Out of equilibrium dynamics of complex systems

Leticia F. Cugliandolo

Sorbonne Université

Laboratoire de Physique Théorique et Hautes Energies

Institut Universitaire de France

leticia@lpthe.jussieu.fr

www.lpthe.jussieu.fr/~leticia/seminars

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Plan of the 1st Lecture

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

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Statistical physics

Advantage

No need to solve the dynamic equations!

Under the *ergodic hypothesis*, after some *equilibration time* $t_{\rm eq}$, *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 $\boldsymbol{P}(\{\boldsymbol{p_i}, \boldsymbol{x_i}\})$

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

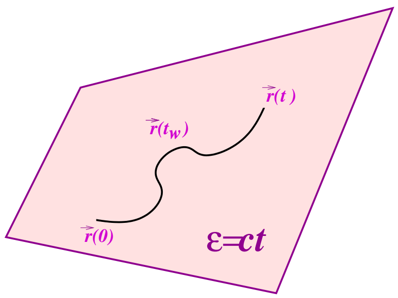
$\langle A \rangle$ should coincide with $\overline{A} \equiv \lim_{\tau \to \infty} \frac{1}{\tau} \int_{t_{\rm eq}}^{t_{\rm eq}+\tau} dt' \, A(\{\boldsymbol{p}_i(t'), \boldsymbol{x}_i(t')\})$

the *time average* typically measured experimentally **Ergodicity**

Boltzmann, late XIX

Statistical physics

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



Isolated system

$$\mathcal{E} = \mathcal{H}(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) = ct$$

Microcanonical ensemble

$$\boxed{P(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) \propto \delta(\mathcal{H}(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) - \mathcal{E})}$$

Flat probability density

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

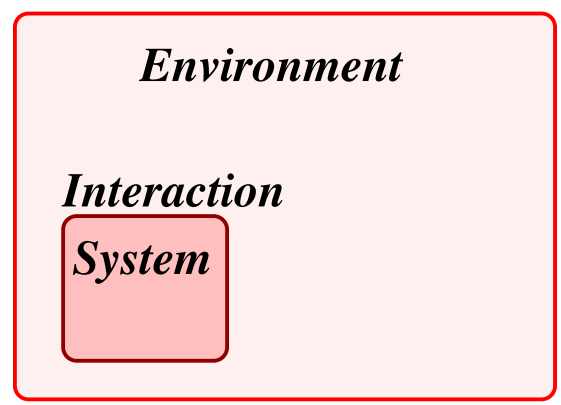
Entropy — Temperature

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

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

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

$$\boxed{P(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) \propto e^{-\beta\mathcal{H}(\{\boldsymbol{p}_i, \boldsymbol{x}_i\})}}$$



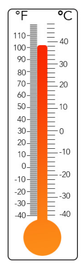
Canonical ensemble

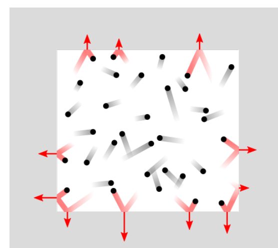
Statistical physics

Accomplishments

- Microscopic definition & derivation of thermodynamic concepts

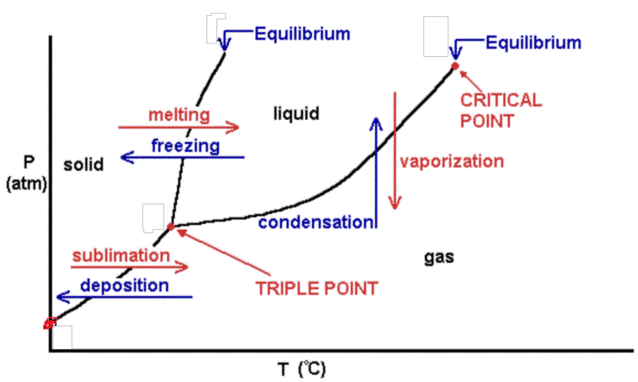
  (temperature, pressure, *etc.*) and laws (equations of state, *etc.*)



$$PV = nRT$$

- 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

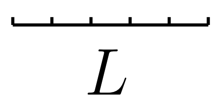
Statistical physics

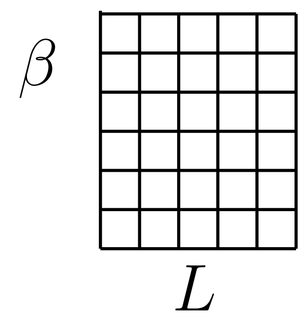
Classical $\Leftrightarrow$ Quantum

Partition function correspondence

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

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





$\beta\hbar$-periodic imaginary time direction

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

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

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

Dynamics $\Rightarrow$ Stat Mech

Different cases

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

General setting

Different cases

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

Isolated systems

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 ?

General setting

Different cases

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

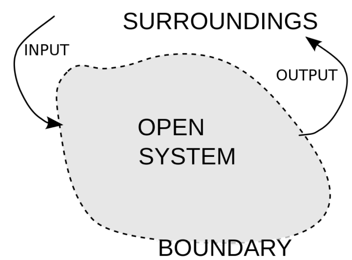
Open systems

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).

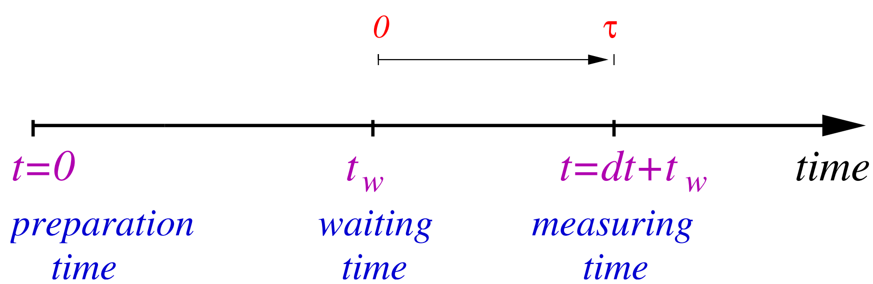
The total energy is conserved, $\mathcal{E} =$ ct but each contribution is not, in particular, $\mathcal{E}_{syst} \neq$ ct, and we'll take $e_0 \ll \mathcal{E}_{syst} \ll \mathcal{E}_{env}$.

In and out of equilibrium

Take a **mechanical point of view** and call $\{\zeta_i\}(t)$ the variables

e.g. the particles' coordinates $\{\boldsymbol{x}_i(t)\}$ and momenta $\{\boldsymbol{p}_i(t)\}$

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

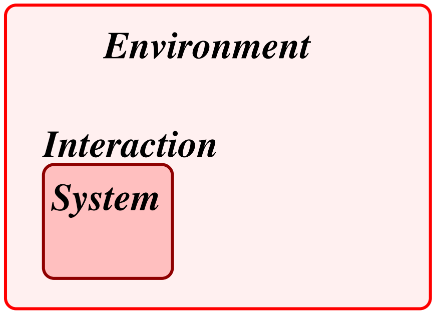


- For $t_w > t_{\rm eq}$: $\{\zeta_i\}(t)$ reach the equilibrium pdf and thermodynamics and statistical mechanics apply (e.g., **temperature** is a well-defined concept).
- For $t_w < t_{\rm eq}$: the system remains out of equilibrium and thermodynamics and (Boltzmann) statistical mechanics **do not**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

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

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

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   - Quenched randomness & glasses
   - Driven systems
   - Active matter

Out of equilibrium

Three possible reasons

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

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

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

- **Driven systems** Energy injection

$$\boxed{\boldsymbol{F}_{\rm ext} \neq -\boldsymbol{\nabla} V(\boldsymbol{x})} \qquad \boxed{\Gamma_1 \neq \Gamma_2}$$

e.g., **active matter**

- **Integrability**

$$\boxed{I_\mu(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) = ct, \qquad \mu = 1, \dots, N}$$

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

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

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Macroscopic systems

Discussion of several macroscopic systems with slow dynamics due to

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

Examples :

Ordering processes

Domain growth, phase separation

Systems with frustrated interactions

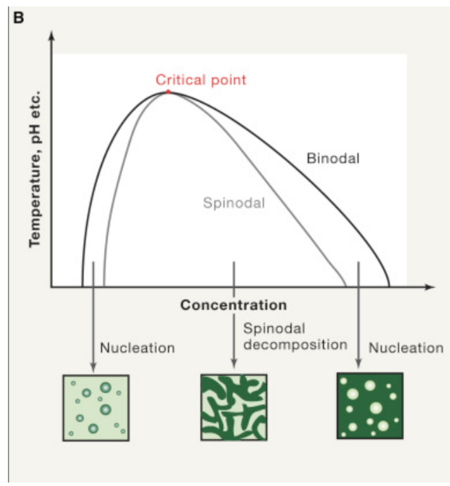
Spin ices

Systems with quenched disorder

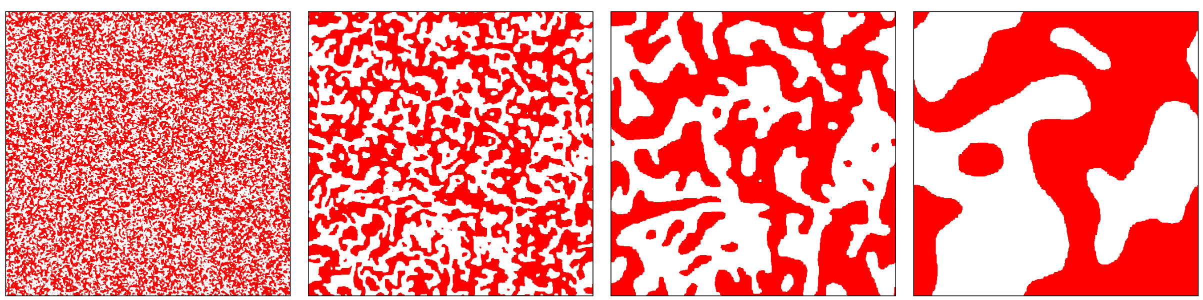
Random ferromagnets, spin-glasses

Phase separation

Quench below the binodal : remnant interfaces



$$t_1 \quad < \quad t_2 \quad < \quad t_3 \quad < \quad t_4 \quad < \quad \ldots$$

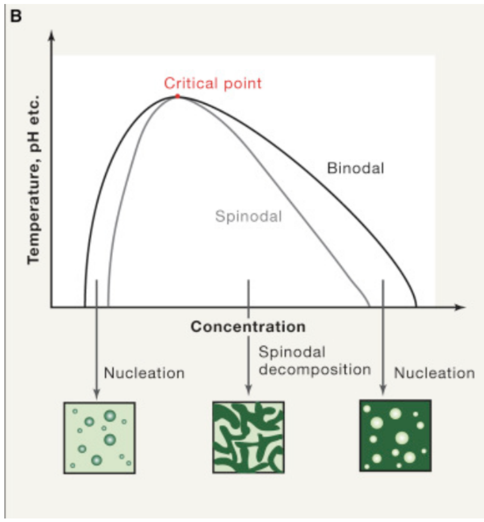


Coarsening process with growing length $\mathcal{R}(t) \simeq t^{1/z} \implies \boxed{t_{\mathbf{eq}} \sim L^z}$

Equilibration time diverges with the system size

Phase separation

Quench below the binodal : universality



Microscopic details are irrelevant

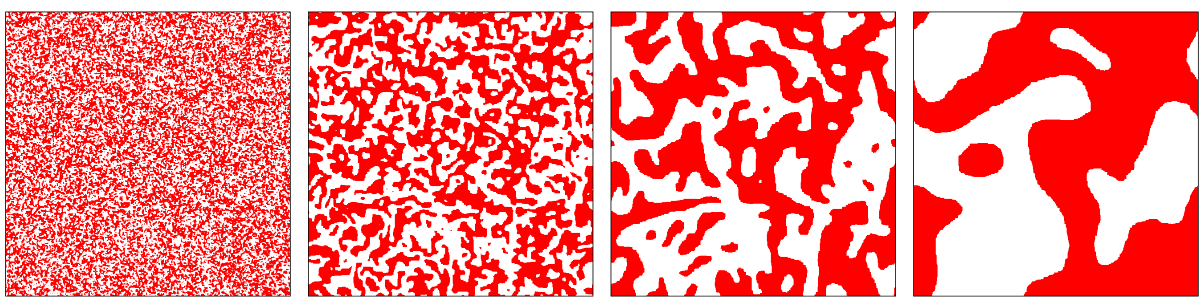
but conservation laws and

dimension of order parameter fix the

$\Longrightarrow$

Dynamic universality class

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



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

Quenched disorder

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

Time scales $t_{\rm micro} \ll t \ll t_q$

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 !

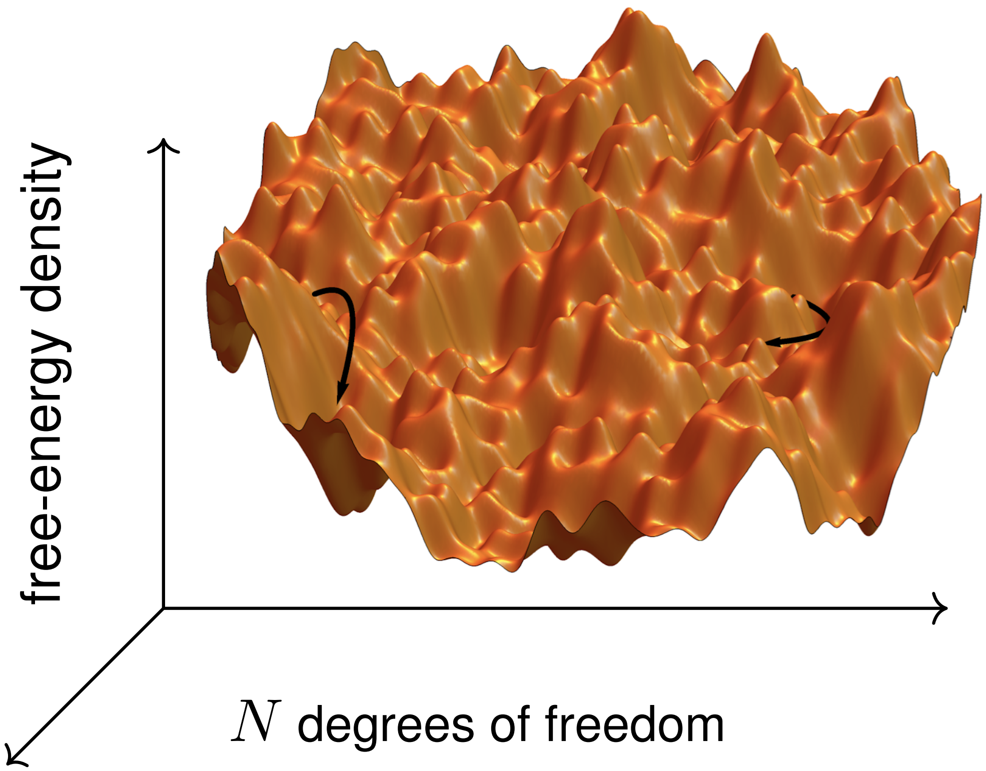


Figure adapted from a picture by **C. Cammarota**

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

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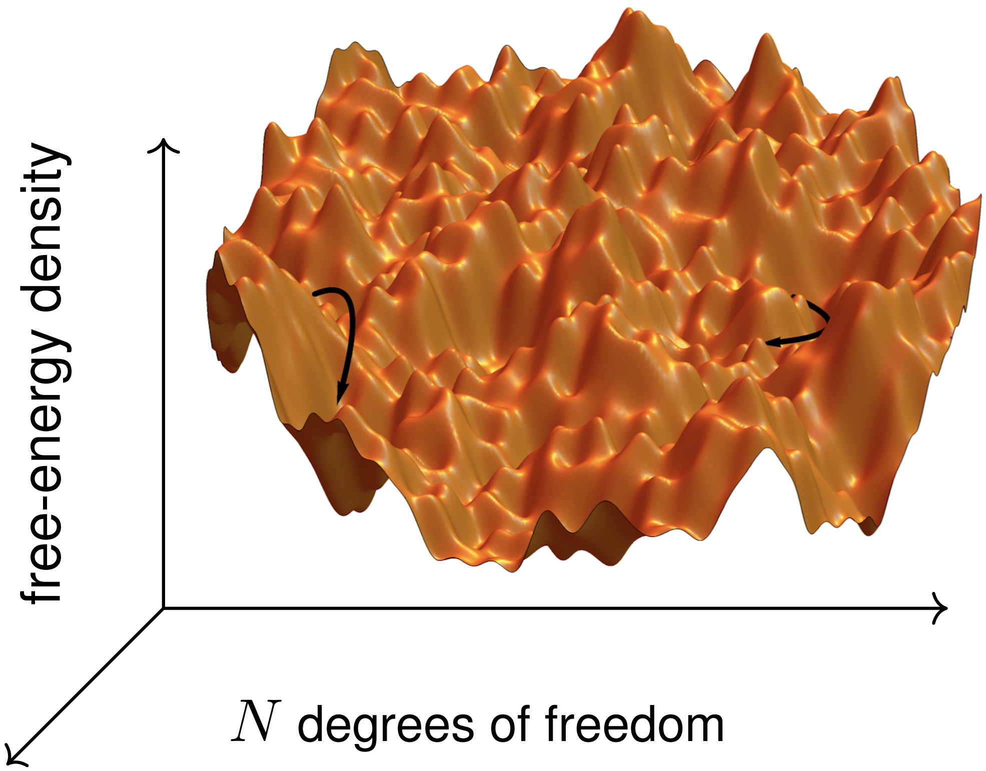


How to reach the absolute minimum ?

Thermal activation, surfing over tilted regions, quantum tunneling ?

Optimisation problem Smart algorithms ? Computer sc - applied math

Spin-glasses

Magnetic impurities (spins) randomly placed in an inert host

Quenched random interactions

Interacting via the RKKY potential

$$V(s_i, s_j) \propto \frac{\sin 2\pi k_F r}{r^3} s_i s_j \qquad J(r) \propto \frac{\sin 2\pi k_F r}{r^3}$$

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

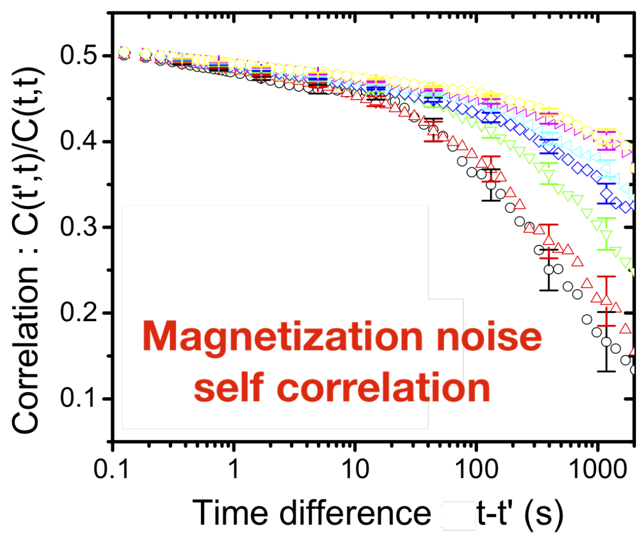
Standard lore : there is a 2nd order static phase transition at T_s separating a paramagnetic from a spin-glass phase.

No dynamic precursors above T_s.

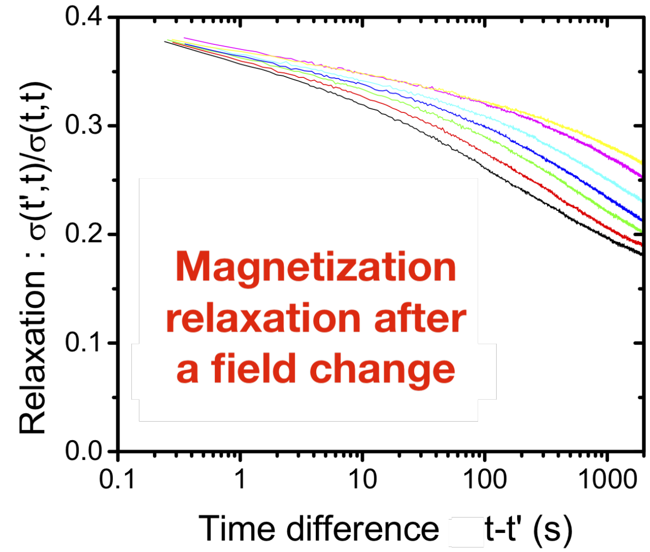
Glassy dynamics below T_s with aging, memory effects, etc.

Rugged free-energy landscapes

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



Correlation



Linear response

0 t' t' t' t' time

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

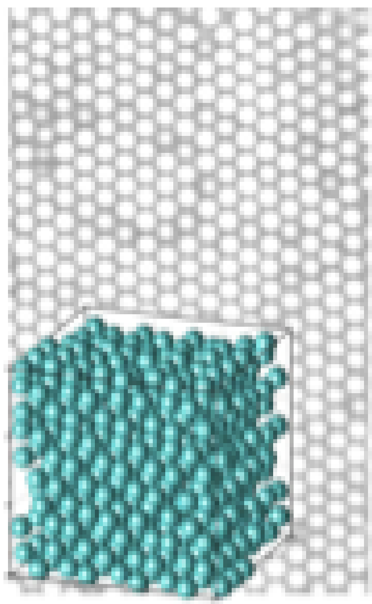
No identifiable growing length $\mathcal{R}(t)$: **glassy microscopic mechanisms ?**

Spin-glass experiments **Hérisson & Ocio 02-04**

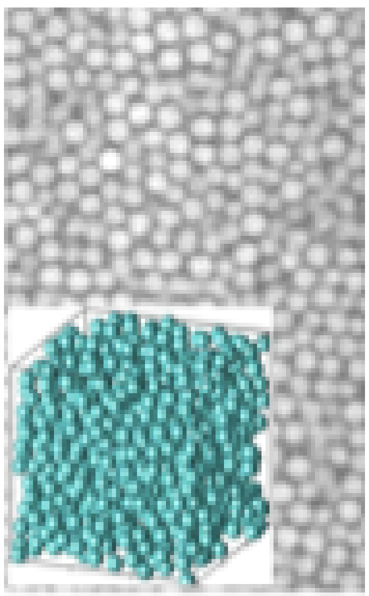
Structural Glasses

e.g., **colloidal ensembles**

Micrometric spheres immersed in a fluid



Crystal



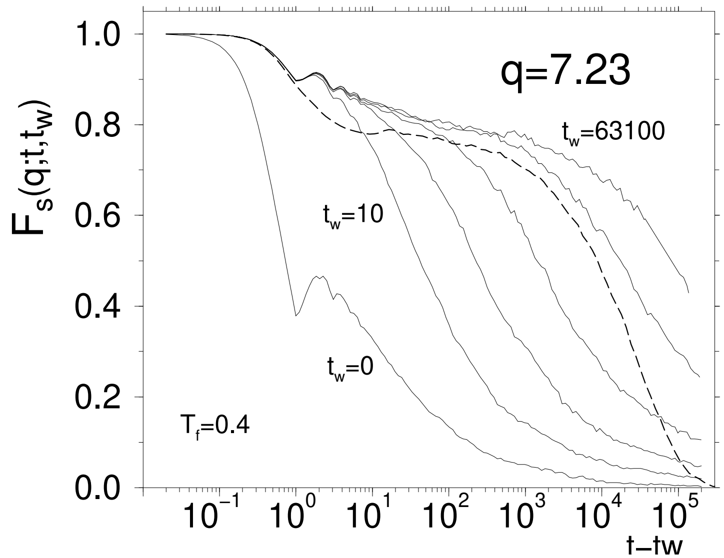
Glass

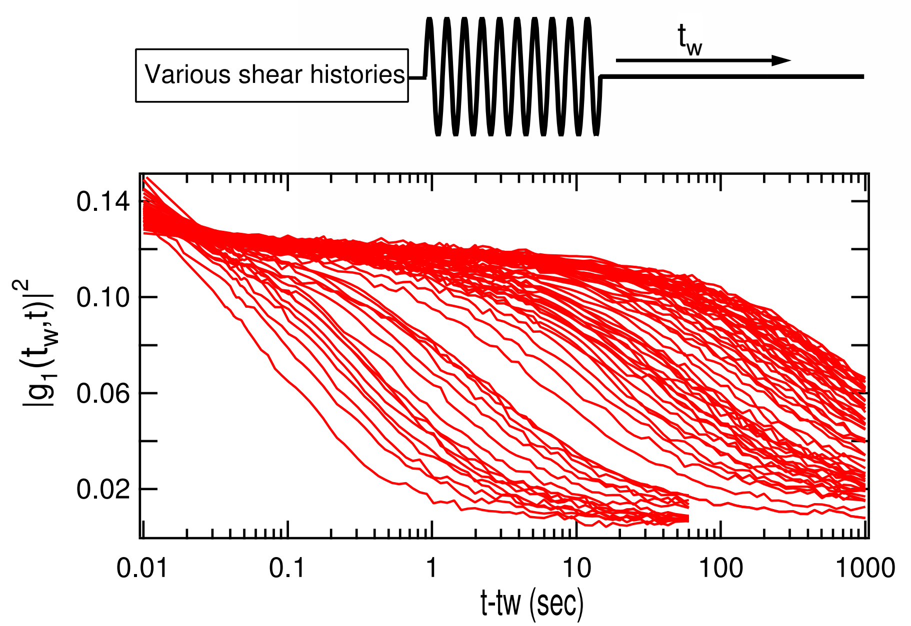
In the glass : no obvious growth of order, slow dynamics with, however, scaling properties

What drives the slowing down ?

Low temp/high densities

Out of equilibrium aging 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.

Long time-scales

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

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$$\boldsymbol{F}_{\rm ext} \neq -\boldsymbol{\nabla} V(\boldsymbol{x}) \qquad \Gamma_1 \neq \Gamma_2$$

e.g., **active matter**

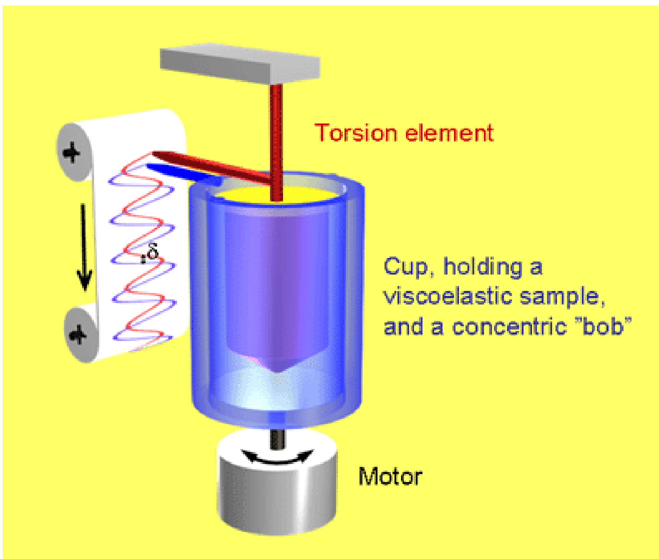
- **Integrability** $$I_\mu(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) = ct, \qquad \mu = 1, \dots, N$$

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

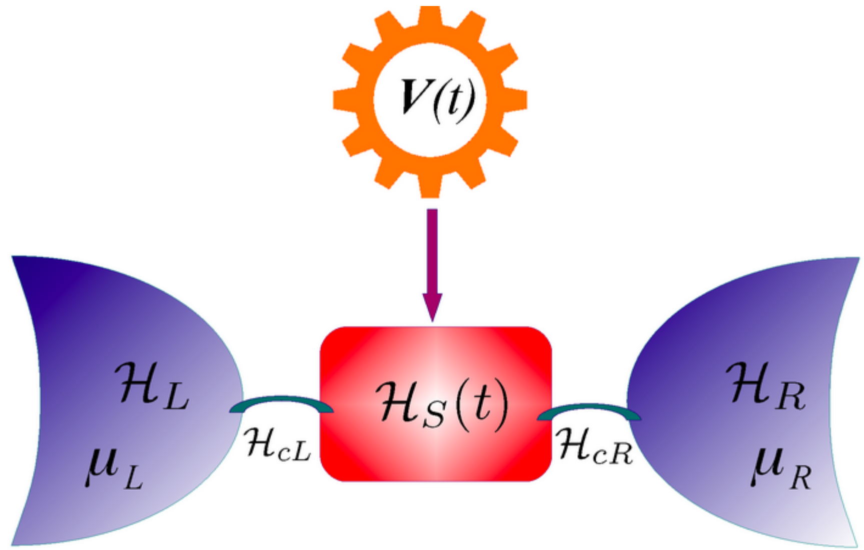
e.g., **1d bosonic gases**

Energy injection

Traditional : from the borders (outside)



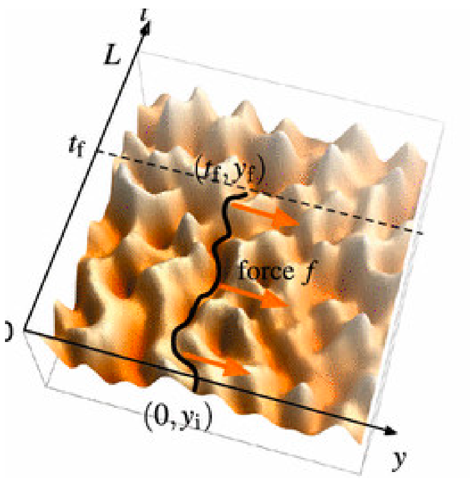
Rheology



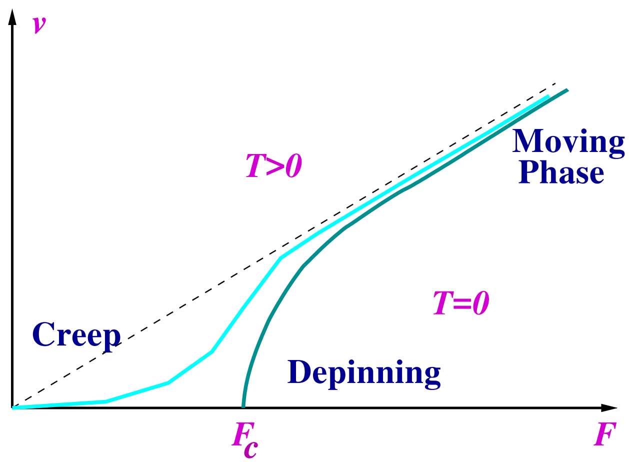
Transport

Drive & transport

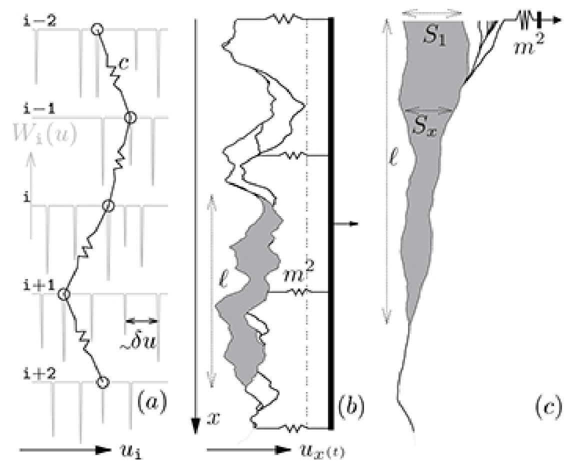
Driven interface over a disordered background



A line



Depinning & creep



avalanches

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

Active matter

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.

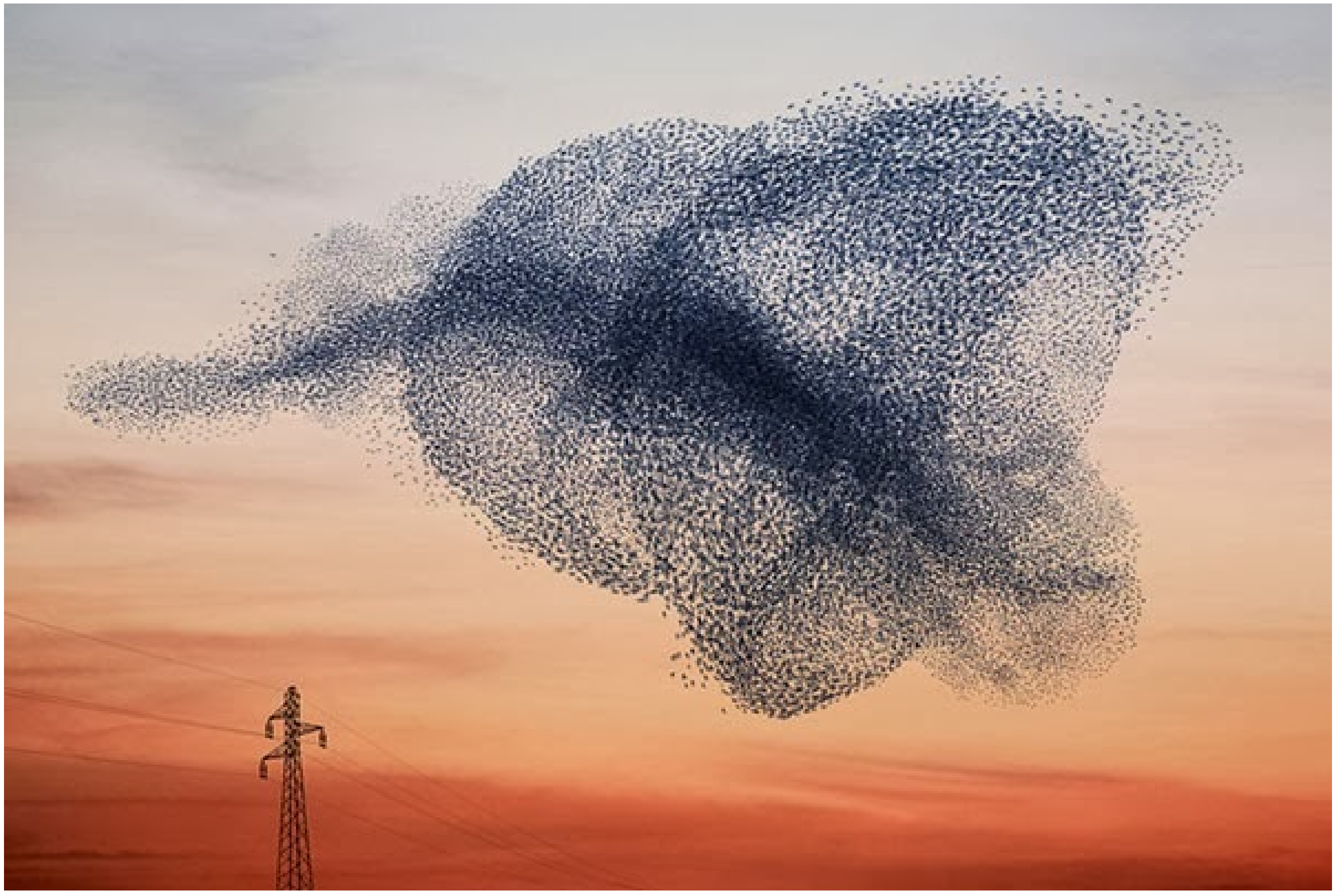
Due to the energy consumption, these systems are intrinsically out of thermal equilibrium.

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.

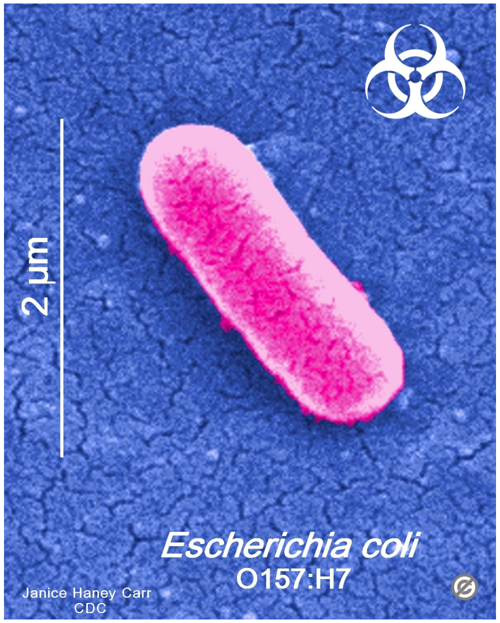
Natural systems

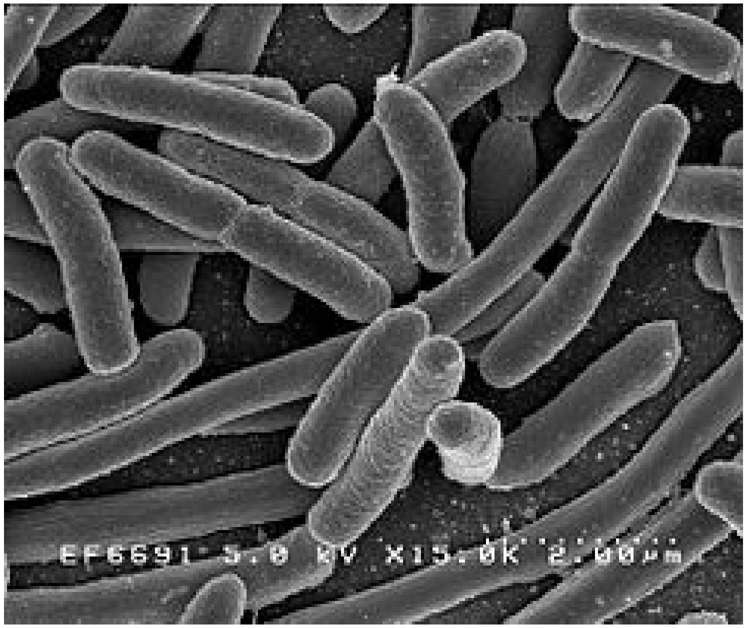
Birds flocking



Natural systems

Bacteria

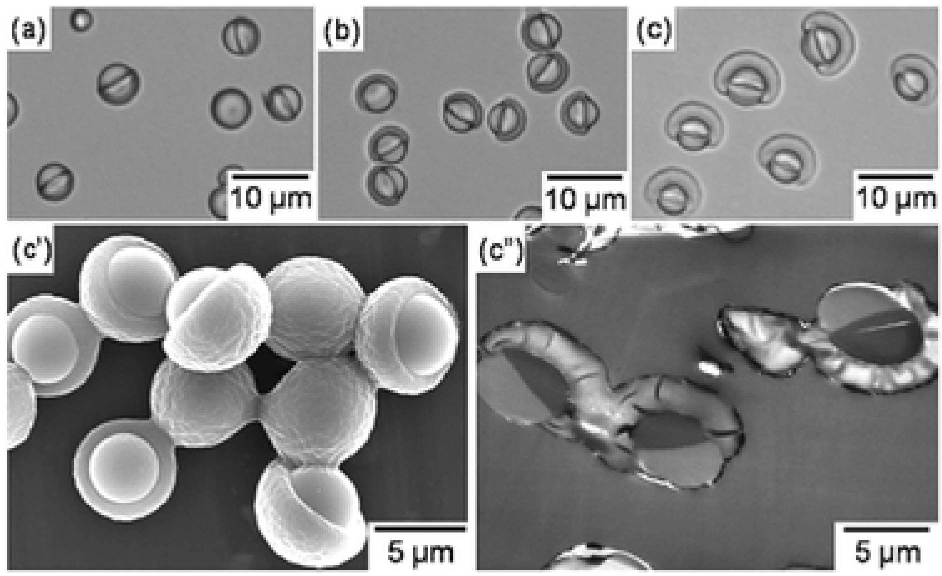




Escherichia coli - Pictures borrowed from the internet.

Artificial systems

Janus particles



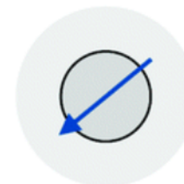
Particles with two faces (Janus God)

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

Active Brownian particles

The standard model – ABPs

Spherical particles with diameter σ_d



Environment $\Longrightarrow$ Langevin dynamics

Scales $\Longrightarrow$ over-damped motion

Self-propulsion $\Longrightarrow$ active force $\boldsymbol{F}_{\rm act}$ along $\boldsymbol{n}_i = (\cos\theta_i(t), \sin\theta_i(t))$

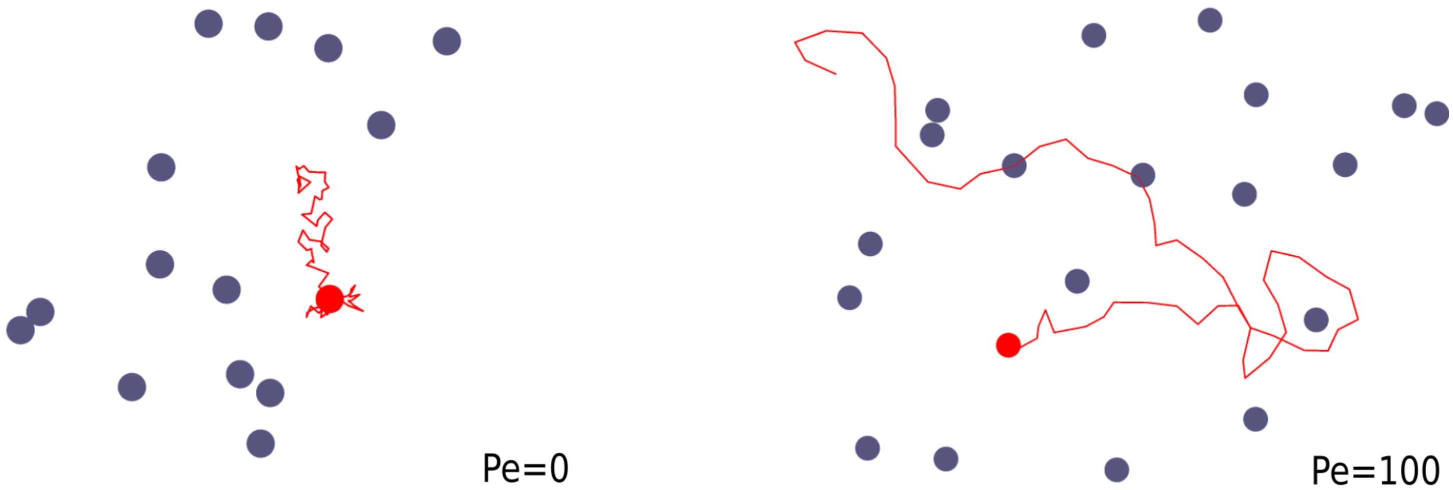
$$\underbrace{\gamma \dot{\boldsymbol{r}}_i}_{\text{friction}} = \underbrace{F_{\rm act}\boldsymbol{n}_i}_{\text{propulsion}} \underbrace{- \boldsymbol{\nabla}_i \sum_{j(\neq i)} U(r_{ij})}_{\text{inter-particle repulsion}} + \underbrace{\boldsymbol{\xi}_i}_{\text{translational white noise}} \qquad \underbrace{\dot{\theta}_i = \eta_i}_{\text{rotational white noise}}$$

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

Bialké, Speck & Löwen 12, Fily & Marchetti 12

Active Brownian particles

Typical motion of ABPs in interaction



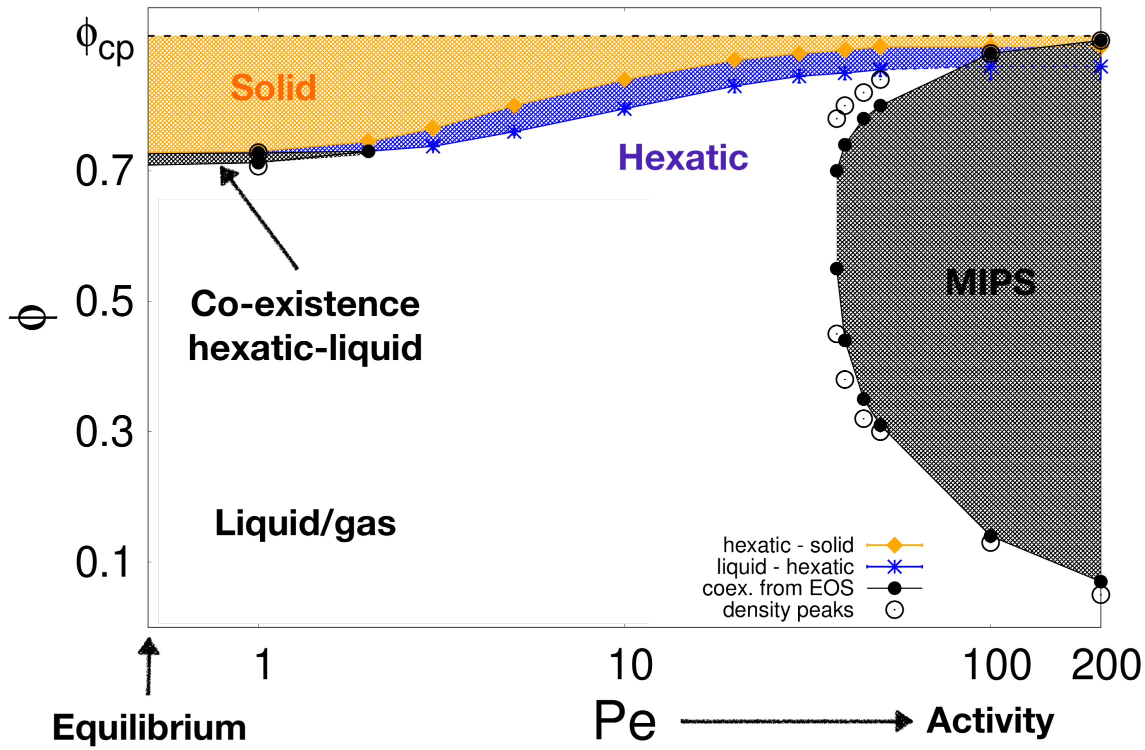
The activity induces a persistent random motion

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

sudden changes in direction

Active Brownian particles

Complex out of equilibrium phase diagram



Motility induced phase separation (MIPS)

gas & dense droplet

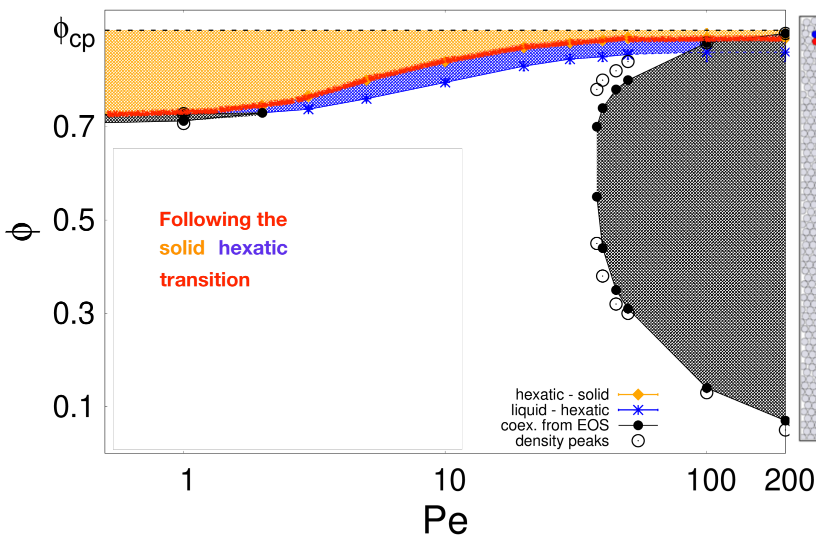
Cates & Tailleur 12

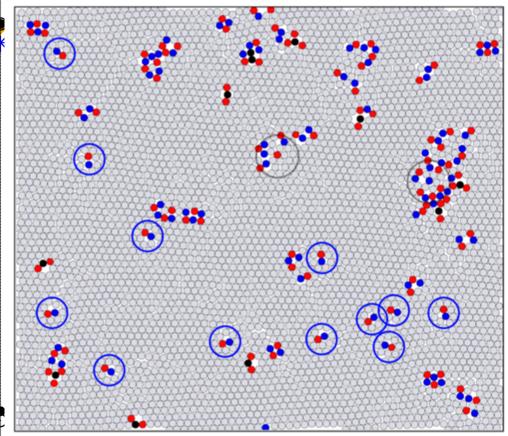
From virial pressure $P(\phi)$, translational and orientational correlations G_T and G_6, distributions of local density and hexatic order ϕ_i and ψ_{6i}, at fixed $k_BT = 0.05$

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

Active Brownian particles

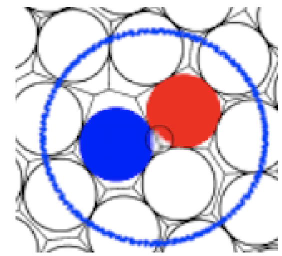
Out of equilibrium phase diagram **First question (out of many !)**





Free dislocation:

a 7-5 neighbor



$\neq$ from $\triangle$ lattice

Solid - **Hexatic** transition at ϕ_{sh}, **driven by unbinding of dislocation pairs**

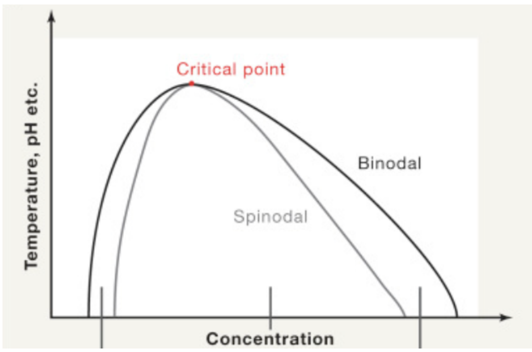
as in Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young universality ?

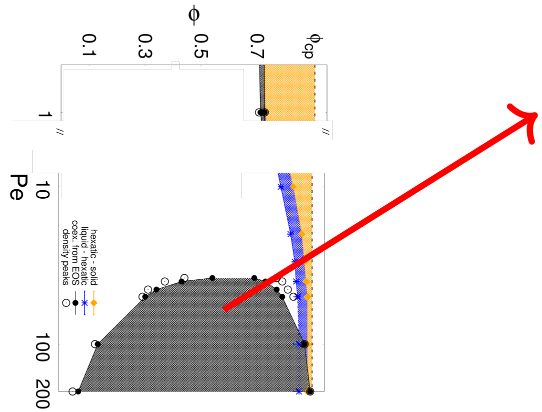
$$\rho_{disloc} \simeq a \, \exp\left[-b\left(\frac{\phi_{sh}}{\phi_{sh}-\phi}\right)^{\nu}\right] \qquad \nu \sim 0.37 \quad \forall \text{Pe ?}$$

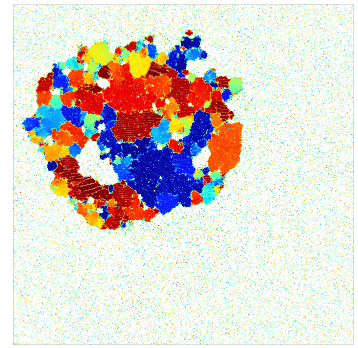
Digregorio, Levis, LFC, Gonnella & Pagonabarraga 21

Active Brownian particles

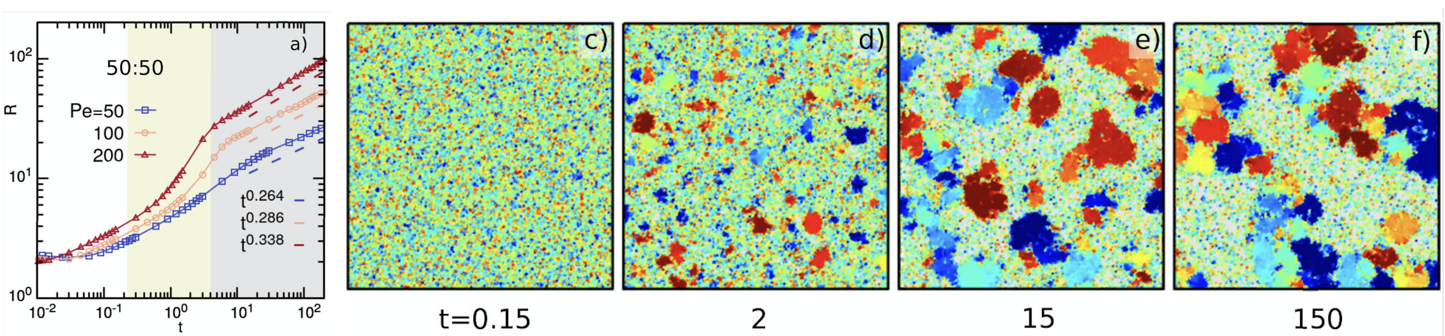
Out of equilibrium phase diagram **So many questions !**







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, ...**

Out of equilibrium

Three possible reasons

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

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

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

- **Driven systems** Energy injection

$$\boldsymbol{F}_{\rm ext} \neq -\boldsymbol{\nabla} V(\boldsymbol{x}) \qquad \Gamma_1 \neq \Gamma_2$$

e.g., **active matter**

- **Integrability** $$I_\mu(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) = ct, \qquad \mu = 1, \dots, N$$

Too many constants of motion inhibit equilibration to the Gibbs ensembles

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

Questions

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

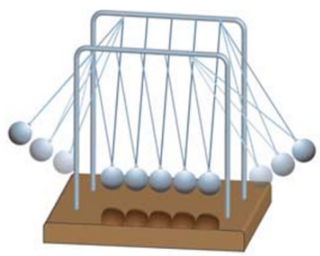
And, an isolated classical system ?

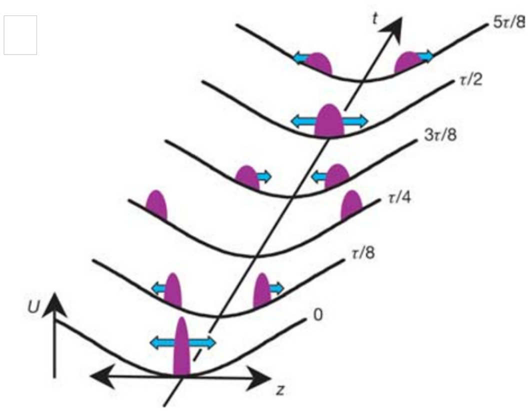
The (old) ergodicity question revisited

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

Motivation

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





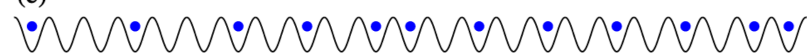
A quantum Newton's cradle
cold atoms in isolation

Kinoshita, Wenger & Weiss 06

Quantum quenches & Conformal field theory

Calabrese & Cardy 06

Numerics of lattice hard core bosons



Rigol, Dunjko, Yurovsky & Olshanii 07

and many others

$1d$ lattice models & 1+1 field theories

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**

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

Classical quenches

Definition & questions

- Take an **isolated** classical system with Hamiltonian H_0, evolve with H
- Initialize it in, say, ψ_0 a configuration, *e.g.* $\{\boldsymbol{x}_i, \boldsymbol{p}_i\}_0$ for a particle system

  ψ_0 could be drawn from a probability distribution, *e.g.* $\mathcal{Z}^{-1}\, e^{-\beta_0 H_0(\psi_0)}$

Does the system reach a steady state ? (in the $N \to \infty$ 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 ($N \to \infty$) model

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

& 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 ρ

in which, in integrable cases, all constants of motion are fixed **Yuzbashyan 18**

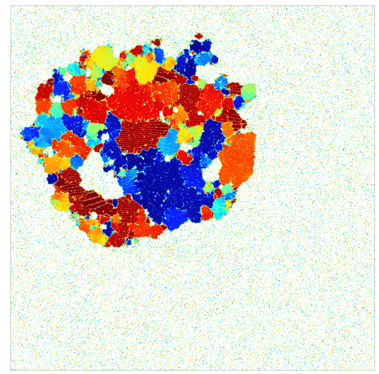
Are local observables characterised by a "canonical" measure ?

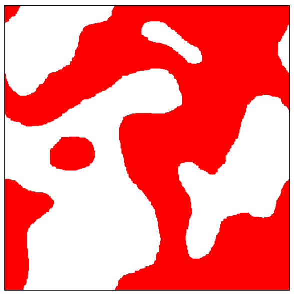
If yes, which ones ?

Out of equilibrium

Explain, describe and, something in common ?

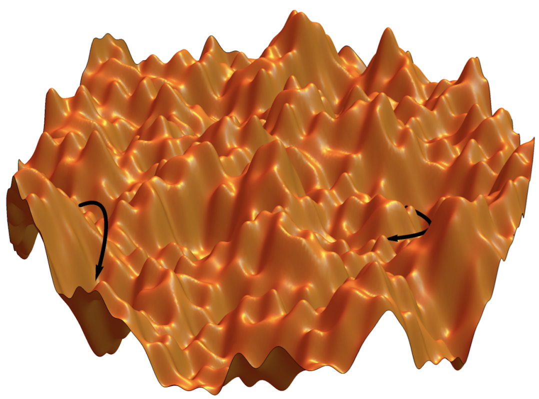
$$\boldsymbol{F} \neq -\boldsymbol{\nabla} V(\boldsymbol{r})$$

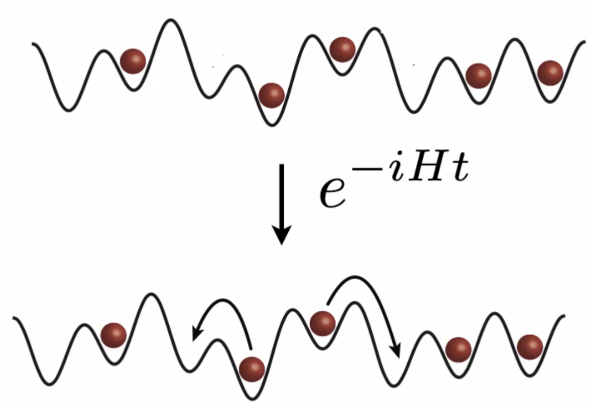




$$\lim_{N \gg 1} t_{\rm eq}(N) \gg t$$

$$I_\mu = \text{ct} \qquad \mu = 1, \dots, N$$





Challenges

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 ?

Methods

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...