics after **quantum quenches** of cold atomic systems
  - rôle of interactions (integrable vs. non-integrable)
- **many-body localisation**
  - novel effects of quenched disorder

## And, an isolated classical system ?

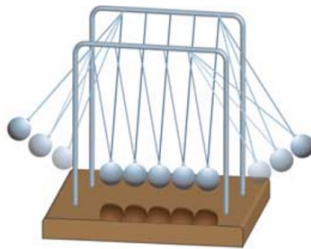
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The (old) ergodicity question revisited

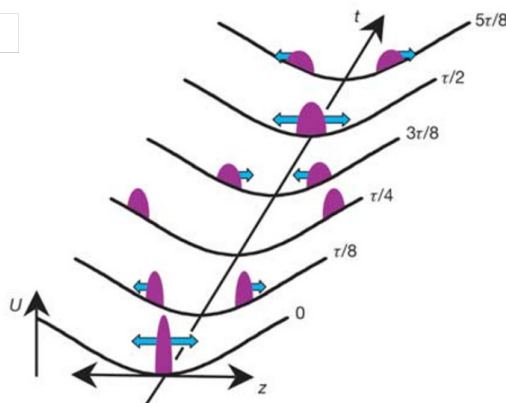
Our contribution **Barbier, LFC, Lozano, Nessi, Picco, Tartaglia 17-21**

# Motivation

Isolated quantum systems: experiments and theory  $\sim 15$ y ago

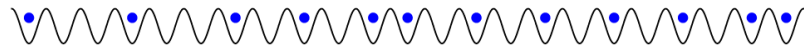


Quantum quenches & Conformal field theory  
**Calabrese & Cardy 06**



Numerics of lattice hard core bosons

(e)



**Rigol, Dunjko, Yurovsky & Olshanii 07**  
and many others

1d lattice models & 1+1 field theories

A quantum Newton's cradle  
cold atoms in isolation  
**Kinoshita, Wenger & Weiss 06**

**Alba, Bernard, Bertini, Calabrese, Cardy, Caux, De Luca, De Nardis, Doyon, Essler, Dubail, Gambassi, Konik, Mussardo, Polkovnikov, Prosen, Silva, Santoro, Spohn...**



# Quantum quenches

## Definition & questions

- Take an isolated quantum system with Hamiltonian  $\hat{H}_0$
- Initialize it in, say,  $|\psi_0\rangle$  the ground-state of  $\hat{H}_0$  (or any  $\hat{\rho}(t_0)$ )
- Unitary time-evolution  $\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}$  with a Hamiltonian  $\hat{H} \neq \hat{H}_0$ .

Does the system reach (locally) a steady state?

Are the expected values of local observables determined by  $e^{-\beta\hat{H}}$ ?

Does the evolution occur as in equilibrium?

Not for integrable models. Alternative, the **Generalized Gibbs Ensemble**

$$\hat{\rho}_{\text{GGE}} = \mathcal{Z}^{-1}(\{\gamma_\mu\}) e^{-\sum_{\mu=1}^N \gamma_\mu \hat{I}_\mu} \quad \& \quad \langle \psi_0 | \hat{I}_\mu | \psi_0 \rangle = \langle \hat{I}_\mu \rangle_{\text{GGE}} \text{ fix } \{\gamma_\mu\}$$



# Classical quenches

## Definition & questions

- Take an **isolated** classical system with Hamiltonian  $H_0$ , evolve with  $H$
- Initialize it in, say,  $\psi_0$  a configuration, e.g.  $\{x_i, p_i\}_0$  for a particle system  
 $\psi_0$  could be drawn from a probability distribution, e.g.  $Z^{-1} e^{-\beta_0 H_0(\psi_0)}$

Does the system reach a steady state ? (in the  $N \rightarrow \infty$  limit)

Is it described by a thermal equilibrium probability  $e^{-\beta H}$  ?

Do at least some local observables behave as thermal ones ?

Does the evolution occur as in equilibrium ?

If not, other kinds of probability distributions ?

# Classical quenches

## Definition & questions

In the steady state of a classical macroscopic ( $N \rightarrow \infty$ ) model

Time averages  $\overline{O(t)} \equiv \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_{t_{\text{st}}}^{t_{\text{st}} + \tau} dt' O(t')$

& statistical averages  $\langle O \rangle \equiv \int \prod_i dx_i \prod dp_i O(x_i, p_i) \rho(x_i, p_i)$

should be equal  $\overline{O(t)} = \langle O \rangle$  for a generalised micro-canonical measure  $\rho$

in which, in integrable cases, all constants of motion are fixed

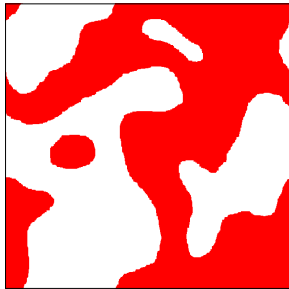
**Yuzbashyan 18**

Are local observables characterised by a “canonical” measure ?

If yes, which ones ?

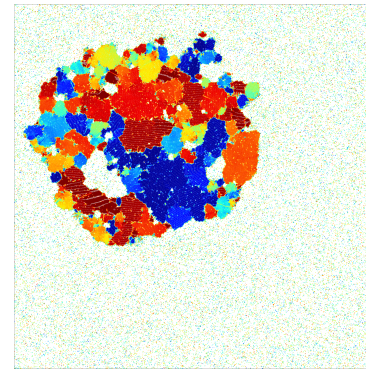
# Out of equilibrium

Explain, describe and, something in common ?

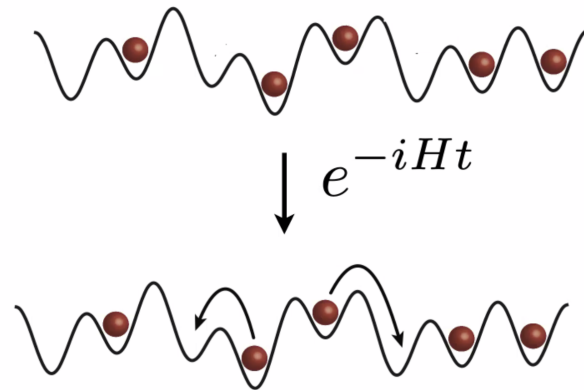
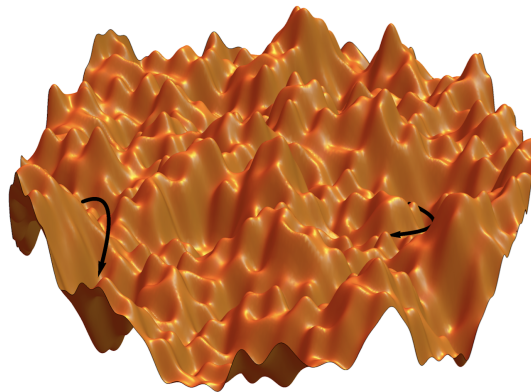


$$\lim_{N \gg 1} t_{\text{eq}}(N) \gg t$$

$$F \neq -\nabla V(r)$$



$$I_\mu = ct \quad \mu = 1, \dots, N$$



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# Challenges

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## in classical non-equilibrium macroscopic systems

- Coarsening

The systems are taken across *usual phase transitions*

The *dynamic mechanisms* are well-understood :

competition between equilibrium phases & topological defect annihilation

The difficulty lies in the calculation of observables in a time-dependent non-linear field theory.

- Glasses & active matter

Are there *phase transitions*?

The *dynamic mechanisms* are not well understood

The difficulty is conceptual (also computational)

- General question

Do these enjoy some kind of thermodynamic properties ?

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# Methods

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## Many body systems

- Coarsening phenomena

Identify the **order parameter**  $\phi(\boldsymbol{x}, t)$  (a field). Write **Langevin or Fokker-Planck** equations for it and analyse them. A difficult problem. Non-linear equations. Neither perturbation theory nor RG methods are OK. Self-consistent resummations tried.

- Glassy systems

The "order parameter" is a composite object depending on two-times. Spin models with quenched randomness yield a mean-field description of the dynamics observed. Classes of systems (ferromagnets, spin-glass and fragile glasses) captured.

- Active matter

Numerics of agent-based models, field theories, expansions...

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# Plan of the 1st Lecture

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1. Equilibrium vs. out of equilibrium classical systems.
2. How can a classical system stay far from equilibrium ?

From single-particle to many-body

Diffusion

Phase-separation & domain growth

Quenched randomness & glasses

Driven systems

Active matter

3. **Plan of the rest of the Course**

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# Plan of the 2nd-4th Lecture

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## 1. Langevin processes

Definition

Properties : irreversibility, dissipation, relaxation, time-scales,

Markov or generation of memory, discretization issues

Single particle observables

Some examples

## 2. Kramers/Fokker-Planck formalism

## 3. Applications

Active Brownian Particles

## 4. Many-body observables

Correlation functions, structure factor

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**End of 1st Lecture**

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# Observables

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## Positional order

The (fluctuating) **local particle number density**

$$\rho(\mathbf{r}_0) = \sum_{i=1}^N \delta(\mathbf{r}_0 - \mathbf{r}_i)$$

with normalisation  $\int d^d \mathbf{r}_0 \rho(\mathbf{r}_0) = N$ .

The **density-density correlation** function  $C(\mathbf{r} + \mathbf{r}_0, \mathbf{r}_0) = \langle \rho(\mathbf{r} + \mathbf{r}_0) \rho(\mathbf{r}_0) \rangle$  that, for homogeneous (independence of  $\mathbf{r}_0$ ) and isotropic ( $\mathbf{r} \mapsto |\mathbf{r}| = r$ ) cases, is simply  $C(\mathbf{r} + \mathbf{r}_0, \mathbf{r}_0) = C(r)$ .

The double sum in  $C(\mathbf{r} + \mathbf{r}_0, \mathbf{r}_0) = \langle \sum_{ij} \delta(\mathbf{r} + \mathbf{r}_0 - \mathbf{r}_i) \delta(\mathbf{r}_0 - \mathbf{r}_j) \rangle$  has contributions from  $i = j$  and  $i \neq j$ :  $C_{\text{self}} + C_{\text{diff}}$

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# Observables

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## Positional order

The density-density **correlation function**

$$C(\mathbf{r} + \mathbf{r}_0, \mathbf{r}_0) = \langle \rho(\mathbf{r} + \mathbf{r}_0) \rho(\mathbf{r}_0) \rangle = \sum_{ij} \langle \delta(\mathbf{r} + \mathbf{r}_0 - \mathbf{r}_i) \delta(\mathbf{r}_0 - \mathbf{r}_i) \rangle$$

is linked to the **structure factor**

$$S(\mathbf{q}) \equiv N^{-1} \langle \tilde{\rho}(\mathbf{q}) \tilde{\rho}(-\mathbf{q}) \rangle = \frac{1}{N} \left\langle \sum_{i=1}^N \sum_{j=1}^N e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right\rangle$$

by

$$N S(\mathbf{q}) = \int d^d r_1 \int d^d r_2 C(\mathbf{r}_1, \mathbf{r}_2) e^{-i\mathbf{q} \cdot (\mathbf{r}_1 - \mathbf{r}_2)}$$

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# Observables

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## Positional order

In isotropic cases, i.e. liquid phases, the pair correlation function

$$\frac{N}{V} g(r) = \text{average number of particles at distance } r \\ \text{from a tagged particle at } r_0$$

is linked to the structure factor

$$S(\mathbf{q}) = \frac{1}{N} \left\langle \sum_{i=1}^N \sum_{j=1}^N e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right\rangle$$

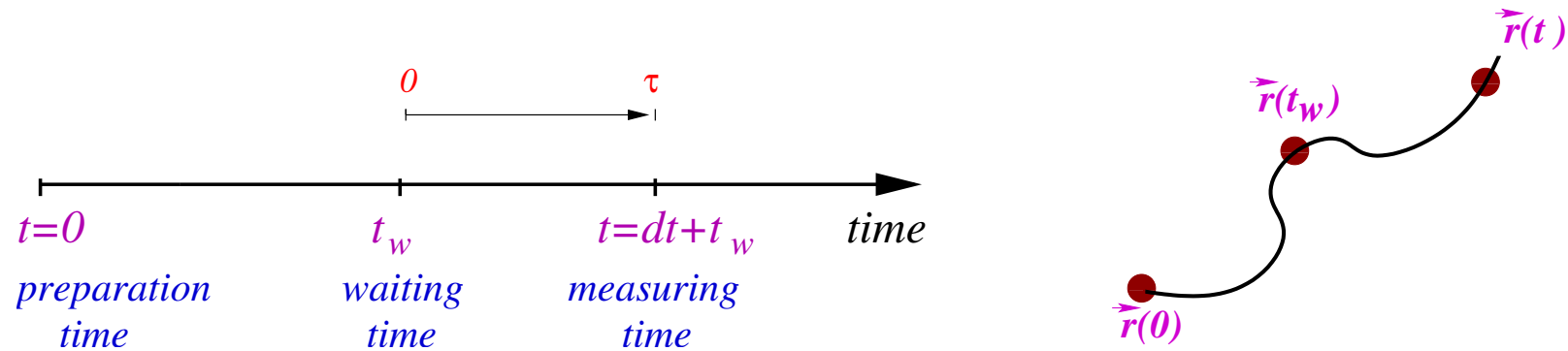
by

$$S(\mathbf{q}) = 1 + \frac{N}{V} \int d^d r g(r) e^{i\mathbf{q} \cdot \mathbf{r}}$$

Peaks in  $g(r)$  are related to peaks in  $S(q)$ . The first peak in  $S(q)$  is at  $q_0 = 2\pi / \Delta r$  where  $\Delta r$  is the distance between peaks in  $g(r)$  (that is close to the inter particle distance as well).

# Two-time observables

## Correlations



$t_w$  not necessarily longer than  $t_{\text{eq}}$ .

The two-time correlation between  $A[\{\mathbf{r}_i(t)\}]$  and  $B[\{\mathbf{r}_i(t_w)\}]$  is

$$C_{AB}(t, t_w) \equiv \langle A[\{\mathbf{r}_i(t)\}] B[\{\mathbf{r}_i(t_w)\}] \rangle$$

average over realizations of the dynamics (initial conditions, random numbers in a MC simulation, thermal noise in Langevin dynamics, etc.)

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# Correlation functions

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One can define a two-time dependent density-density correlation

$$\langle \rho(\boldsymbol{x}, t) \rho(\boldsymbol{y}, t_w) \rangle$$

The angular brackets indicate a “thermal” average ; i.e.

over different dynamical histories (runs of simulation/experiment)

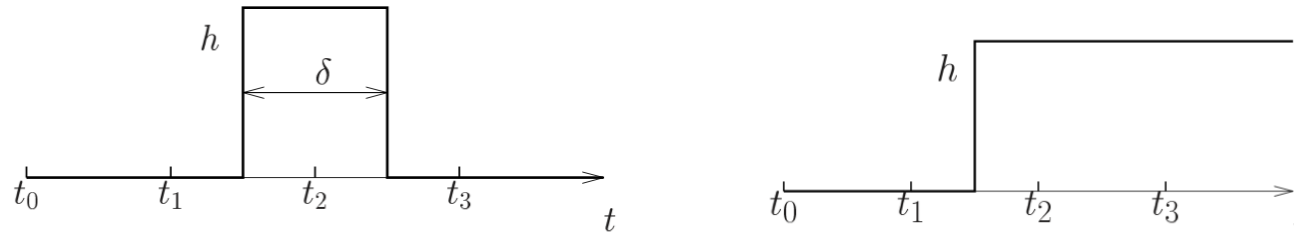
Upon averaging one expects :

isotropy (all directions are equivalent)

invariance under translations of the reference point  $\boldsymbol{x}$ .

Thus,  $\langle \rho(\boldsymbol{x}, t) \rho(\boldsymbol{y}, t_w) \rangle \Rightarrow g(r; t, t_w)$ , with  $r = |\boldsymbol{x} - \boldsymbol{y}|$ . Its Fourier transform is  $F(q; t, t_w)$  and it has a self part  $F_s(q; t, t_w)$  that at equal times becoes the structure factor

# Response to perturbations



The **perturbation** couples **linearly** to the observable  $B[\{\mathbf{r}_i\}]$

$$H \rightarrow H - hB[\{\mathbf{r}_i\}]$$

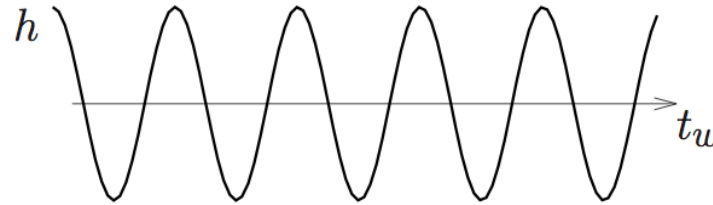
The **linear instantaneous response** of another observable  $A(\{\mathbf{r}_i\})$  is

$$R_{AB}(t, t_w) \equiv \left\langle \left. \frac{\delta A[\{\mathbf{r}_i\}](t)}{\delta h(t_w)} \right|_{h=0} \right\rangle$$

The **linear integrated response** or **dc susceptibility** is

$$\chi_{AB}(t, t_w) \equiv \int_{t_w}^t dt' R_{AB}(t, t')$$

# ac response to perturbations



$$\chi(\omega, t_w) = \int_0^{t_w} dt' R(t_w, t') h(\omega, t') = \int_0^{t_w} dt' R(t_w, t') e^{i\omega t'}$$

$$\chi'(\omega, t_w) = \text{Re}\chi(\omega, t_w) \text{ (in phase)}$$

$$\chi''(\omega, t_w) = \text{Im}\chi(\omega, t_w) \text{ (out of phase)}$$

are related by Kramers-Krönig  $\chi''(\omega, t_w) = -\pi^{-1} P \int d\omega' \frac{\chi'(\omega', t_w)}{\omega' - \omega}$

In equilibrium  $\chi(\omega, t_w) \rightarrow \chi(\omega)$

# Disordered spin systems

## Classical $p$ -spin model

$$H_{syst} = - \sum_{i_1 < \dots < i_p}^N J_{i_1 i_2 \dots i_p} s_{i_1} s_{i_2} \dots s_{i_p}$$

Ising,  $s_i = \pm 1$ , or spherical,  $\sum_{i=1}^N s_i^2 = N$ , spins.

Sum over all  $p$ -uplets on a complete graph: fully-connected model.

Random exchanges  $P(J_{i_1 i_2 \dots i_p}) = e^{-\frac{1}{2} J_{i_1 i_2 \dots i_p}^2 (2N^{p-1} / (p! J^2))}$

Extensions to random graphs possible: dilute models.

$p = 2$  Ising: Sherrington-Kirkpatrick model for spin-glasses

$p = 2$  spherical  $\approx$  mean-field ferromagnet

$p \geq 3$  Ising or spherical: models for fragile glasses



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# Methods

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for classical and quantum disordered systems

## Statics

TAP Thouless-Anderson-Palmer

Replica theory

Cavity or Peierls approx.

Bubbles & droplet arguments

functional RG

}

}

}

fully-connected (complete graph)

Gaussian approx. to field-theories

dilute (random graph)

finite dimensions

## Dynamics

Generating functional for classical field theories (MSRJD).

Schwinger-Keldysh closed-time path-integral for quantum dissipative models  
(the previous is recovered in the  $\hbar \rightarrow 0$  limit).

Perturbation theory, renormalization group techniques, self-consistent approx.

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# Methods

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for classical and quantum disordered systems

## Statics

TAP Thouless-Anderson-Palmer

Replica theory

Cavity or Peierls approx.

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## Dynamics

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Perturbation theory, renormalization group techniques, self-consistent approximations

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# Some references

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## Spin-glasses

*Slow Dynamics and Aging in Spin Glasses*, E. Vincent, J. Hammann, M. Ocio, J-P Bouchaud and L. F. Cugliandolo, arXiv:cond-mat/9607224 (Sitges Conference Proceedings, published by Springer-Verlag).

## Theory and methods

*Dynamics of glassy systems*, L. F. Cugliandolo, arXiv :cond-mat/0210312 (Les Houches Summer School 2002, published in the Les Houches collection).

and unpublished notes (see webpage & [www.lpthe.jussieu.fr/~leticia](http://www.lpthe.jussieu.fr/~leticia))

## Growing lengths

*Growing length scales in aging systems*, F. Corberi, L. F. Cugliandolo, and H. Yoshino, arXiv :1010.0149 (Leiden work-shop, published by Oxford University Press)