Out of equilibrium physics

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Aim

Give you an idea of what a theoretical physicist,

with knowledge of field theory & statistical physics

works on these days.

Plan

1. From Newton dynamics to Statistical Physics ($N \gg 1$).
   - Microscopic definition of entropy, temperature, etc.
     Thermodynamics recovered. Phase transitions shown.
   - Interest in long-range interactions, quenched disorder & frustration effects, exactly solvable models & quantum phase transitions.

2. Put time back in the game.
   - Can a macroscopic system remain out of equilibrium ?
   - A few classical examples : Brownian motion, phase separation & glasses, active samples.
   - A few quantum problems : impurity motion in quantum environments ; the equilibration (or not) of quantum closed systems *and back to square one*.

Part 1.

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Newton dynamics

Take $i = 1, \ldots, N$ point-like particles with Hamiltonian

$$\mathcal{H} = \sum_i \frac{p_i^2}{2m_i} + \sum_{i \neq j} V(|\vec{x}_i - \vec{x}_j|)$$

Given the initial conditions $\{\vec{p}_i(0), \vec{x}_i(0)\}$:

solve $2dN$ first-order or dN second-order differential equations.

For $N = 1, 2, 3, \ldots$ one can try to extract some information analytically *dynamical systems* but already $N = 3$ can be very hard (and rich).

For $N \gg 1$ no hope to progress this way until computers became available in the, say, 70s *molecular dynamics* (still, $N \simeq 10^3 - 10^4$).

Statistical physics

No need to solve the dynamic equations!

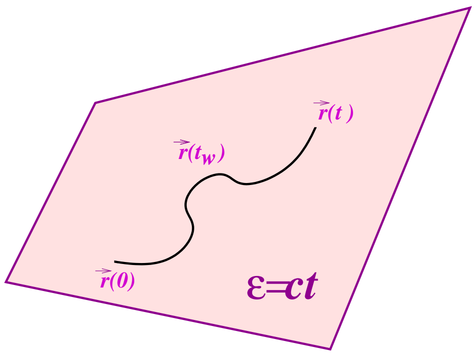
Under certain circumstances, *ergodic hypothesis*, after some equilibration time, t_{eq}, the macroscopic observables can be, on average, obtained with a *static* calculation, as an average over all configurations in phase space weighted with a probability distribution function $P(\{\vec{p}_i, \vec{x}_i\})$:

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

Recipes for $P(\{\vec{p}_i, \vec{x}_i\})$ are given and depend upon the conditions under which the system evolves, whether it is isolated or in contact with an environment.

L. Boltzmann, late XIX

Ensembles



Isolated system $\Rightarrow$ total energy is conserved

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

Flat probability density

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

Microcanonical distribution

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

Entropy   Temperature

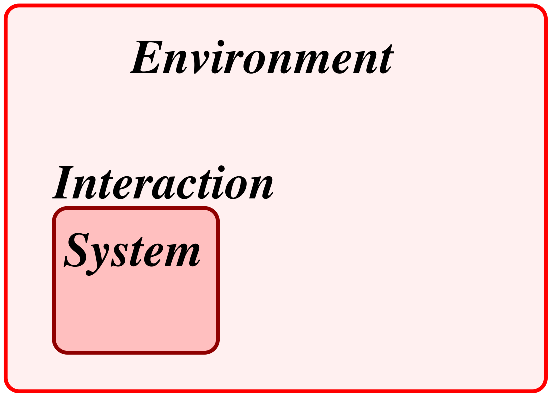
$$\mathcal{E} = \mathcal{E}_{syst} + \mathcal{E}_{env} + \mathcal{E}_{int}$$

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

$$\mathcal{E}_{syst} \ll \mathcal{E}_{env}$$

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

Canonical ensemble



Statistical physics

- Microscopic definition of thermodynamic concepts (entropy, temperature, *etc.*)
- Microscopic derivation of thermodynamic properties (equations of state, *etc.*)
- Theoretical understanding of collective effects.
- Mathematical proof of the existence of phase transitions: sharp changes in the macroscopic behavior of a system when an external (*e.g.* the temperature of the environment) or an internal (*e.g.* a constant in the interaction potential) parameter is changed. The best known example is the solid – liquid – gas phase diagram.
- Calculations can be very difficult but the theoretical framework is set beyond any doubt.

Statistical physics

Generalized formalism

From the particle description $\{\vec{p}_i, \vec{x}_i\}$ to a field-theoretic one $\{\vec{\Pi}(\vec{x}), \vec{\phi}(\vec{x})\}$ with matter density and velocity density fields.

Given an effective Hamiltonian density $\mathcal{H}[\vec{\Pi}, \vec{\phi}]$, construct the probability density in the relevant ensemble, typically the canonical one, and focus on the free-energy density $-\beta f = \ln Z$ with the partition function $Z = \int \mathcal{D}\vec{\Pi}\mathcal{D}\vec{\phi}\, e^{-\beta\mathcal{H}}$.

Quantum fluctuations (bosons) can be included by upgrading the fields to operators, $\Pi_a \mapsto \hat{\Pi}_a$ and $\phi_b \mapsto \hat{\phi}_b$, satisfying canonical commutation relations, $[\hat{\Pi}_a(\vec{x}), \hat{\phi}_b(\vec{x}')] = -i\hbar\delta_{ab}\delta(\vec{x} - \vec{x}')$, and constructing $\hat{\varrho} = Z^{-1}e^{-\beta\hat{H}}$ with $Z = \mathrm{Tr}\hat{\varrho}$. Other subtleties (fermions, spin...) not to be discussed here. Mapping from quantum model in d-dimensions to a classical one in $d+1$-dimensions $\Rightarrow$

Statistical Field Theory – Thermal Quantum Field Theory

Methods

Analytic

Perturbation theory (if there is a small parameter).

Mean-field (effective medium approximation, long-range interactions), e.g. **Curie-Weiss** model for ferromagnetic transition, **early 20th century**.

Self-consistent approximations, e.g. Gaussian closures, Hartree-Fock & large N methods. Improvements over naive mean-field.

Renormalization group techniques for critical behavior. **K. Wilson, 75**

Conformal field theory & integrability for $2d$ cases. **Lieb, Baxter, Cardy** *et al*

Numerical

Monte Carlo methods: incomplete but intelligent sampling of the partition sum.

Goals: Order parameters, phase diagrams, critical behavior, thermodyn...

Statistical physics

Some problems of current research

Disordered systems (in which some parameters in the Hamiltonian are taken from a probability distribution) : functional order parameters and many other peculiarities.

– Applications beyond physics to social sciences, econophysics, computer science, *e.g.* combinatorial optimisation.

Glassy systems prove existence or non-existence of a phase transition.

Exact results in low d classical and quantum integrable models.

Quantum phase transitions as classical ones or not ?

Understanding observed phenomena e.g. high-T_c superconductivity.

Part 2.

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Discussion

- A few variables ruled by Newton dynamics : dynamical systems

- My aim here: exhibit examples of many-body systems in which a part acts as an equilibrium bath but the rest cannot equilibrate with it.
  - One goal: understand the evolution at a mesoscopic scale.
  - Another goal: derive, if possible, generalisations of thermodynamic concepts for these cases and later check whether these are generic for some class of out of equilibrium systems.

Out of equilibrium

How can a classical system stay out of equilibrium ?

- The equilibration time goes beyond the experimentally accessible times.

$$\boxed{t_{eq} \gg t}$$

No confining potential, *e.g.* harmonic oscillator in the $\omega \to 0$ limit:

$t_{eq_x} = \gamma/(M\omega^2) \to \infty$. *e.g.*, **Diffusion processes**.

Macroscopic systems in which the equilibration time grows with

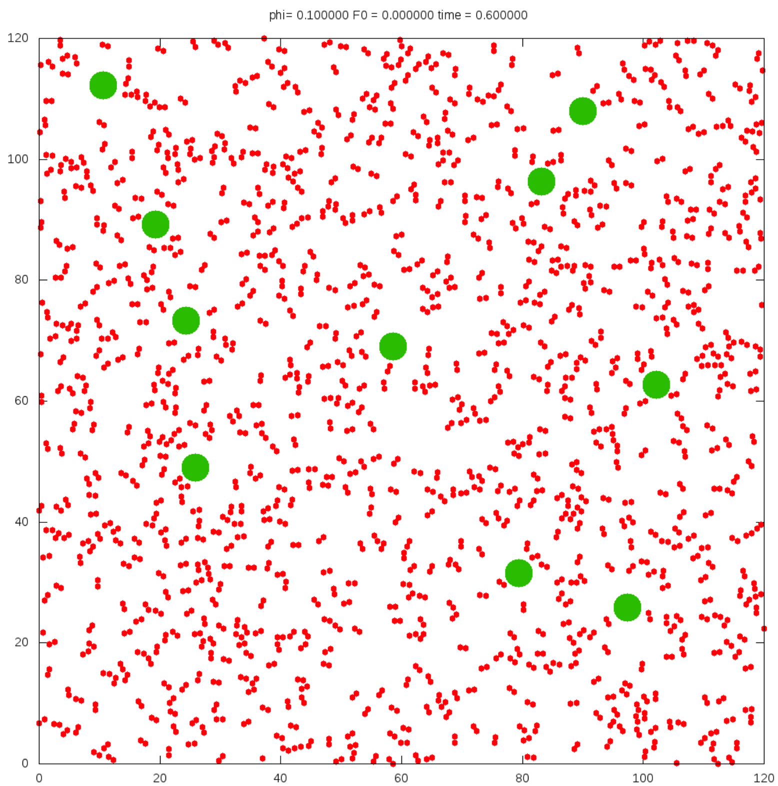
the system size, $\boxed{\lim_{N\gg 1} t_{eq}(N) \gg t}$

e.g., **Critical dynamics, coarsening, glassy physics**.

- **Driven systems** $\boxed{\vec{F} \neq -\vec{\nabla} V(\vec{r})}$

e.g., **Sheared liquids, vibrated powders, active matter**.

Brownian motion



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 ● imbedded in, say, a molecular liquid.

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

Langevin approach

Stochastic Markov dynamics

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

$$\boxed{m\dot{v}_a = -\gamma_0 v_a + \xi_a}$$

with $a = 1, \ldots, d$ (the dimension of space), m the particle mass,
γ_0 the friction coefficient,
and $\vec{\xi}$ 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,
$2\langle E(t) \rangle = m\langle v^2(t) \rangle \neq 0$.

Brownian motion

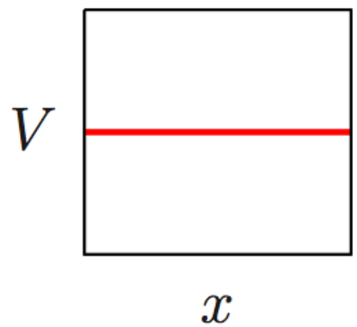
Markov normal diffusion

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

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

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



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

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

The particle is out of equilibrium !

Stochastic dynamics

Open systems

- Stochastic equation, noise, fluctuations Stochastic calculus
- Dissipation, breakdown of time-reversal invariance, irreversibility.
- Similar equations are proposed as phenomenological equations for the evolution of more complex systems, even macroscopic ones, coupled to even larger environments that act as baths.

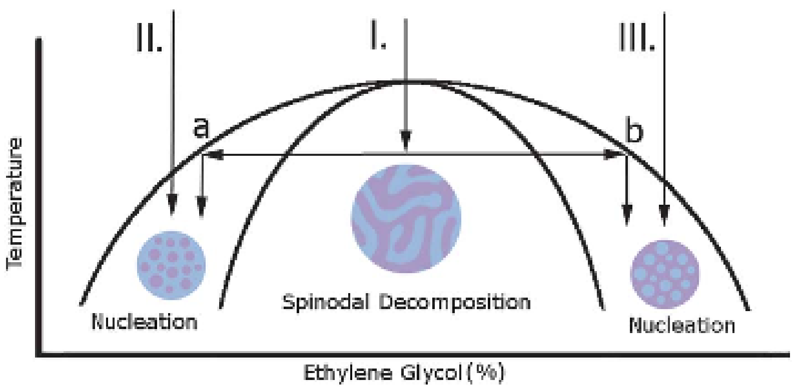
$$\underbrace{m\ddot{\vec{\phi}}(\vec{x},t)}_{\text{Inertia}} + \underbrace{\gamma_0\dot{\vec{\phi}}(\vec{x},t)}_{\text{Dissipation}} = \underbrace{F(\vec{\phi})}_{\text{Deterministic}} + \underbrace{\vec{\xi}(\vec{x},t)}_{\text{Noise}}$$

Effective Langevin equation: time is present, no usual thermodynamics.

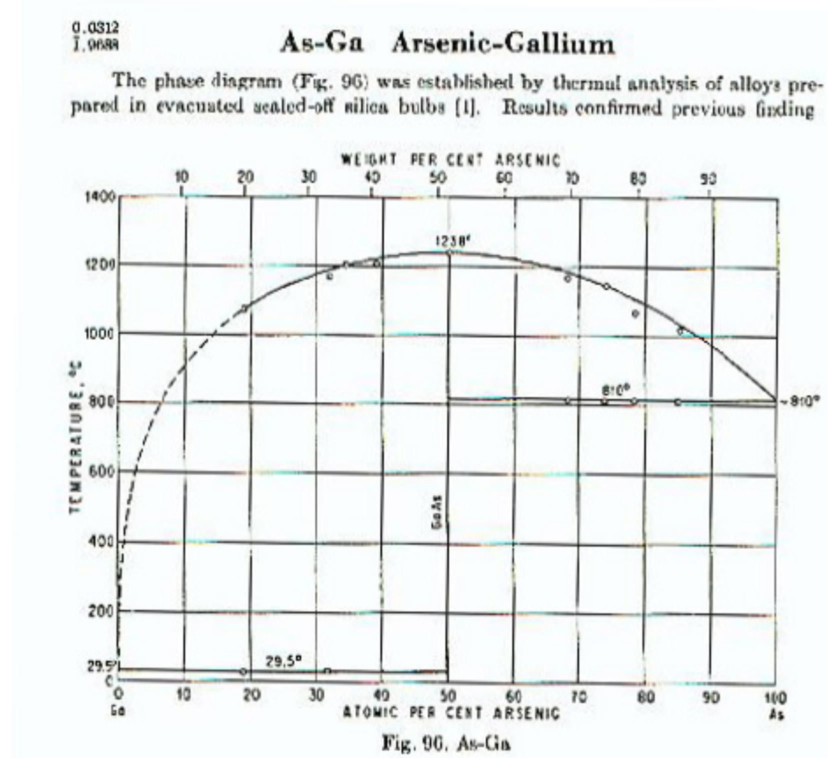
Demixing transitions

Many-body interacting system

Two species ● and ●, repulsive interactions between them.



Sketch

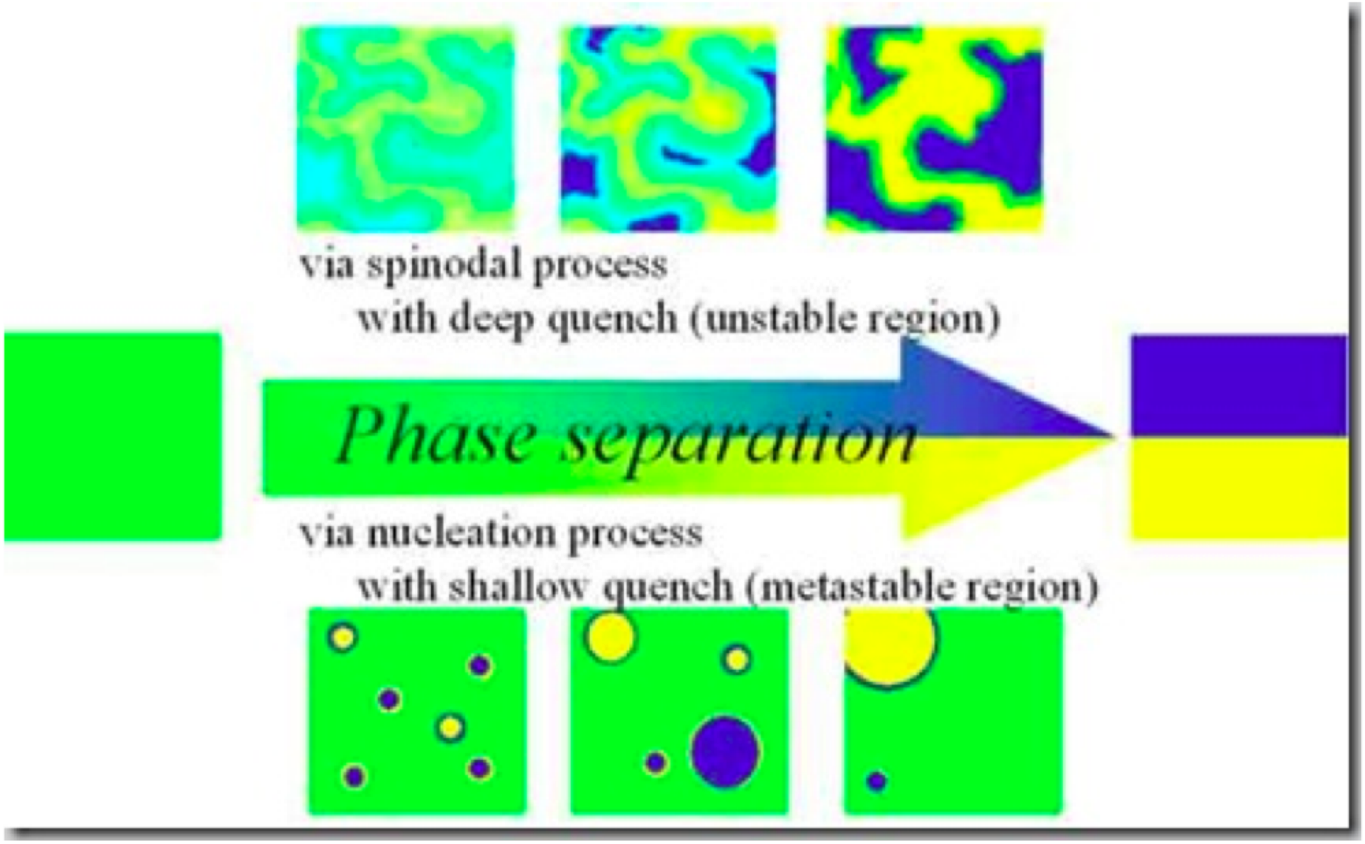


Experimental phase diagram

Binary alloy, **Hansen & Anderko, 54**

Phase separation

Phase ordering kinetics



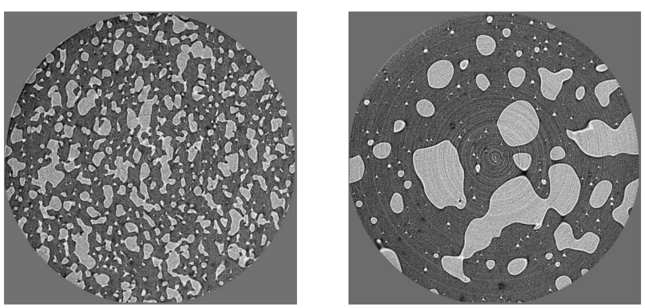
Phase ordering kinetics

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 $\mathcal{V} \to \infty$.

In this case we understand the mechanisms for relaxation : reduction of the local curvature of the interfaces and matter diffusion.



The domains get rounder

The regions get darker and lighter

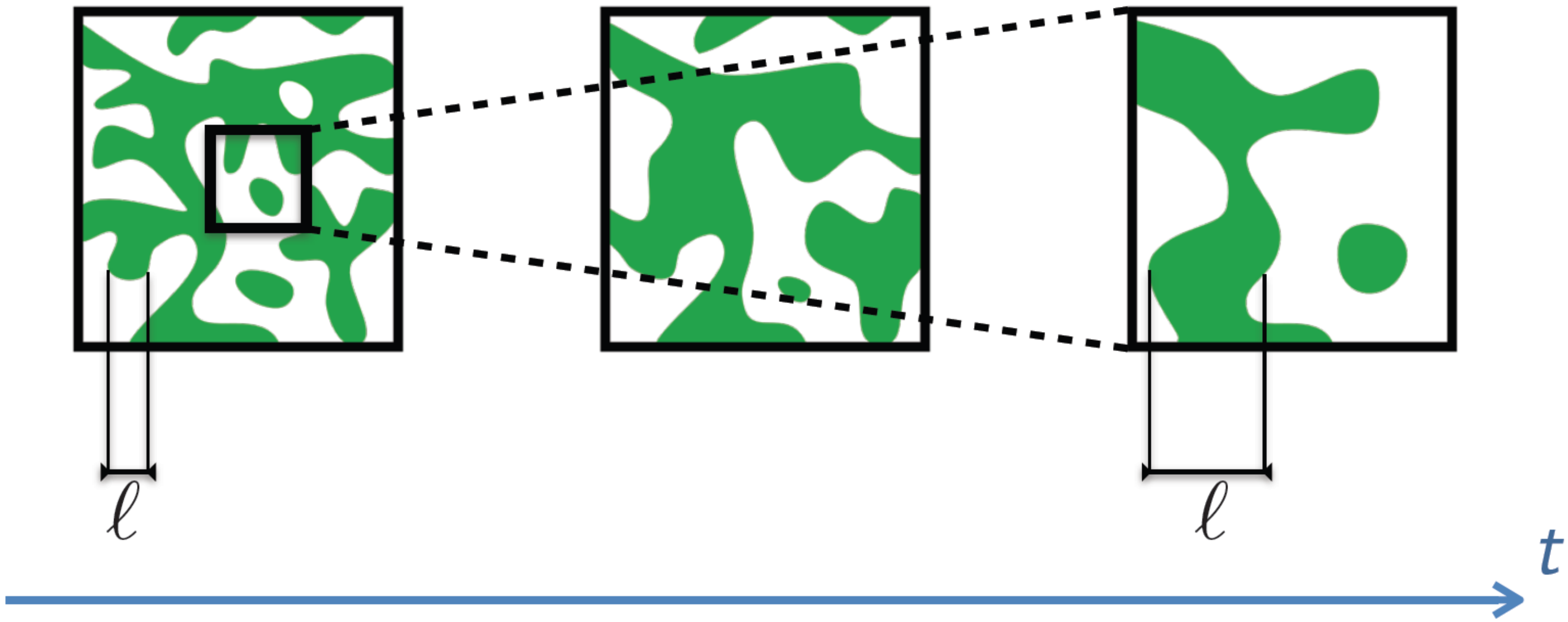
Lifshitz-Slyozov 60s & Huse 93

$R(t) \simeq t^{1/3}$

Dynamic scaling

Dynamic scaling

in phase ordering kinetics



Growing length $\ell(t)$ and equilibrium reached for $\ell(t_{eq}) \simeq L$

Typically $\ell(t) \simeq t^{1/z}$ and $t_{eq} \simeq L^z$

Excess energy w.r.t. the equilibrium one stored in the domain walls ; $\Delta\mathcal{E}(t) \simeq \ell^{-a}(t)$

Vortex dynamics

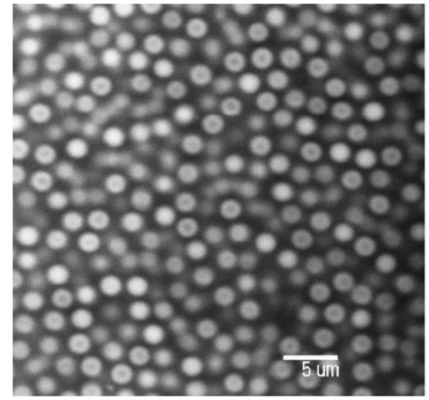
Quenched 3d xy model

M. Kobayashi & LFC

What do glasses look like ?

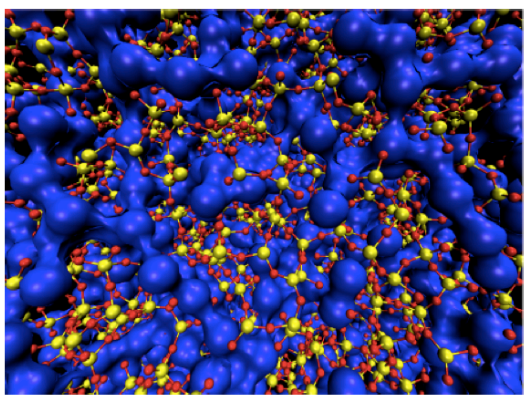
Experiments

Granular matter

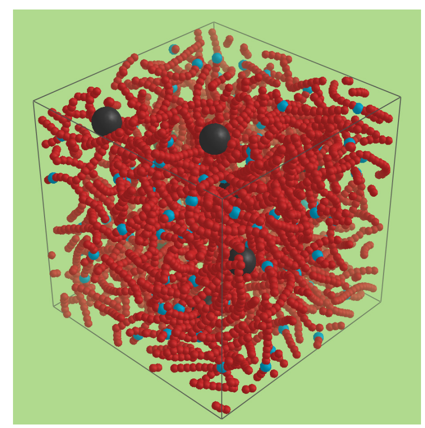


Confocal microscopy - colloids

Simulation



Molecular (Sodium Silicate)

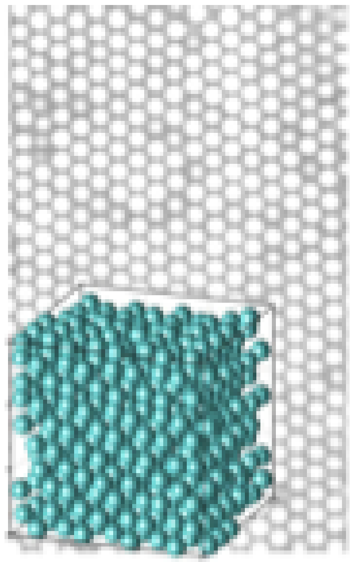


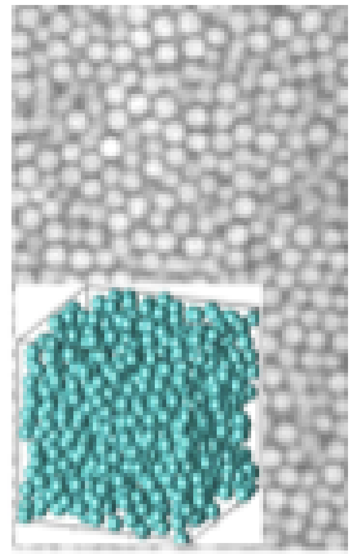
Polymer melt

Glasses

e.g., **colloidal ensembles**

Micrometric spheres immersed in a fluid





Crystal Glass

In the glass : no obvious growth of order, solid-like behaviour though liquid-like structure, slow dynamics with, however, scaling properties.

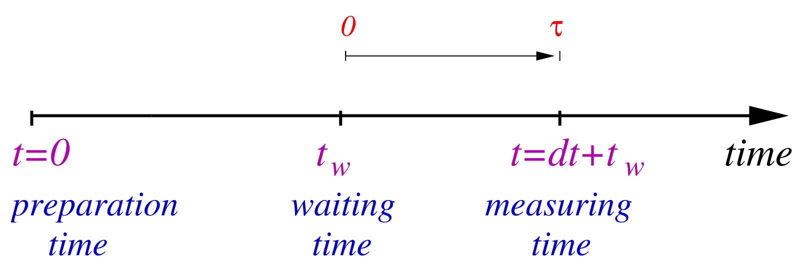
What drives the slowing down ?

Non-potential forces

Apply external non-potential forces, $\vec{f}_i \neq -\vec{\nabla}_i V(\{\vec{x}\})$:

energy injection into the system.

Let the system evolve under $\vec{f}_i$ from some initial condition.



- Typically, for $t_w > t_{st}$: the system reaches a non-equilibrium steady state in which thermodynamics and (Boltzmann) statistical mechanics do not obviously apply.

Dynamic phase transitions ? Which is the stationary measure ?

Bacteria colony

Active matter

Rabani, Ariel & Be'er, 13

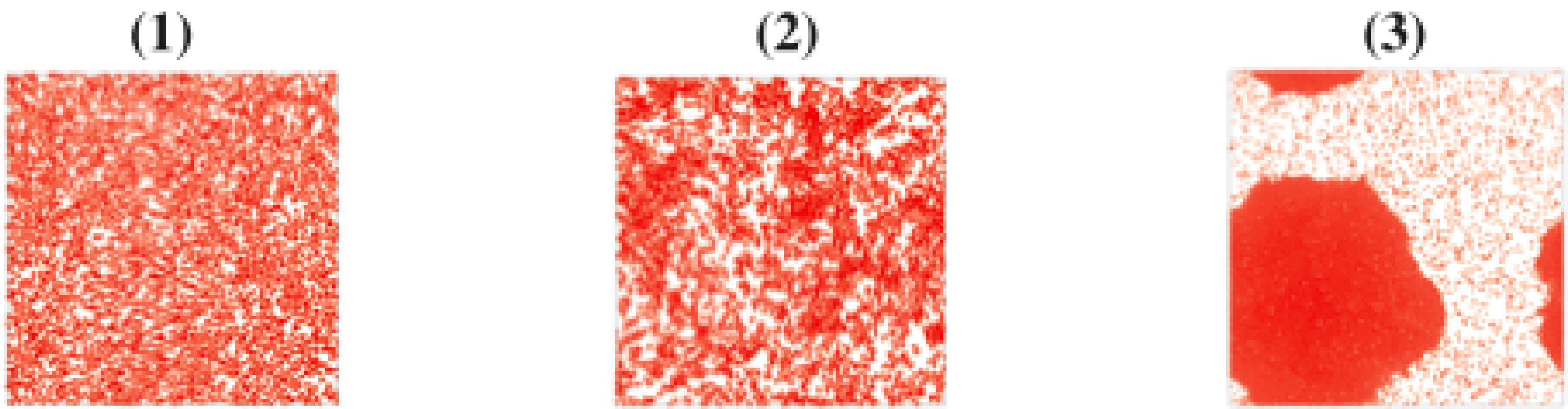
Active dumbbells

Molecular dynamics

Active dumbbells

Phase segregation

Fixed density and fixed activity.



$T = 0.5$ Mixed

$T = 0.05$ Large density fluctuations

$T = 0.01$ Segregation dense-gas

G. Gonnella, A. Lamura & A. Suma, 13

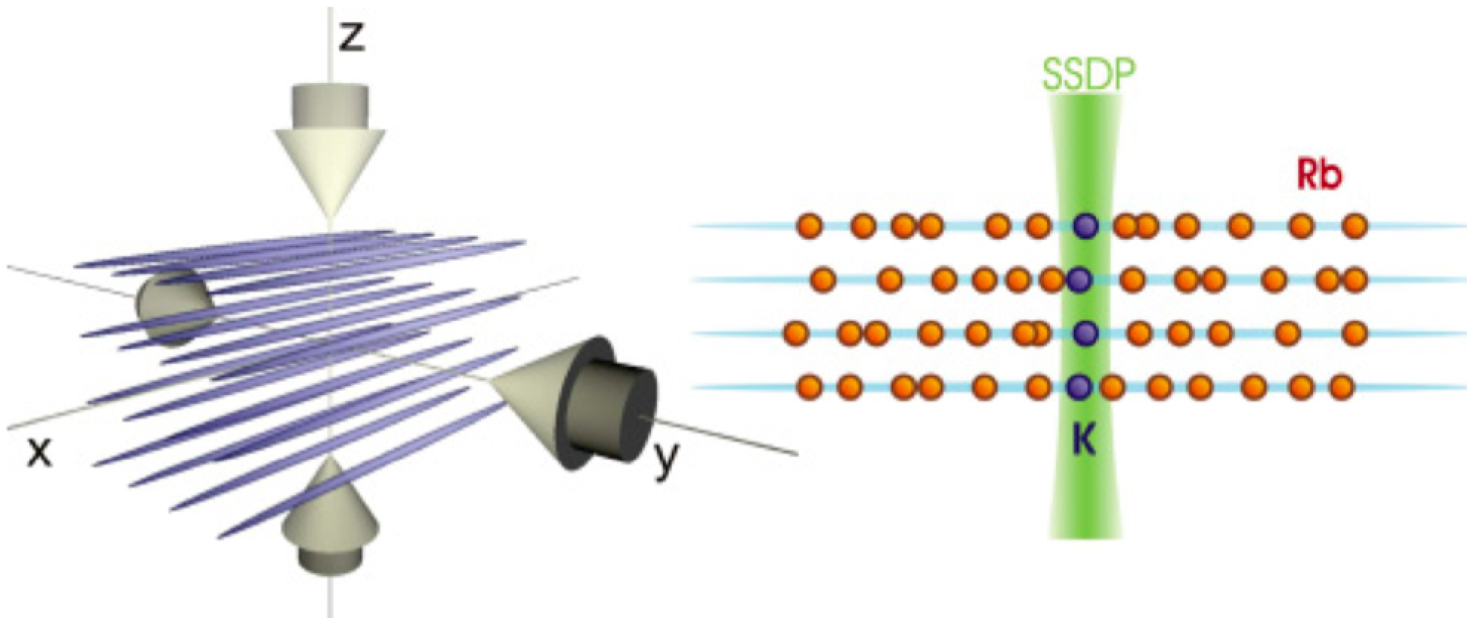
Active dumbbells

Spherical tracers to probe the dynamics of the “active bath"

G. Gonnella, G. L. Laghezza, A. Lamura, A. Suma & LFC

A quantum impurity

in a one dimensional harmonic trap



K atom : the impurity (1.4 on average per tube)

Rb atoms : the bath (180 on average per tube)

all confined in one dimensional tubes

$T \simeq 350$ nK

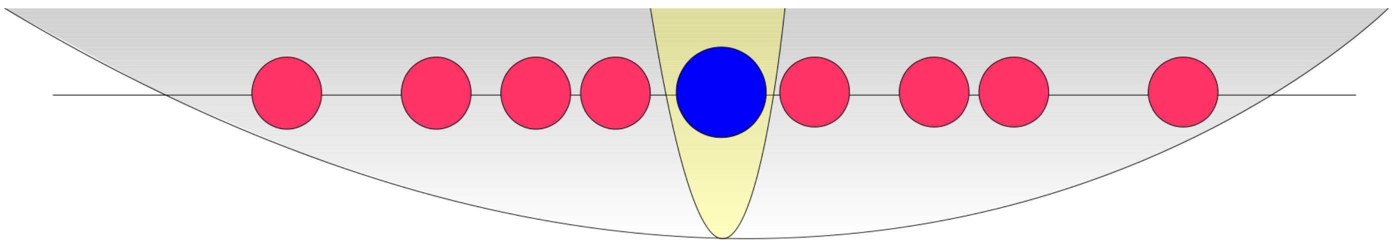
$\hbar\beta\sqrt{\kappa_0/m} \simeq 0.1$

Catani ***et al.*** **12 (Firenze)**

Experiment

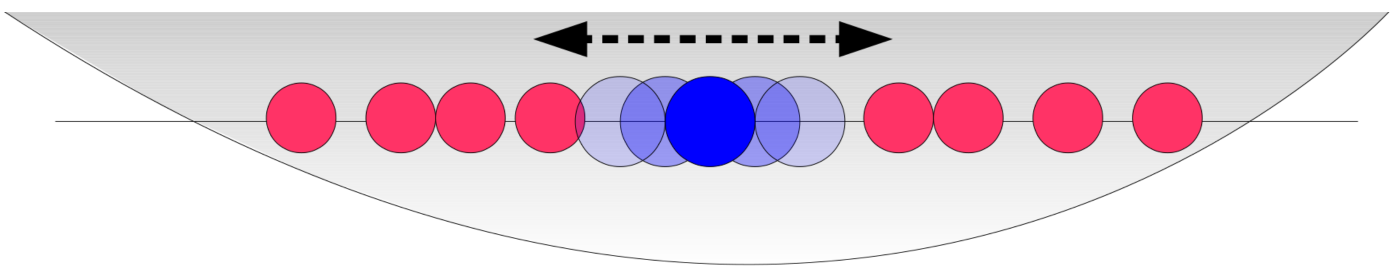
Sketch

Initially, the impurity is localized at the centre of the harmonic potential.



At $t = 0$, the impurity is released.

It subsequently undergoes quantum Brownian motion in the quasi $1d$ harmonic potential.



Experimental protocol

A quench of the system

Initial equilibrium of the coupled system :

$$\hat{\varrho}(t_0) \propto e^{-\beta \hat{\mathcal{H}}_0}$$

with
$$\hat{\mathcal{H}}_0 = \hat{\mathcal{H}}^0_{syst} + \hat{\mathcal{H}}_{env} + \hat{\mathcal{H}}_{int}$$

and
$$\hat{\mathcal{H}}^0_{syst} = \frac{1}{2m}\,\hat{p}^2 + \frac{1}{2}\kappa_0\,\hat{x}^2$$

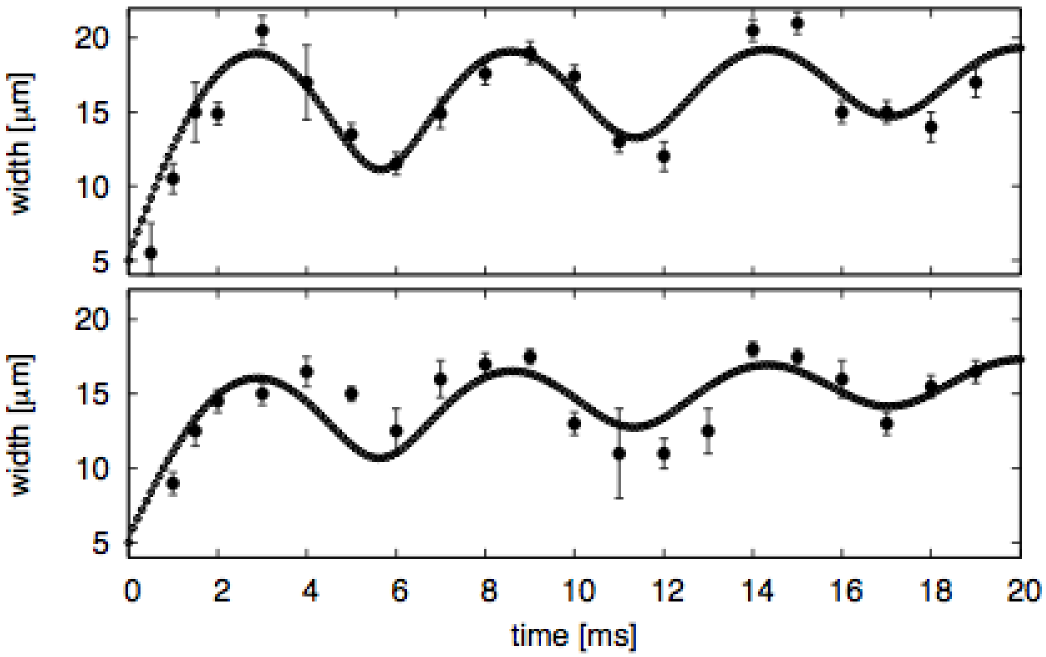
At time $t_0 = 0$ the impurity is released, the laser blade is switched-off and the atom only feels the *wide* confining harmonic potential $\kappa_0 \longrightarrow \kappa$ as well as the bath made by the other species.

What are the subsequent dynamics of the particle ?

Use it to characterise the environment

Breathing mode

Theory vs. experiment



$w/\omega_L = 1$

$w/\omega_L = 4$

Dynamics with m^* and κ^*, interpolation to $\lim_{t\to\infty}\langle x^2(t)\rangle \to k_BT/\kappa$:

$$\langle x^2(t)\rangle = \frac{\hbar^2\kappa_0}{4k_BT}\mathcal{R}(t) - \frac{\kappa^*}{k_BT}\mathcal{C}_{eq}^2(t) + \frac{k_BT}{\kappa^*} + (1 - e^{-\Gamma t})\left(\frac{k_BT}{\kappa} - \frac{k_BT}{\kappa^*}\right)$$

Bonart & LFC EPL 13

Closed quantum systems

Quantum quenches

- Take an isolated quantum system with Hamiltonian $\hat{\mathcal{H}}_0$
- Initialize it in, say, $|\psi_0\rangle$ the ground-state of the $\hat{\mathcal{H}}_0$
- Evolve this state with the Hamiltonian $\hat{\mathcal{H}}$

Does the system reach equilibrium ?

Note that it the **ergodic theory** question posed in the quantum context (and back to square one).

Motivated by cold-atom experiments & exact solutions of $1d$ quantum models.

Methods

Analytic : dynamic generating functional

Perturbation theory (if there is a small parameter).

Mean-field (effective medium approximation, long-range interactions).

Self-consistent approximations, e.g. Gaussian closures, Hartree-Fock & large N methods. Improvements over naive mean-field.

Dynamic renormalization group techniques for critical behavior. **Janssen, 80s**

Numerical

Classical : molecular dynamics, Monte Carlo methods.

Quantum : time-dependent density-functional RG for low-d systems.

Goals : Dynamic phase diagrams & collective effects,

"thermodynamic-like" properties

Thermodynamics ?

Model independent concepts and laws

- Fluctuation theorems, work relations.

Morris, Evans, Gallavotti, Cohen, Jarzinsky, Crooks, Sasa...

- Effective temperatures.

LFC, Kurchan, Peliti...

- Stochastic thermodynamics

Sekimoto, Maes, Seifert...

Wrap-up

Collective phenomena out of equilibrium.

- Understand concrete chosen systems.
- Find general rules.

Close exchanges between theoreticians and experimentalists.

Technically difficult both theoretically as experimentally.

M2 Systèmes complexes

Master recherches

- Physique théorique des systèmes complexes (PCS) parcours international avec le Politecnico di Torino. Martine Ben Amar, Jean-Baptiste Fournier, Emmanuel Trizac
- Modélisation statistique et algorithmique. Dominique Mouhanna
- Microfluidique. Marie-Caroline Jullien, Patrick Tabeling
- Mécanique/Physique (à partir de la rentrée 2015). Matteo Ciccotti

Master Pro

- Fluides complexes et Milieux divisés. Anke Lindner, Florent Carn