Dynamics of Quantum Systems

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Lectures & Exercises Thursday 14:00 - 18:00

Exam during the January week (Monday-Thursday)

Oral presentation + questions

80% attendance required

Dynamics of Quantum Systems

Leticia F. Cugliandolo

LPTHE, Sorbonne Université, Paris, France

— Introduction.

(Closed and open systems. How to be out of equilibrium. Why quantum.)

— Quantum Mechanics.

(Concepts and notation. Many-body systems. Time evolution.)

— Generic properties.

(Expectation values and correlations, linear response & Kubo formula, Onsager & KMS relations, causality & Kramers-Kronig, fluctuation-dissipation thm.)

— Open systems.

(Decoherence, reduced system, entanglement, Lindblad equation, Feynman-Vernon model)

— Generating functionals.

(Closed time path or Schwinger-Keldysh formulation)

— Equilibration or not of closed quantum systems.

(Random matrix theory, quantum chaos vs. integrability, localization)

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

3. And a quantum system ?

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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 $\boldsymbol{P}(\{\boldsymbol{p}_i, \boldsymbol{x}_i\})$

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

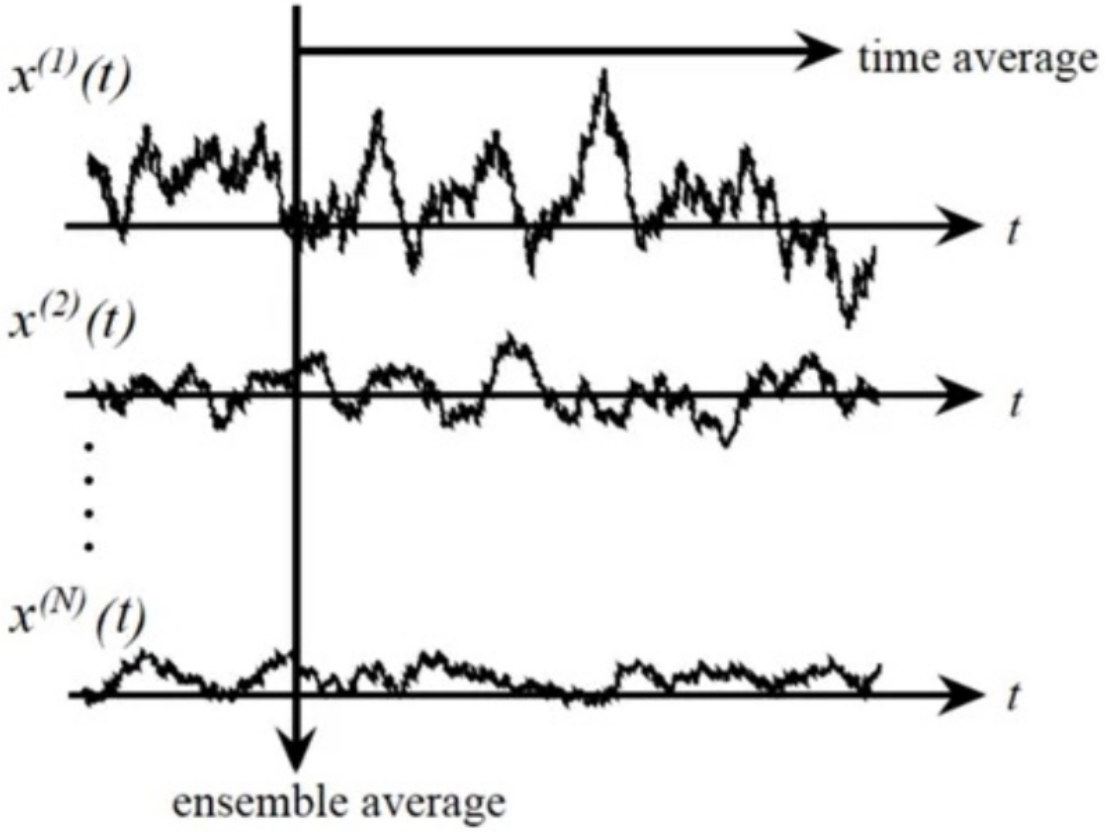
$\langle A \rangle$ should coincide with $\overline{A} \equiv \lim_{\tau \to \infty} \frac{1}{\tau} \int_{t_{\rm eq}}^{t_{\rm eq}+\tau} dt' \; A(\{\boldsymbol{p}_i(t'), \boldsymbol{x}_i(t')\})$

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

Boltzmann, late XIX

Statistical physics

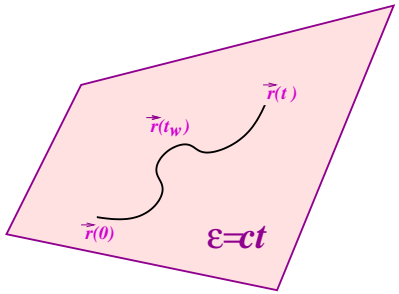
Advantage



Ex. 1.1

Statistical physics

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



Isolated system

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

Microcanonical ensemble

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

Flat probability density

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

Entropy

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

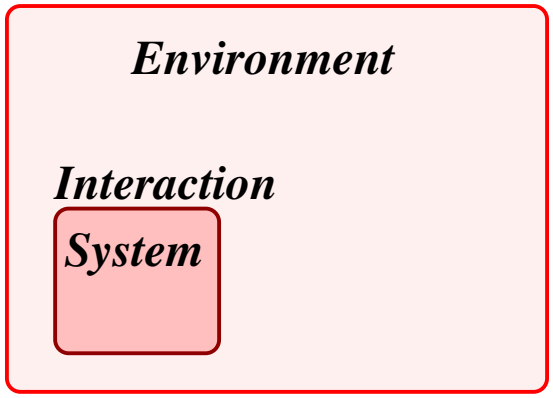
Temperature

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

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

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

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



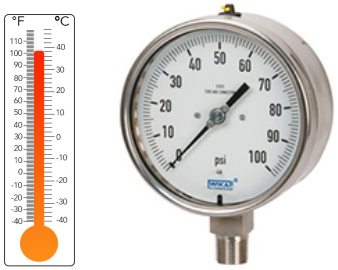
Canonical ensemble

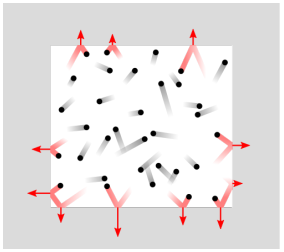
Statistical physics

Accomplishments

- Microscopic definition & derivation of thermodynamic concepts

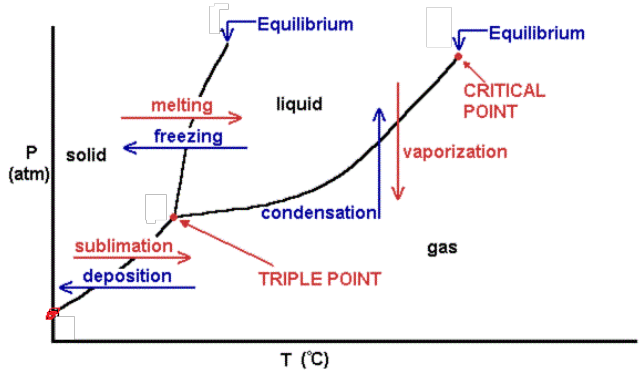
  (temperature, pressure, *etc.*) and laws (equations of state, *etc.*)





$$PV = nRT$$

- 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

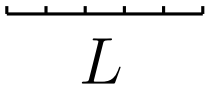
Classical $\Leftrightarrow$ Quantum

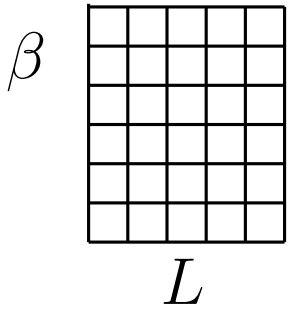
Partition function correspondence

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

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

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





$\beta\hbar$-periodic imaginary time direction

$\phi(\boldsymbol{x})$

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

Matsubara 55, Trotter 59, Feynman-Hibbs 65 & Suzuki 76

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**

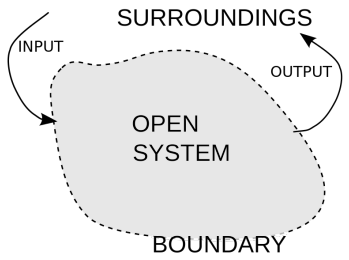
Open systems

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).

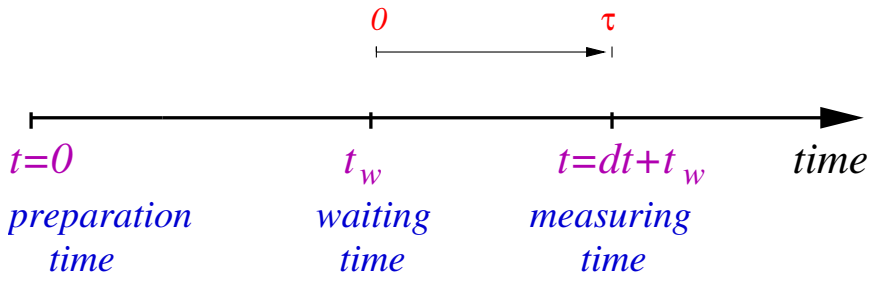
The total energy is conserved, $\mathcal{E} =$ ct but each contribution is not, in particular, $\mathcal{E}_{syst} \neq$ ct, and we'll take $e_0 \ll \mathcal{E}_{syst} \ll \mathcal{E}_{env}$.

In and out of equilibrium

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

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

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

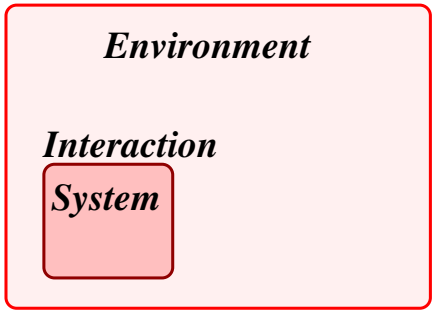


- For $t_w > t_{\rm eq}$: $\{\boldsymbol{\zeta}_i\}(t)$ reach the equilibrium pdf and thermodynamics and statistical mechanics apply (e.g., **temperature** is a well-defined concept).
- For $t_w < t_{\rm eq}$: the system remains out of equilibrium and thermodynamics and (Boltzmann) statistical mechanics **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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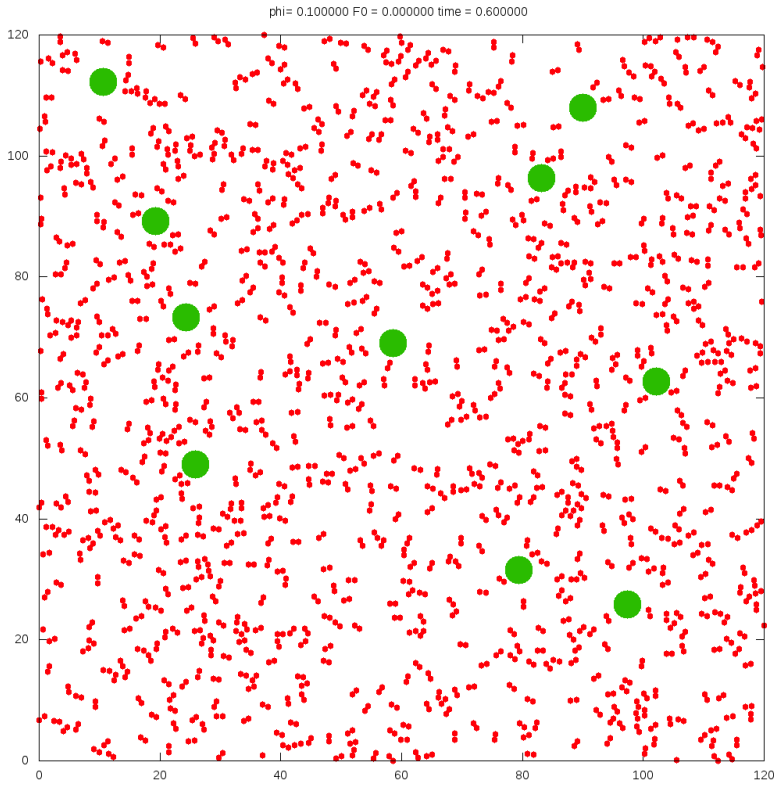
   From single-particle to many-body

   - Diffusion
   - Phase-separation & domain growth
   - Quenched randomness & glasses
   - Driven systems
   - Active matter

3. And a quantum system ?

Microscopic system

Brownian motion : diffusion



First example of dynamics of an *open system*

The system : the Brownian particle

The bath : the liquid

Interaction : collisional or potential

Canonical setting

A few Brownian particles or tracers ● embedded in a liquid.

Late XIX, early XX (Brown, Einstein, Langevin, Smoluchowski)

Langevin approach

Stochastic Markov dynamics

From Newton's equation $\boldsymbol{F} = m\boldsymbol{a} = m\dot{\boldsymbol{v}}$ and $\boldsymbol{v} = \dot{\boldsymbol{x}}$

$$m\dot{v}_a = \underbrace{-\gamma_0 v_a + \xi_a}_{\text{force from the bath}}$$

with $a = 1, \ldots, d$ (the dimension of space), m the mass of the particle, and γ_0 the friction coefficient,

ξ is the time-dependent thermal noise with Gaussian statistics,

zero average $\langle \xi_a(t) \rangle = 0$ at all times t,

and delta-correlations $\langle \xi_a(t) \xi_b(t') \rangle = 2\,\gamma_0 k_B T\, \delta_{ab}\, \delta(t - t')$.

Dissipation for $\gamma_0 > 0$ the averaged energy is not conserved,

$$d_t \langle \mathcal{E}_{syst}(t) \rangle = -\frac{2\gamma_0}{m} \left(2\langle \mathcal{E}_{\text{syst}}(t) \rangle - k_B T \right)$$

Brownian motion

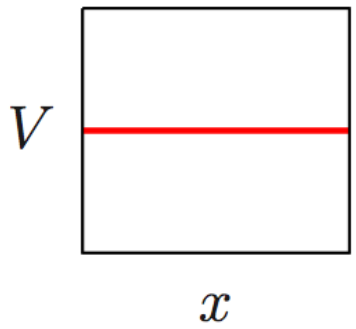
Normal diffusion

For simplicity, take a one dimensional system, $d = 1$.

The relation between friction coefficient γ_0 and amplitude of the noise correlation $2\gamma_0 k_B T$ ensures equipartition for the velocity variable

$$m\langle v^2(t)\rangle \to k_B T \quad \text{for} \quad t \gg t_r^v \equiv \frac{m}{\gamma_0}$$ **Langevin 1908**

But the position variable x diffuses since $e^{-\beta V}$ is not normalizable.



$$\langle x^2(t)\rangle \to 2D\,t \quad (t \gg t_r^v = m/\gamma_0)$$

$$D = k_B T/\gamma_0$$ diffusion constant.

The particle is out of equilibrium !

Brownian motion

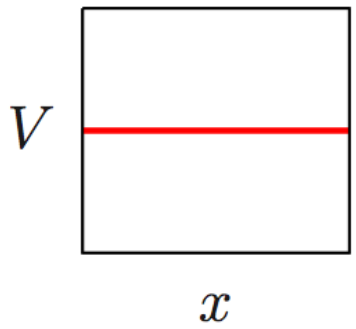
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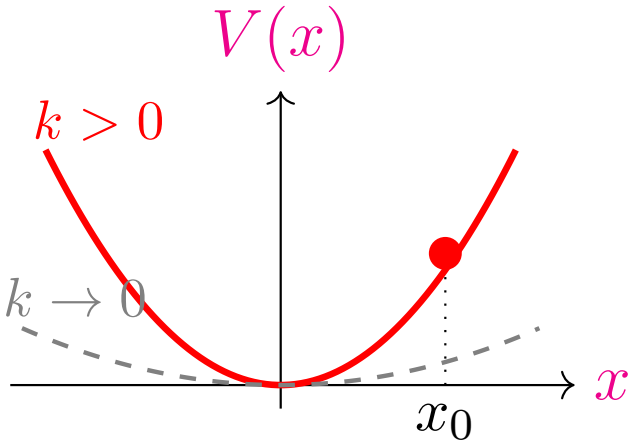
$$\langle x^2(t)\rangle \to 2D\,t \quad (t \gg t_r^v = m/\gamma_0)$$

$$D = k_B T/\gamma_0$$ diffusion constant.

Coexistence of equilibrium (v) and out of equilibrium (x) variables

Brownian motion

Exercise: an over-damped particle in a harmonic trap



$$\boxed{\gamma_0 \, \dot{x}(t) = -k \, x(t) + \xi(t)}$$

$$\langle \xi(t) \rangle = 0 \;\; \langle \xi(t) \xi(t') \rangle = 2\gamma_0 k_B T \, \delta(t - t')$$

Initial condition $x(0) = x_0$

- Compute $\langle x^2(t) \rangle$
- Discuss the limits $t \to \infty$ at fixed $k > 0$ and $k \to 0$ at fixed t
- Do the two limits commute ?

  Compare with $\langle x^2(t) \rangle \to 2Dt, \;\; D = k_B T / \gamma_0$.

Diffusion never equilibrates, a trapped particle does

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**

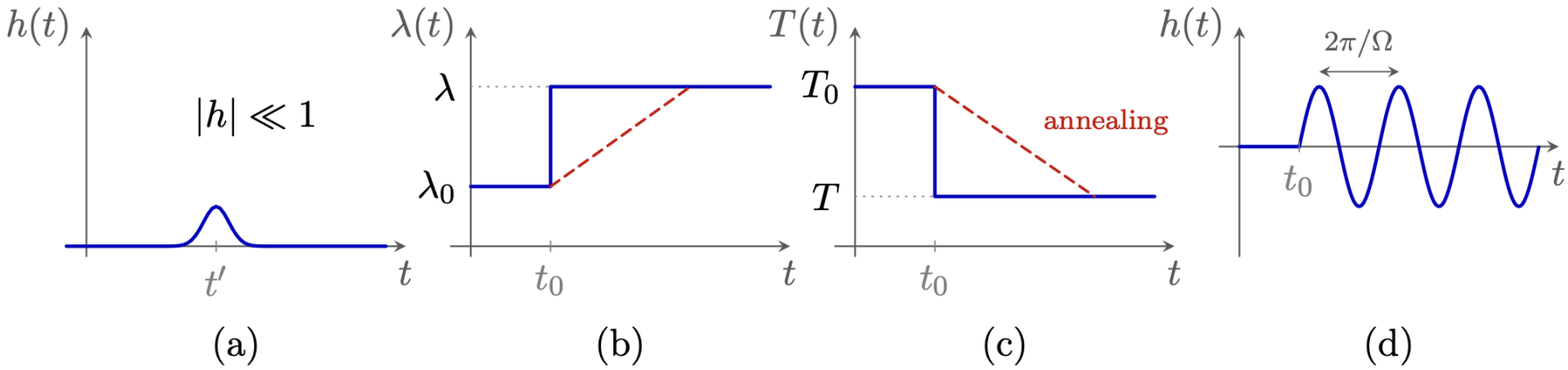
$$\boxed{I_\mu(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) = ct, \qquad \mu = 1, \ldots, N}$$

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

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

Perturbations

Possibilities



Does the system relax to a steady state ?

Is the one of equilibrium ?

Is it a non-equilibrium steady state ?

Out of equilibrium

Three possible reasons

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- **Driven systems** Energy injection

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- **Integrability**

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

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

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

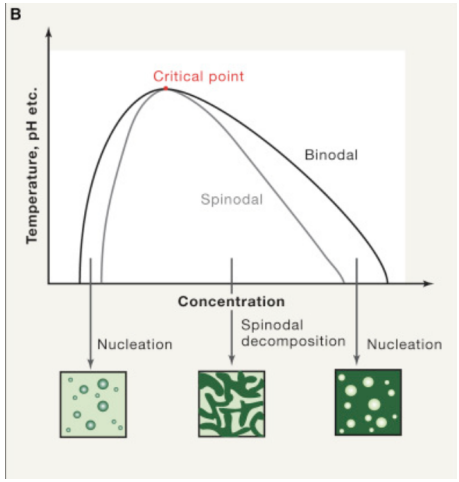
Spin ices

Systems with quenched disorder

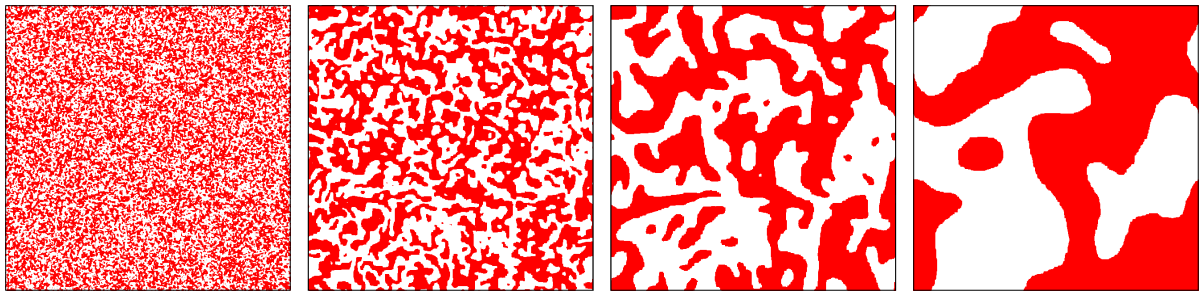
Random ferromagnets, spin-glasses

Phase separation

Quench below the binodal : remnant interfaces



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

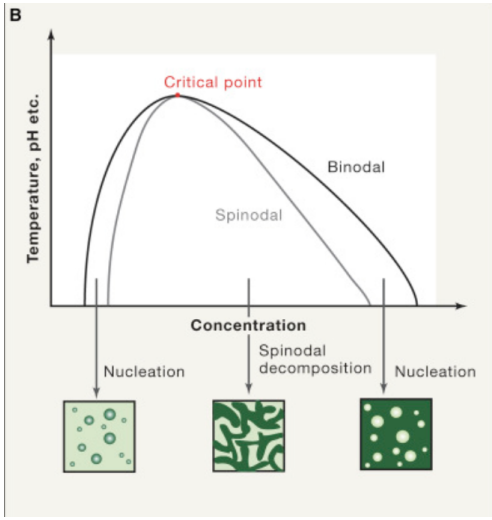


Coarsening process with growing length $\mathcal{R}(t) \simeq t^{1/z} \implies \boxed{t_{\mathrm{eq}} \sim L^z}$

Equilibration time diverges with the system size L

Phase separation

Quench below the binodal: universality



Microscopic details are irrelevant

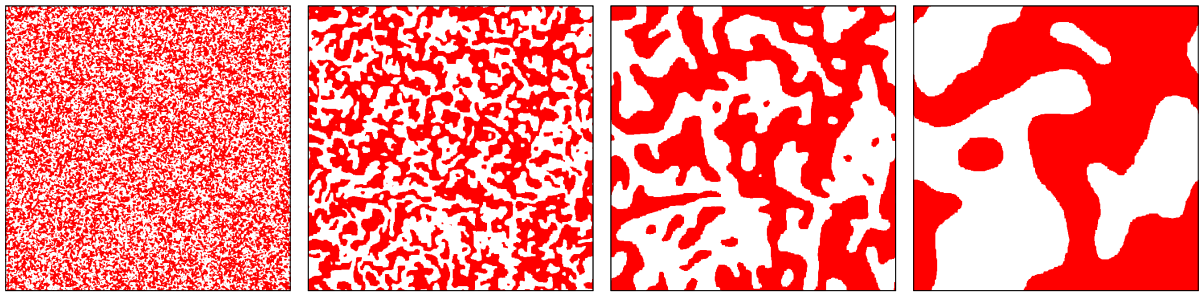
but conservation laws and

dimension of order parameter fix the

$\Longrightarrow$

Dynamic universality class

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



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 $\boxed{t_{\rm micro} \ll t \ll t_q}$

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 !

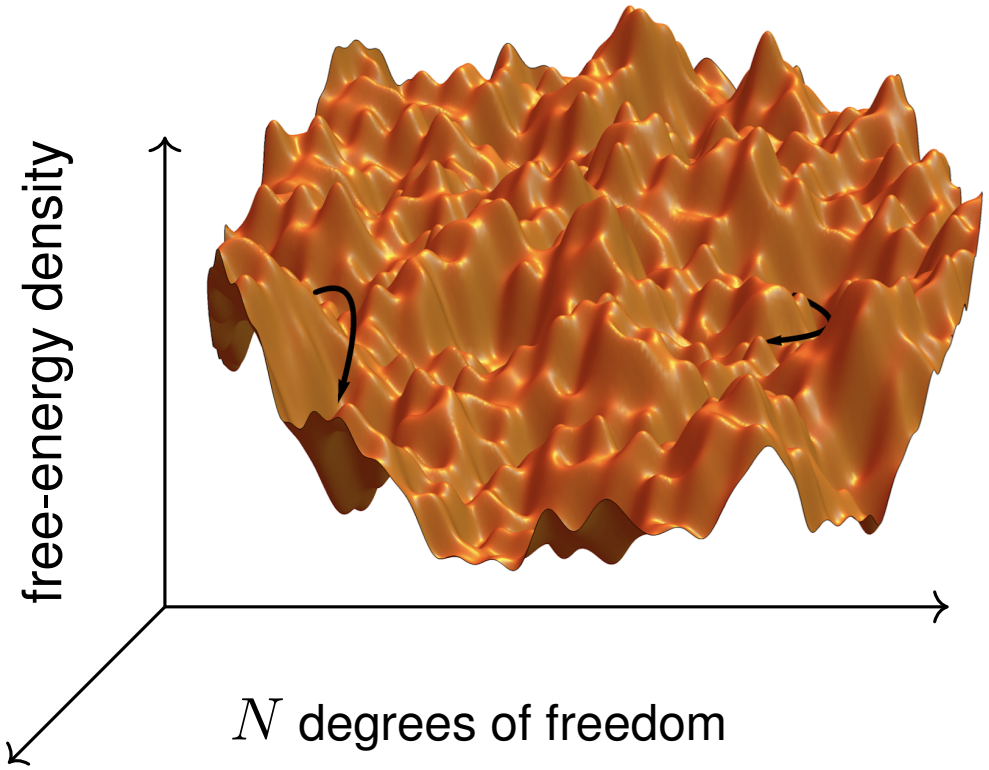


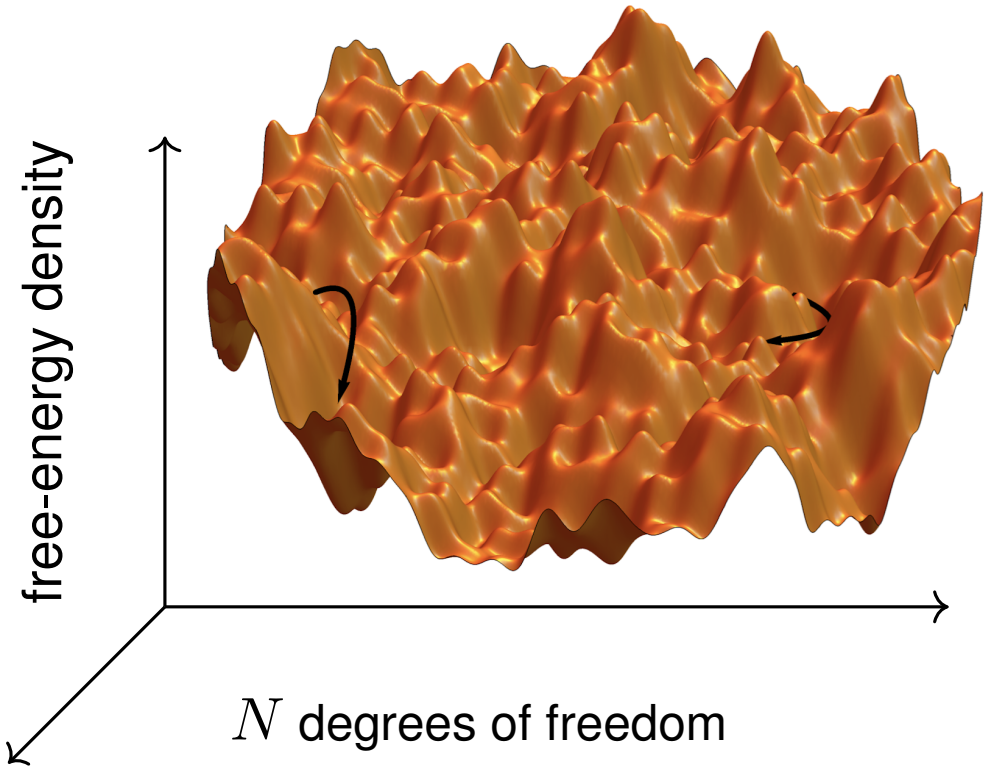
Figure adapted from a picture by **C. Cammarota**

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

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**

Spin-glasses

Magnetic impurities (spins) randomly placed in an inert host

Quenched random interactions

Interacting via the RKKY potential

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

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

Standard lore : there is a 2nd order static phase transition at T_s

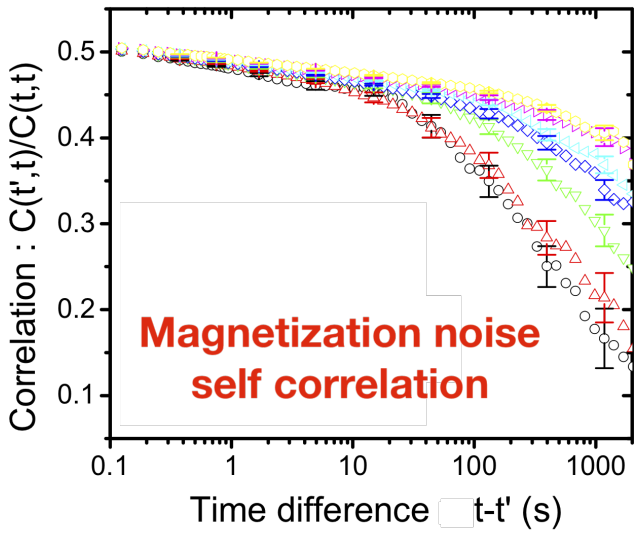
separating a paramagnetic from a spin-glass phase.

No dynamic precursors above T_s.

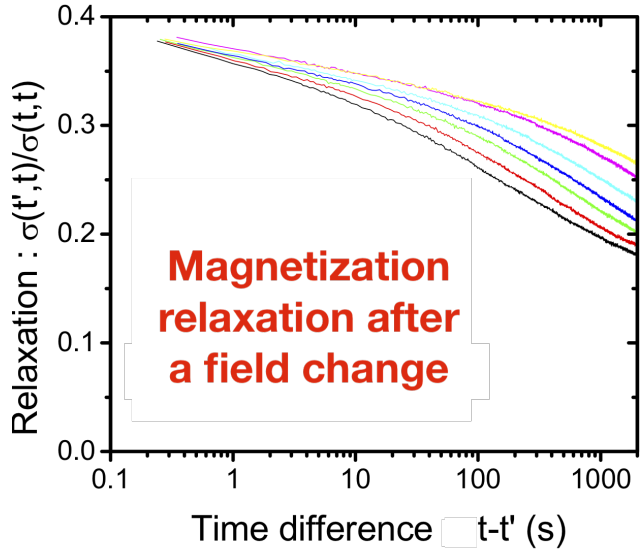
Glassy dynamics below T_s with aging, memory effects, etc.

Rugged free-energy landscapes

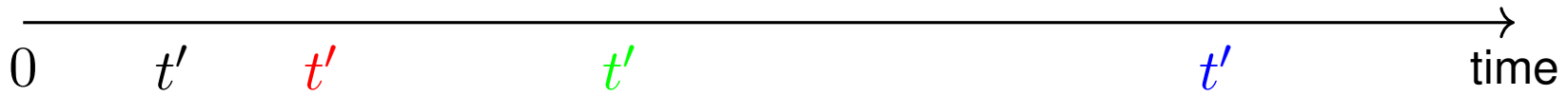
Glassy physics: slow relaxation & loss of stationarity (aging)



Correlation



Linear response



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

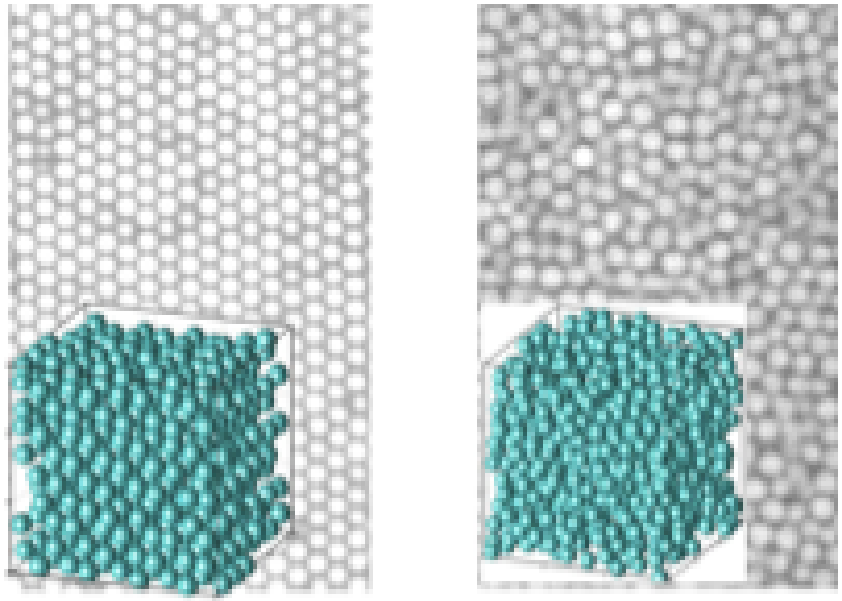
No identifiable growing length $\mathcal{R}(t)$: **glassy microscopic mechanisms ?**

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

Structural Glasses

e.g., **colloidal ensembles**

Micrometric spheres immersed in a fluid



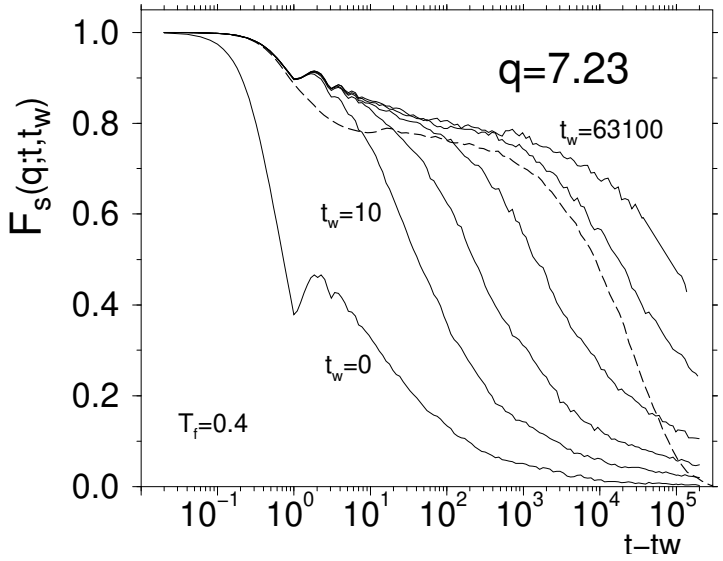
Crystal Glass

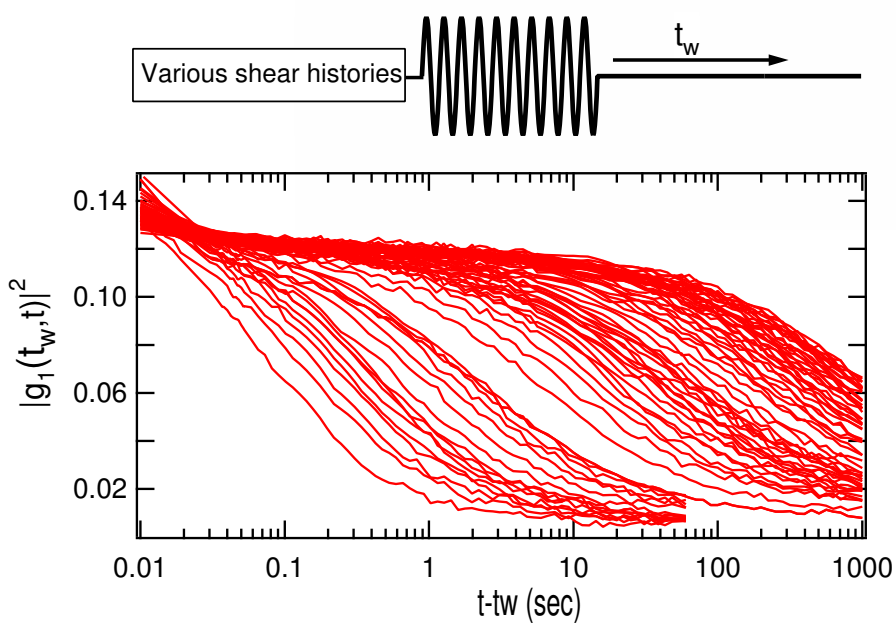
In the glass : no obvious growth of order, slow dynamics with, however, scaling properties

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.

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**

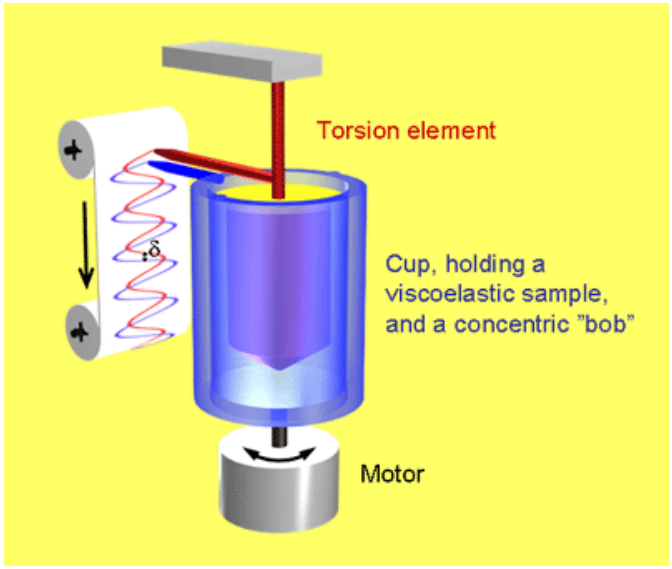
$$I_\mu(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) = ct, \qquad \mu = 1, \ldots, N$$

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

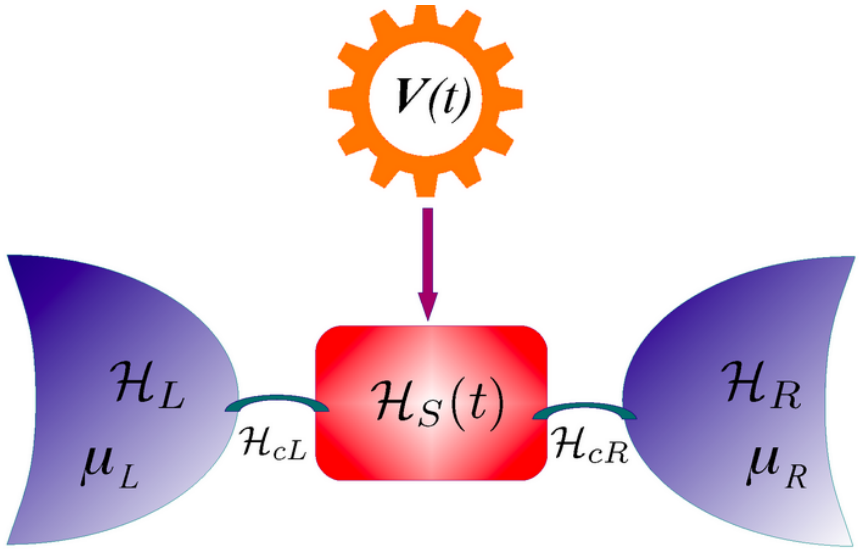
e.g., **1d bosonic gases**

Energy injection

Traditional: from the borders (outside)



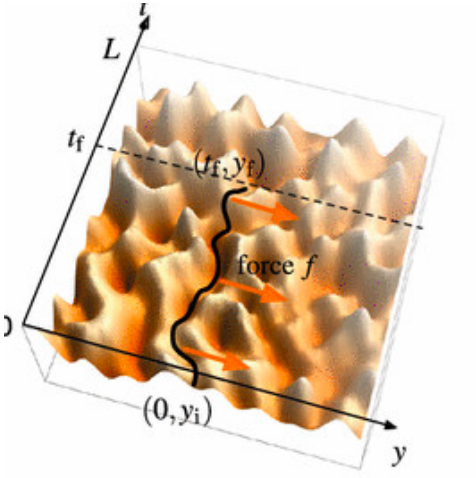
Rheology

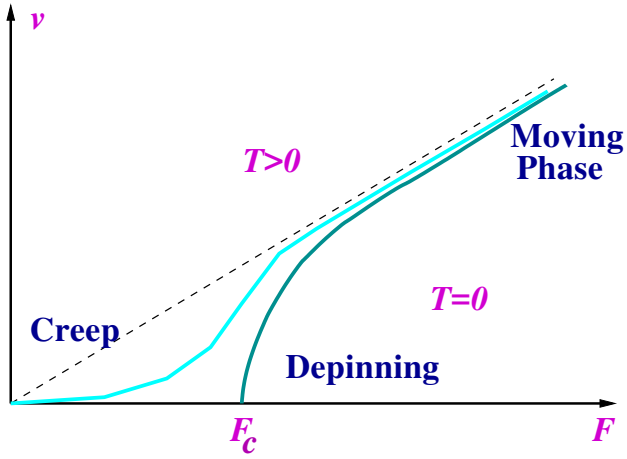


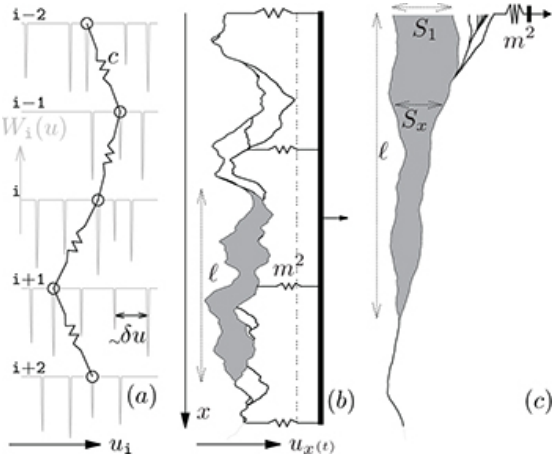
Transport

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.

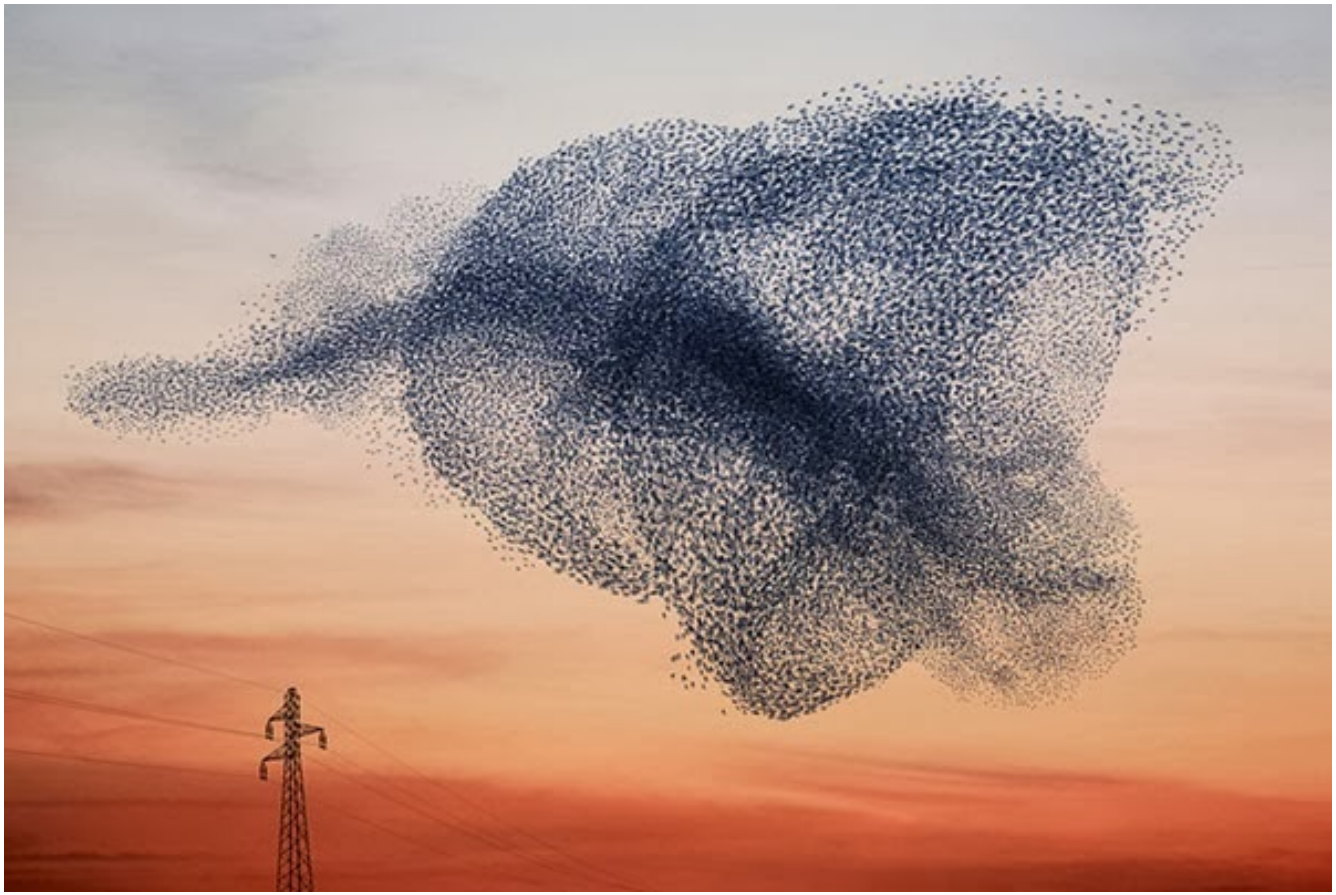
Due to the energy consumption, these systems are intrinsically out of thermal equilibrium.

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.

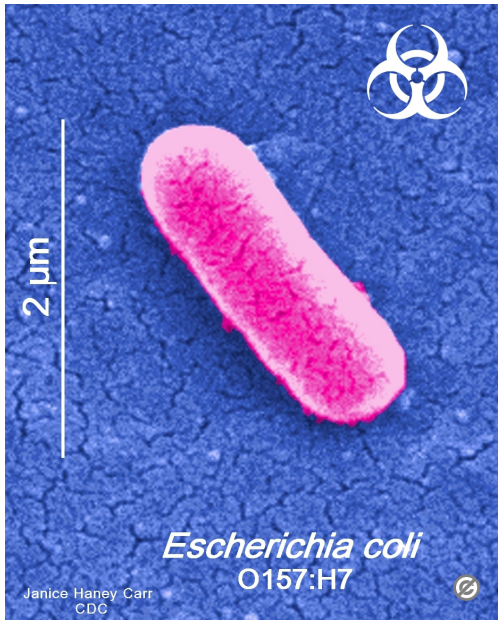
Natural systems

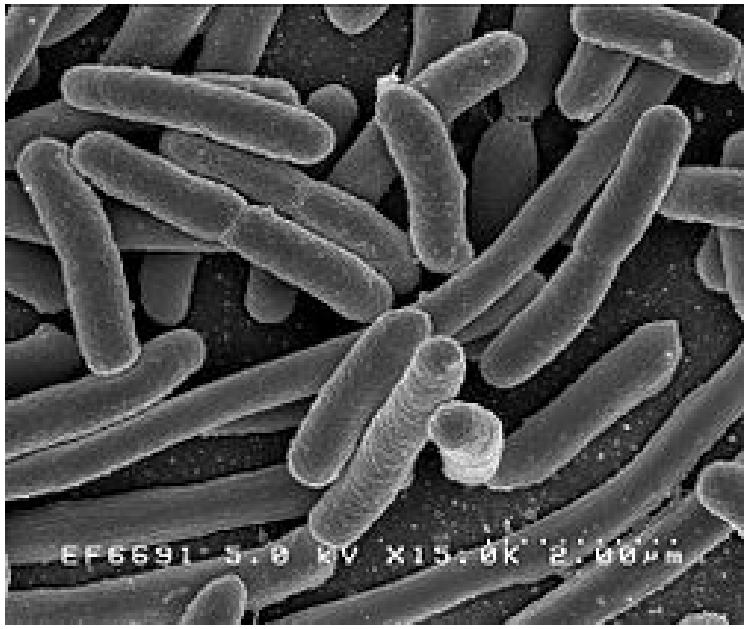
Birds flocking



Natural systems

Bacteria



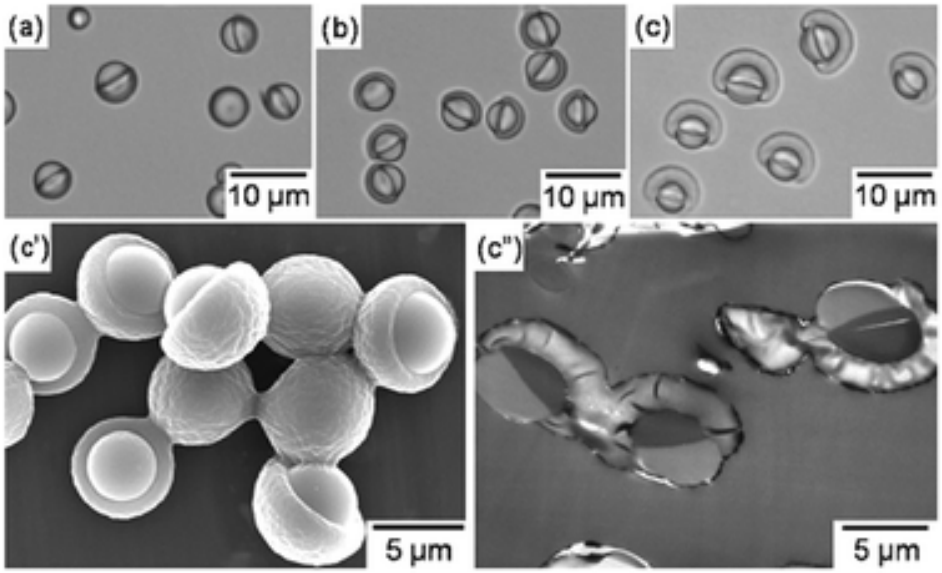


Escherichia coli - Pictures borrowed from the internet.

Artificial systems

Janus particles





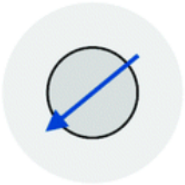
Particles with two faces (Janus God)

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 $\boldsymbol{n}_i = (\cos\theta_i(t), \sin\theta_i(t))$

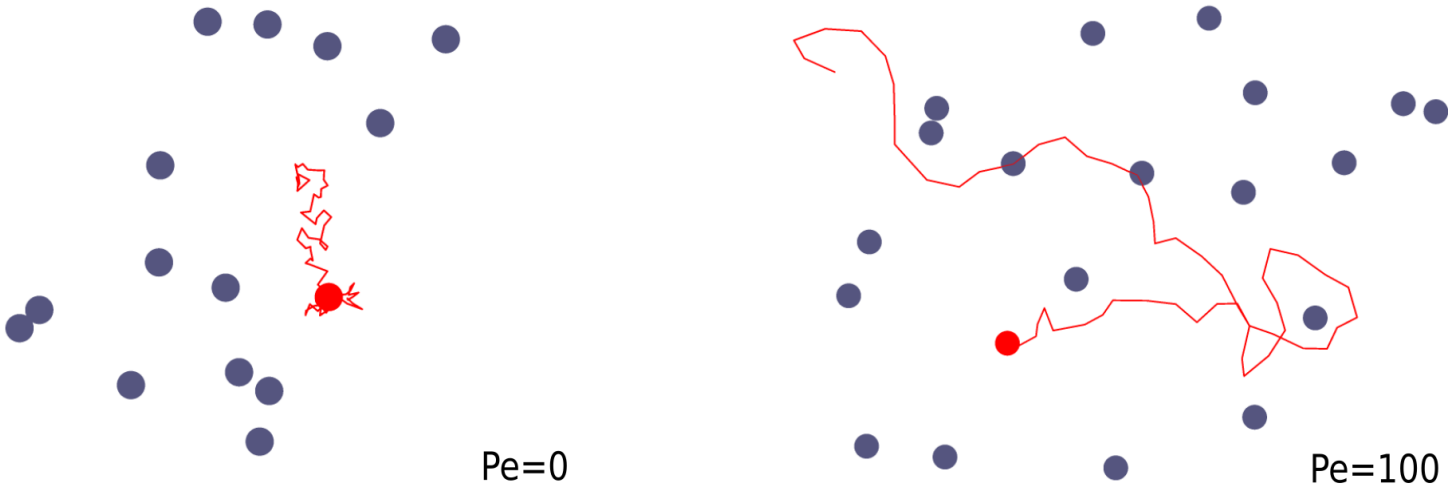
$$\underbrace{\gamma \dot{\boldsymbol{r}}_i}_{\text{friction}} = \underbrace{F_{\rm act}\boldsymbol{n}_i}_{\text{propulsion}} - \underbrace{\boldsymbol{\nabla}_i \sum_{j(\neq i)} U(r_{ij})}_{\text{inter-particle repulsion}} + \underbrace{\boldsymbol{\xi}_i}_{\substack{\text{translational}\\ \text{white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

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

Bialké, Speck & Löwen 12, Fily & Marchetti 12

Active Brownian particles

Typical motion of ABPs in interaction



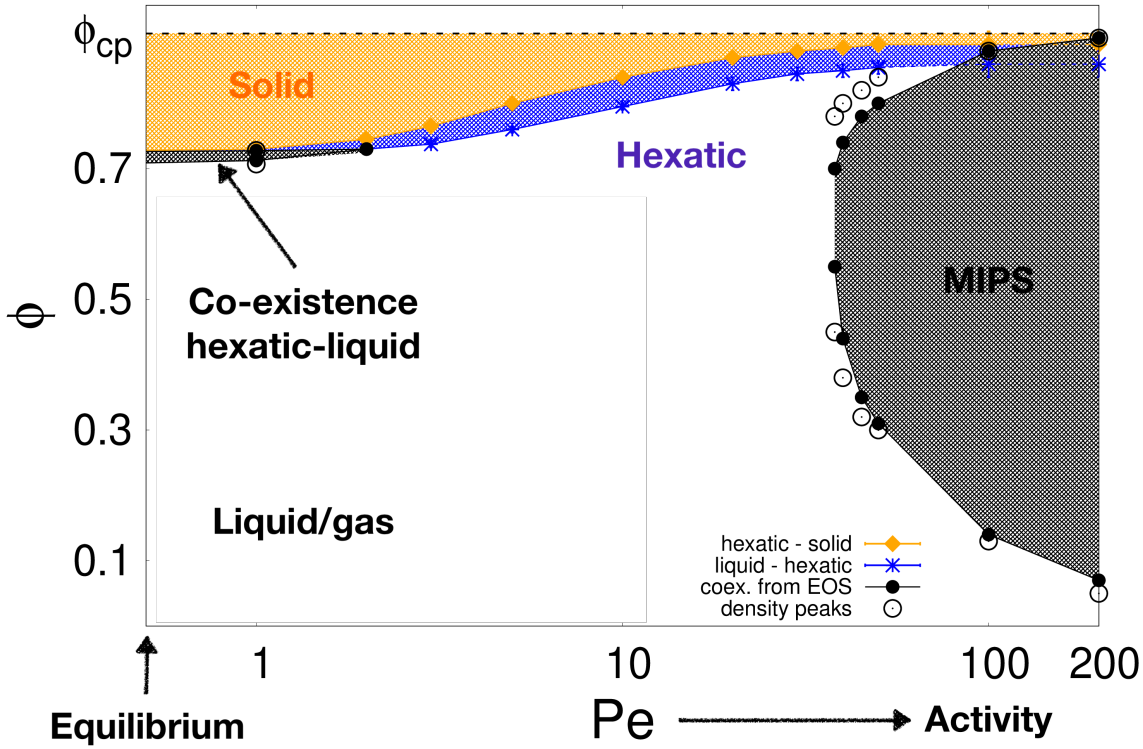
The activity induces a persistent random motion

Long running periods $\ell_p \propto$ Pe σ_d and

sudden changes in direction

Active Brownian particles

Complex out of equilibrium phase diagram



Motility induced phase separation (MIPS) gas & dense droplet

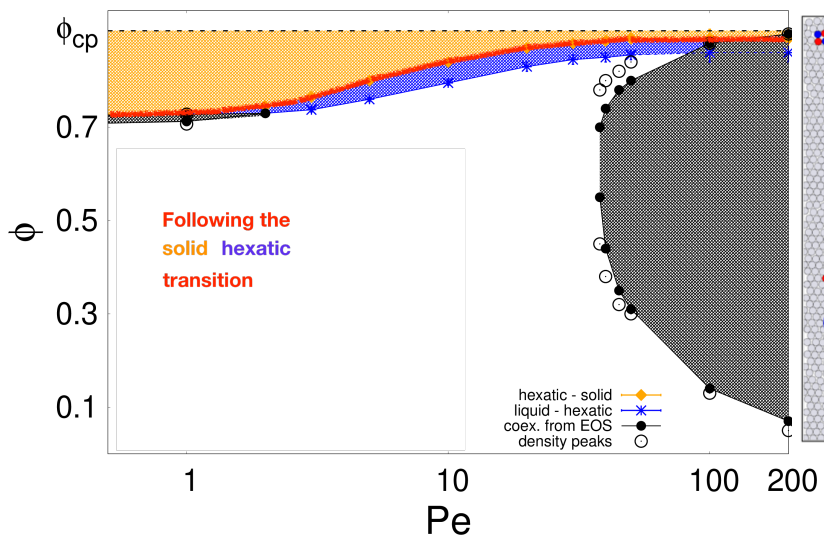
Cates & Tailleur 12

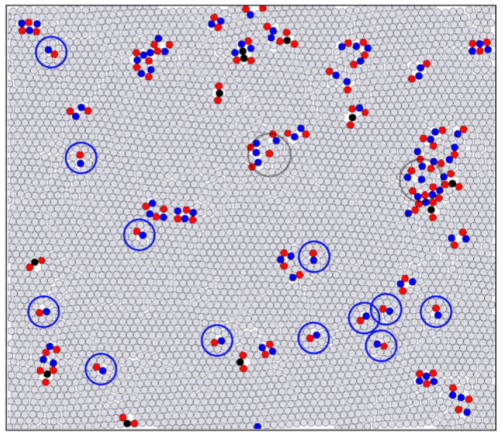
From virial pressure $P(\phi)$, translational and orientational correlations G_T and G_6, distributions of local density and hexatic order ϕ_i and ψ_{6i}, at fixed $k_B T = 0.05$

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

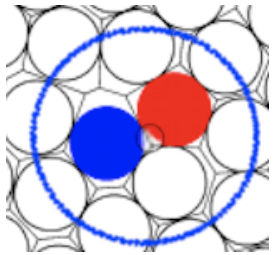
Active Brownian particles

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





Free dislocation:
a 7-5 neighbor



$\neq$ from $\triangle$ lattice

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

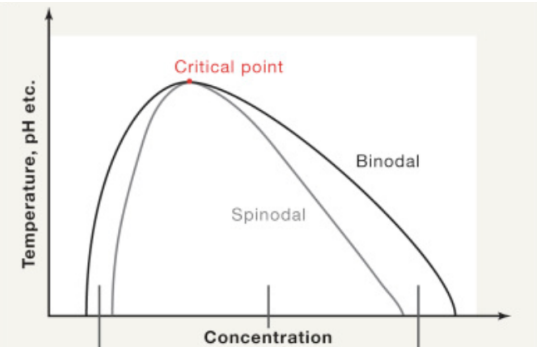
as in Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young universality ?

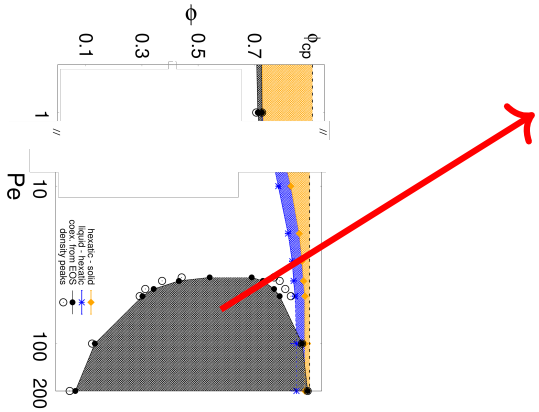
$$\rho_{disloc} \simeq a \exp\left[-b\left(\frac{\phi_{sh}}{\phi_{sh}-\phi}\right)^{\nu}\right] \qquad \nu \sim 0.37 \quad \forall \text{Pe}\,?$$

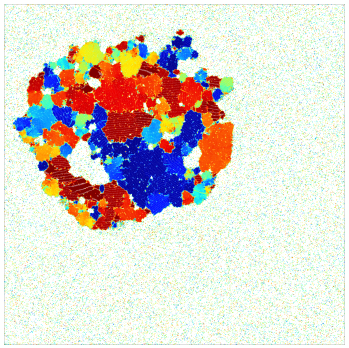
Digregorio, Levis, LFC, Gonnella & Pagonabarraga 21

Active Brownian particles

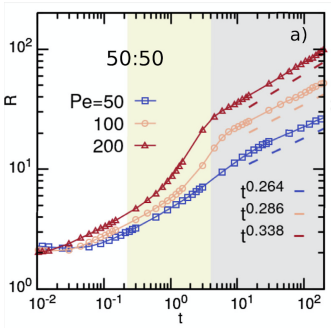
Out of equilibrium phase diagram So many questions !

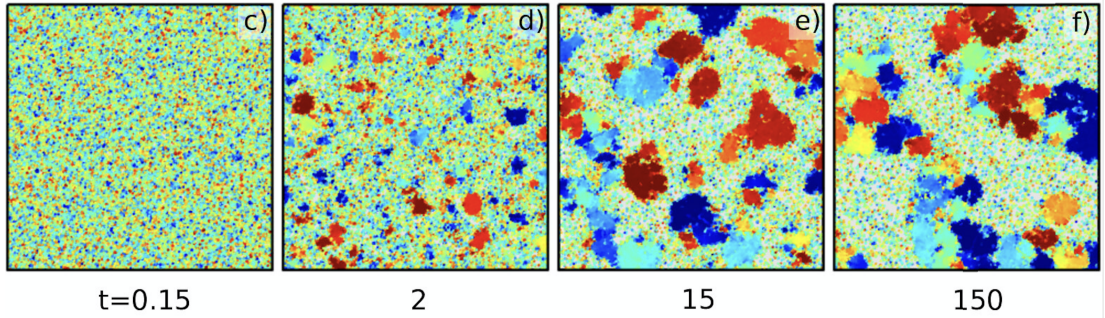






Dynamics of formation of the dense phase ? but bubbles, hexatic order, ...





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,

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

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

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

e.g., **active matter**

- **Integrability**

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

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**

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**

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

Classical quenches

Definition & questions

- Take an **isolated** classical system with Hamiltonian H_0, evolve with H
- Initialize it in, say, 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 ?

Classical Statistical Physics

non-Integrable vs. Integrable Systems

Easier to work in canonical - open - conditions

Focus on a **non-integrable** system with energy $\mathcal{H}(\{\boldsymbol{p}_j, \boldsymbol{x}_j\}) = \mathcal{E}$ conserved

Equivalence of ensembles implies that (non-conserved) observables can also be calculated with Boltzmann's canonical measure

$$P_{\rm GB}(\{\boldsymbol{p}_j, \boldsymbol{x}_j\}) = \mathcal{Z}_{\rm GB}^{-1}\, e^{-\beta \mathcal{H}(\{\boldsymbol{p}_j, \boldsymbol{x}_j\})}$$

and β be such that $\mathcal{E} = \langle \mathcal{H}(\{\boldsymbol{p}_j, \boldsymbol{x}_j\}) \rangle_{\rm GB}$

In **integrable systems**, a Generalized Canonical Distribution is proposed

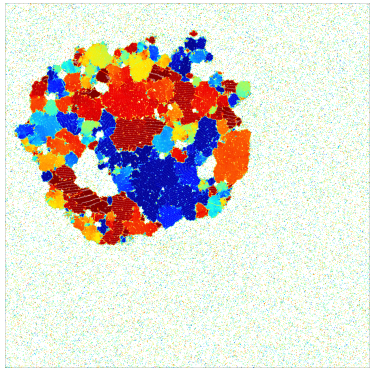
$$P(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) = \mathcal{Z}_{\rm GGE}^{-1}\, e^{-\sum_i \gamma_i I_i(\{\boldsymbol{p}_j, \boldsymbol{x}_j\})}$$

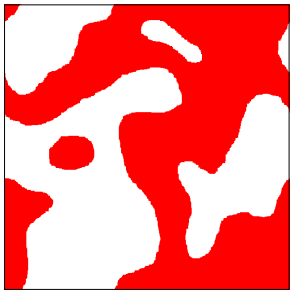
and $\{\gamma_i\}$ be such that $\mathcal{I}_i = \langle I_i(\{\boldsymbol{p}_j, \boldsymbol{x}_j\}) \rangle_{\rm GGE}$ with $i = 1, \ldots, N$

Out of equilibrium

Explain, describe and, something in common ?

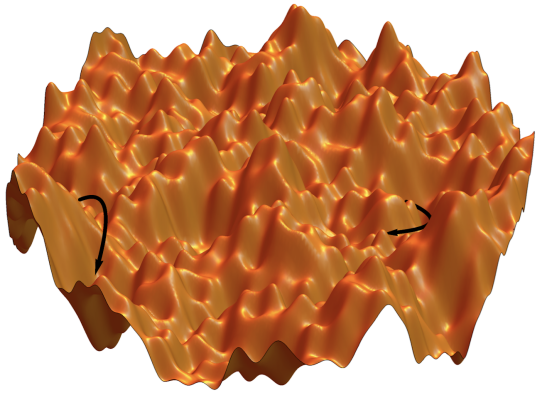
$$\boldsymbol{F} \neq -\boldsymbol{\nabla} V(\boldsymbol{r})$$

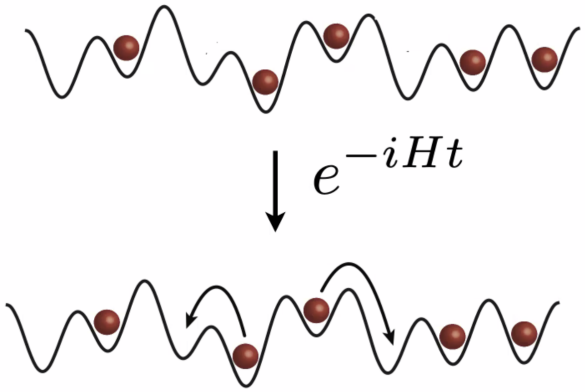




$$\lim_{N \gg 1} t_{\mathrm{eq}}(N) \gg t$$

$$I_\mu = \mathrm{ct} \qquad \mu = 1, \ldots, N$$





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...

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

3. **And a quantum system ?**

Why quantum ?

What changes with respect to classical dynamics

Quantum effects matter when

$\hbar\omega \gtrsim k_B T$ or $\lambda_T = h/\sqrt{2\pi m k_B T} \gtrsim$ inter-particle distance

Basically, at very low temperatures

- No trajectories $\hat{\rho}(t),\ i\hbar\,\partial_t\hat{\rho} = [\hat{H},\hat{\rho}]$

  observables do not commute $\langle \hat{A}(t)\hat{B}(t')\rangle \neq \langle \hat{B}(t')\hat{A}(t)\rangle$

  response from commutators $R(t,t') = \frac{i}{\hbar}\,\theta(t-t')\,\langle[\hat{A}(t),\hat{B}(t')]\rangle$

- Zero-point fluctuations survive at $T = 0$,

  e.g. harmonic oscillator

$$\langle x^2\rangle_{\rm eq} = \frac{\hbar}{2m\omega}\coth\frac{\beta\hbar\omega}{2} \quad \xrightarrow{T\to 0} \quad \frac{\hbar}{2m\omega} \quad \xrightarrow{\hbar\to 0} \quad \frac{k_B T}{m\omega^2}$$

Why quantum ?

What changes with respect to classical dynamics

- **Entanglement** system + environment pure, but

  $\hat{\rho}_S = \mathrm{Tr}_{\mathrm{env}}\, \hat{\rho}$ mixed $\Rightarrow$ decoherence

- **Unitarity** isolated : $\hat{\rho}(t)$ never relaxes

  Only local observables may thermalize (ETH)

- **Quantum FDT** in equilibrium, symmetrized correlation vs. response

  $$C_{\mathrm{sym}}(\omega) = \hbar \coth \frac{\beta\hbar\omega}{2}\, \chi''(\omega) \quad \xrightarrow{\hbar\to 0} \quad \frac{2k_B T}{\omega}\, \chi''(\omega)$$

  coloured noise at low T

Same questions, new ingredients

Closed Quantum System

Evolution of a pure state

An isolated closed macroscopic quantum system in a **pure state** $|\psi(0)\rangle$

follows **unitary evolution** $|\psi(t)\rangle = e^{-\mathrm{i}\hat{\mathcal{H}}t/\hbar}|\psi(0)\rangle$ which ensures that the state remains **pure** and $|\psi(0)\rangle$ is never forgotten

But thermodynamics tells us that systems lose memory of their initial states

Classically : ergodicity, trajectories explore the phase space energy shell

The **density operator** is a projector $\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)|$

and the **entropy** $S = -\mathrm{Tr}(\hat{\rho}\ln\hat{\rho})$ of a pure state is strictly zero at all times.

Thermodynamics tells us that entropy should be maximized but $S_{\mathrm{pure}}(t) = 0$

Way out ?

Focus on a Sub-System

Reduced density operator & von Neumann entropy

Full system $\hat{\mathcal{H}} = \hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B + \hat{\mathcal{H}}_{\rm int}$

in a pure state $|\psi\rangle$

The density operator is $\hat{\rho} = |\psi\rangle\langle\psi|$

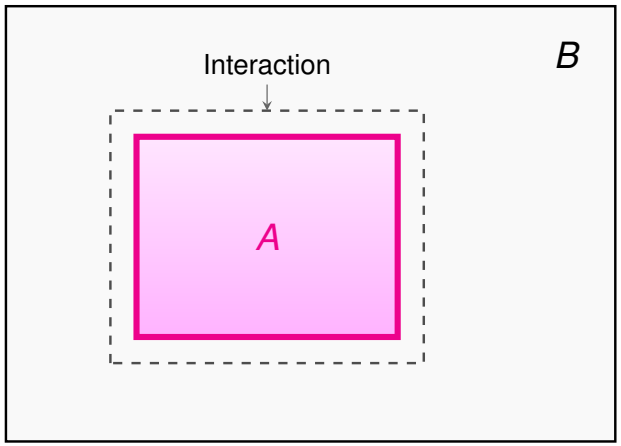
and $S_{|\psi\rangle} = 0$

The reduced density op. of sub-system *A*

$\hat{\rho}_A^{\rm red} = {\rm Tr}_B \hat{\rho}$

can be mixed $\hat{\rho}_A^{\rm red} \neq |\psi\rangle_A \, {}_A\langle\psi|$

with $S_A^{\rm red} = -{\rm Tr}_A(\hat{\rho}_A^{\rm red} \ln \hat{\rho}_A^{\rm red}) \neq 0$



B* can act as a bath on *A

Consequence : A pure state under unitary evolution can “look" thermal to a local observer without ever becoming a mixed state

Still, which is the measure $\hat{\rho}_A^{\mathrm{red}}$?

It depends on the full system being integrable or not

A huge question

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**

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e.g., **active matter**

- **Integrability**

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

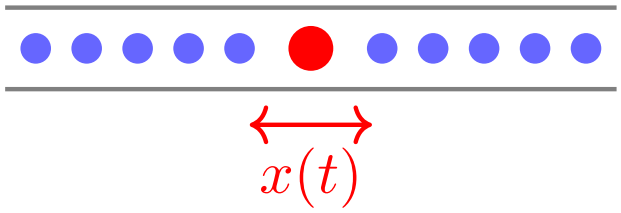
Too many constants of motion inhibit equilibration to the Gibbs ensembles

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

Quantum diffusion

One impurity atom immersed in a quasi one-dimensional gas

The host gas is a Luttinger liquid and its phonons act as a quantum bath



Integrating out the phonons $\Rightarrow$

quantum Langevin / Schwinger–Keldysh

retarded friction & coloured quantum noise

Ohmic case:

$$\nu(\omega) = \gamma_0 \hbar\omega \coth \frac{\beta\hbar\omega}{2}$$

$$\xrightarrow{\hbar\to 0} \quad 2\gamma_0 k_B T$$

Free quantum Brownian particle, Ohmic bath at $T = 0$: $\langle \Delta x^2(t) \rangle \simeq \frac{\hbar}{\pi\gamma_0} \ln t/t_0$

vs. classical $2Dt$

Hakim & Ambegaokar 85, Grabert, Schramm & Ingold 88

Impurity in a 1D Bose gas: **Bonart & LFC**, 12; experiment (K in Rb): **Catani** *et al.* 12

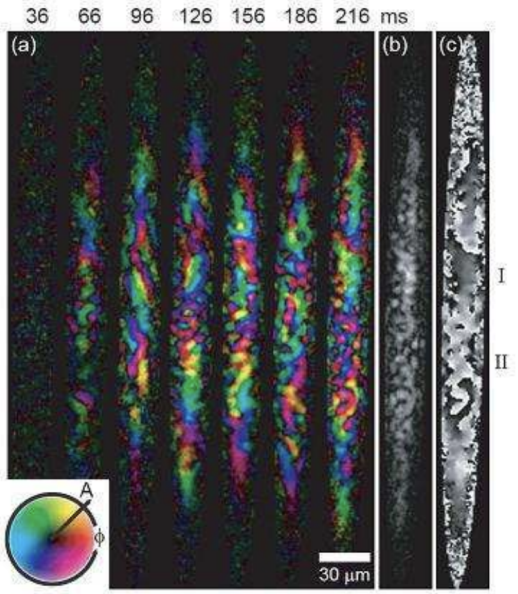
Quantum noise is coloured: no white-noise limit at low T

Quantum domain growth

Quench across a quantum phase transition

Local order is chosen at random : domains of the equivalent ordered states form and grow

$C(r,t) \simeq f\big(r/R(t)\big)$ with $R(t) \sim t^{1/z}$ dynamic scaling



Experiment : spinor ^{87}Rb BEC ($F = 1$), quench of the quadratic Zeeman energy q across the polar $\rightarrow$ ferromagnetic transition. In situ imaging of magnetization domains, textures and vortices.

Self-similar scaling far from equilibrium

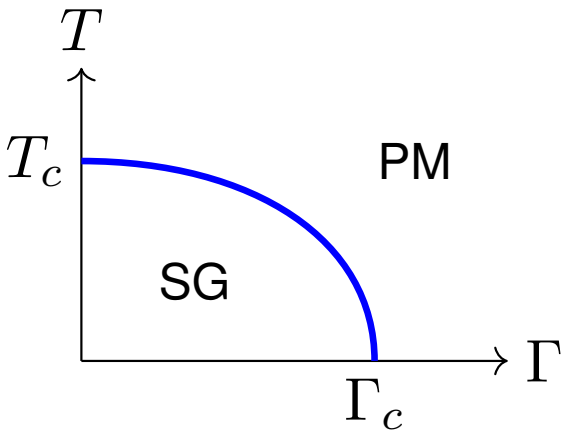
Sadler *et al.* 06

$R(t) \ll L \rightarrow \infty$ **: never equilibrates in the thermodynamic limit**

Quantum spin glasses

Random couplings and a transverse field

$$H = -\sum_{i<j} J_{ij}\, \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x \qquad J_{ij} \text{ random}$$



Coupled to a bath and quenched into the SG phase : quantum aging $C(t, t_w)$, $R(t, t_w)$

Quantum FDT violated, with $T_{\rm eff} > T$ in the aging regime, also at $T = 0$

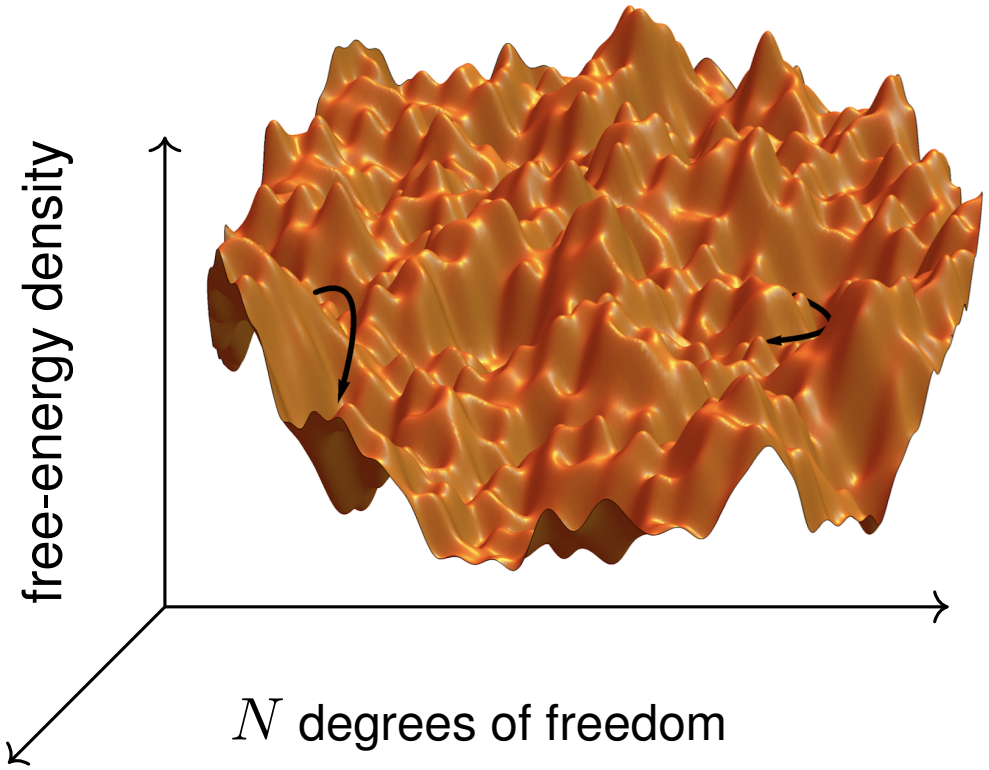
At low T the transition can become first order.

Experiments: $LiHo_xY_{1-x}F_4$, **Wu** *et al.* 91, **Brooke** *et al.* 99 Theory: **LFC & Lozano** 98

Slow relaxation with quantum fluctuations: aging and $T_{\rm eff}$

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 ?

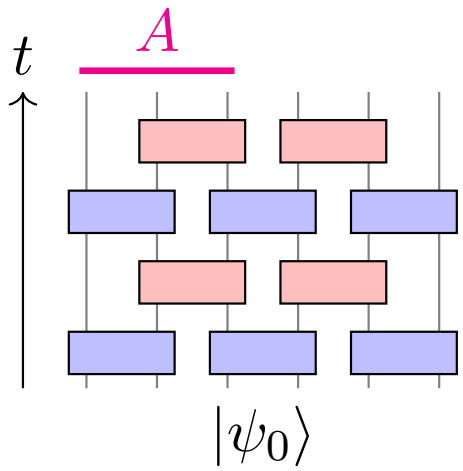
Optimisation problem Smart algorithms ? **Computer sc - applied math**

Quantum circuits

Minimal models of unitary many-body dynamics

Chain of L qubits, discrete time, two-qubit gates in a brickwork

isolated system with random gates



$$|\psi(t)\rangle = \prod_{\text{layers}} \bigotimes_i \hat{U}_{i,i+1} \, |\psi_0\rangle$$

$\hat{U}_{i,i+1}$ Haar random

Global state stays pure but subsystems equilibrate

$$\hat{\rho}_A(t) = \mathrm{Tr}_{\bar{A}} \, |\psi(t)\rangle\langle\psi(t)| \;\to\; \mathbb{I}/2^{|A|}$$

to infinite temperature

Entanglement growth, scrambling, measurements, etc.

Nahum, Ruhman, Vijay & Haah 17, **Nahum, Vijay & Haah** 18, **von Keyserlingk** *et al.* 18 **Khemani, Vishwanath & Huse** 18, **Li, Chen & Fisher** 18

Experiments: **Arute** *et al.* 19, Mi *et al.* 21

Pure global state, thermal subsystems : what does equilibrium mean ?

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**

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

Too many constants of motion inhibit equilibration to the Gibbs ensembles

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Quantum dynamics

Periodically driven (Floquet) systems

Time-periodic Hamiltonian, $\hat{H}(t+\tau) = \hat{H}(t)$: energy is not conserved

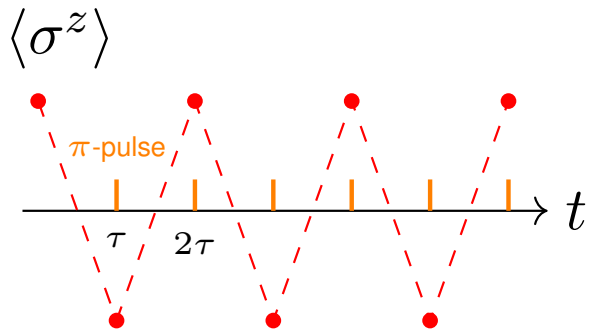
Stroboscopic evolution

$$\hat{U}(\tau) = \mathcal{T} e^{-\frac{i}{\hbar}\int_0^\tau dt'\, \hat{H}(t')} \equiv e^{-\frac{i}{\hbar}\hat{H}_F \tau}$$

Floquet Hamiltonian $\hat{H}_F$

Isolated, interacting, generic heat to $T = \infty$

high frequency : long **prethermal** plateau



Example : discrete time crystal

Disordered interacting spin chain +

imperfect π-pulses $(\pi - \epsilon)$:

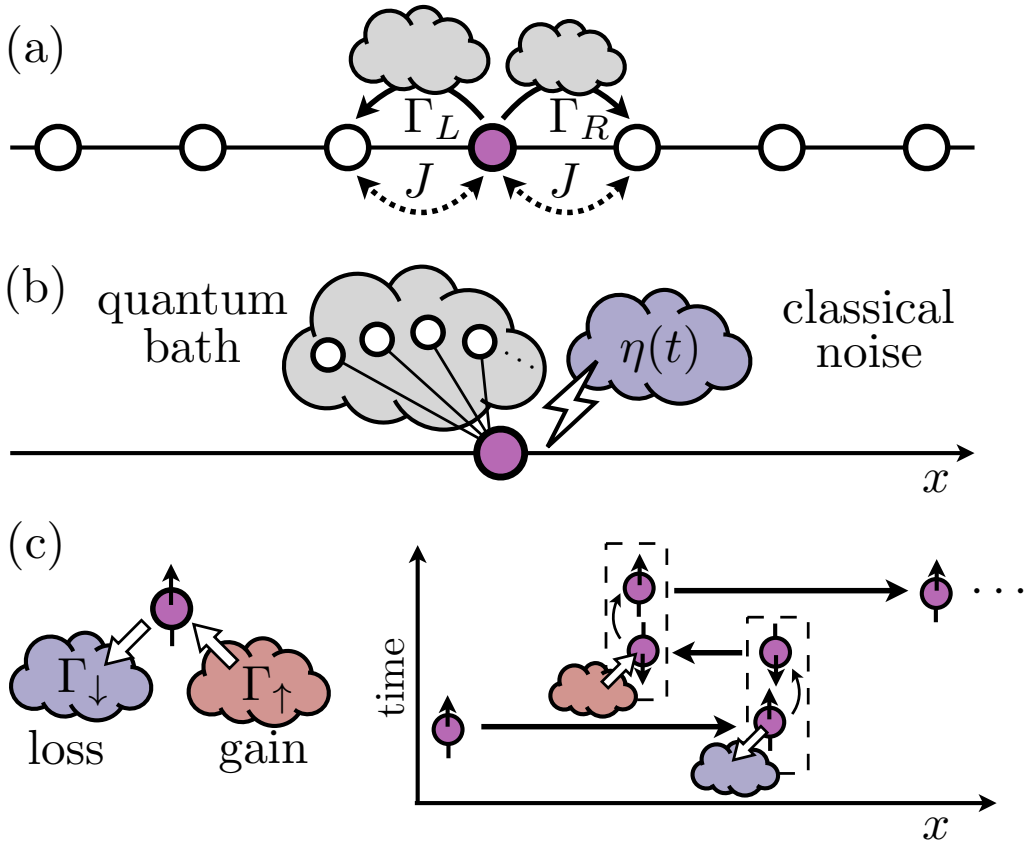
$\langle \sigma_i^z(n\tau) \rangle \propto (-1)^n$ period doubling

D'Alessio & Rigol 14, **Lazarides, Das & Moessner** 14, **Mori, Kuwahara & Saito** 16
Abanin *et al* 17, **Khemani** *et al* 16, **Else, Bauer & Nayak** 16

Driven : no equilibrium state ; at best a stroboscopic steady state

Quantum Active Particles

Sketches of three models - playing with the environments



Gipouloux, Brunelli, LFC, Fazio & Schirò 26

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,

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

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- **Driven systems** Energy injection

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- **Integrability**

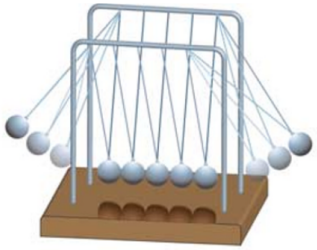
$$\boxed{I_\mu(\{\boldsymbol{p}_i, \boldsymbol{x}_i\}) = ct, \qquad \mu = 1, \ldots, N}$$

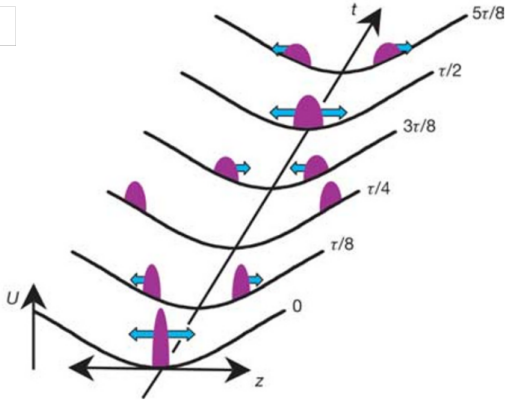
Too many constants of motion inhibit equilibration to the Gibbs ensembles

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

Motivation

Isolated quantum systems: experiments and theory $\sim$ 20y ago





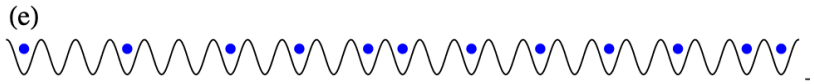
A quantum Newton's cradle cold atoms in isolation

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**

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

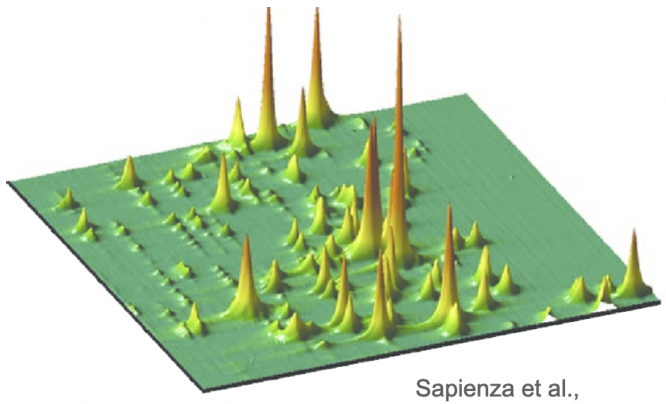
Anderson Localization

Single particle - no interactions

$$H = \sum_{ij} \underbrace{t_{ij}}_{j \to i \text{ hopping}} c_i^\dagger c_j + \sum_i \underbrace{\epsilon_i}_{\text{random energies}} \underbrace{c_i^\dagger c_i}_{\text{fermion number}}$$

i.i.d. random local energies from $\epsilon_i \in [-W/2, W/2]$

Competition between kinetic and random disordered terms



Sapienza et al.,
Science 327, 1352 (2010)

Real space localization, for $L \to \infty$

$\psi_E(\vec{r}) \sim e^{-|\vec{r}-\vec{r}_o|/\xi}$

$d \leq 2$ for infinitesimal disorder $\forall\, E$

$d > 2$ metal/insulator transition $W < W_c$

Center/edge states extended/localized

Anderson, *Absence of Diffusion in Certain Random Lattices*, Phys. Rev. 109, 1492 (1958)

Many-body Localization

Interactions

From the **real-space** Hamiltonian with interactions

$$H = \sum_{ij} t_{ij}\, c_i^\dagger c_j \;+\; \sum_i \epsilon_i\, c_i^\dagger c_i + \sum_{ij} \underbrace{V_{ij}\;\; c_i^\dagger c_i c_j^\dagger c_j}_{\text{fermion}-\text{fermion } \textbf{interaction}}$$

to the **Fock-space** Hamiltonian

$$H' = \sum_{\alpha\neq\beta} \underbrace{T_{\alpha\beta}}_{\text{state change}} \;\; |\alpha\rangle\langle\beta| \;+\; \sum_{\alpha} \underbrace{E_\alpha}_{\text{correlated energies}} \;\; |\alpha\rangle\langle\alpha|$$

e.g. $|\alpha\rangle = |n_1, n_2, \ldots, n_N\rangle$

n_i occupation numbers

of the N real-space sites

$T_{\alpha\beta}$ hierarchical

Fock space is a **graph**

with 2^N sites

Altshuler, Gefen, Kamenev & Levitov, *Quasiparticle Lifetime in a Finite System : A Nonperturbative Approach*, Phys. Rev. Lett. 78, 2803 (1997)

Many-Body Localization (MBL)

Interactions

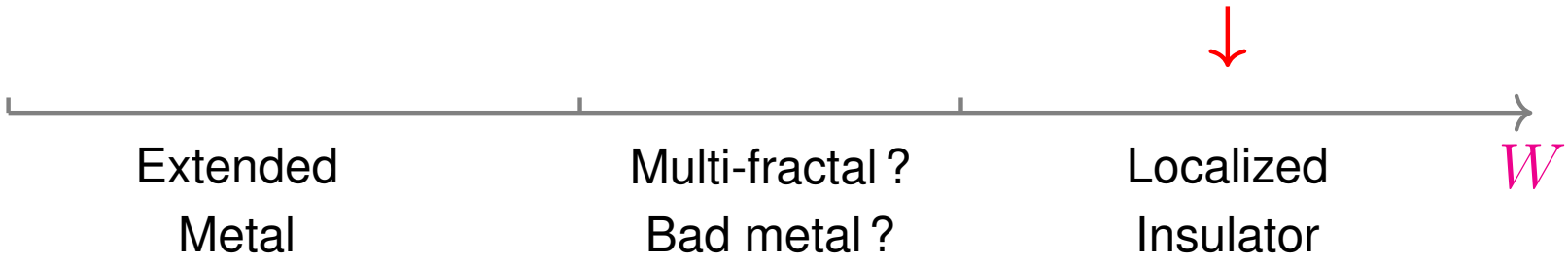
Fock-space Hamiltonian

$$H' = \underbrace{\sum_{\alpha \neq \beta} \underbrace{T_{\alpha\beta}}_{\text{state change}} \; |\alpha\rangle\langle\beta|}_{\text{Non-local}} + \underbrace{\sum_{\alpha} \underbrace{E_{\alpha}}_{\text{corr. energies}} \; |\alpha\rangle\langle\alpha|}_{\text{Local}}$$

Anderson model on a graph

At energy E

Localization in Fock space



Basko, Aleiner & Altshuler, *Metal-insulator transition in a weakly interacting many-electron system with localized single-particle states*, Ann. Phys. 321, 1126 (2006). **Alet & Laflorencie**, *Many-body localization: an introduction and selected topics*, Comptes Rendus Physique 19, 498 (2018)