Out of equilibrium physics

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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!

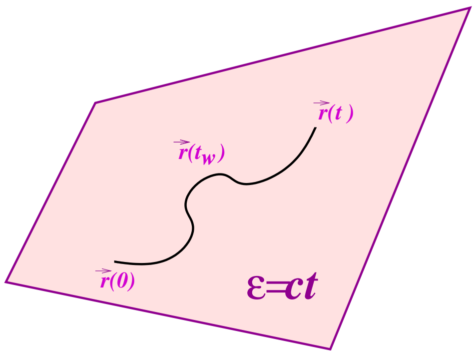
Under certain circumstances, *ergodic hypothesis*, after some equilibration time, t_{eq}, the macroscopic observables can be, on average, obtained with a *static* calculation, as an average over all configurations in phase space weighted with a probability distribution function $P(\{\vec{p}_i, \vec{x}_i\})$:

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

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

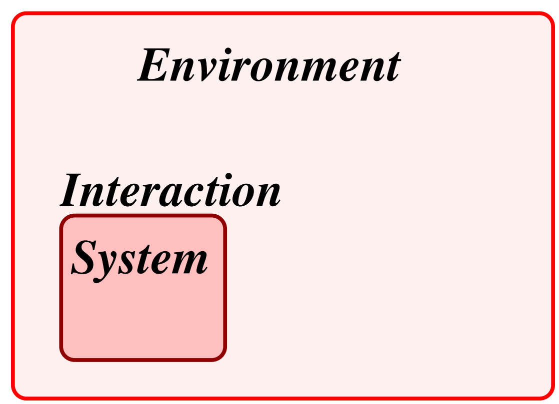
$$\mathcal{E} = \mathcal{E}_{syst} + \mathcal{E}_{env} + \mathcal{E}_{int}$$

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

Ensemble inequivalence for systems with long-range interactions (talk to T. Dauxois).

Disordered systems (spin-glasses) and functional order parameters.

– Applications beyond physics to social sciences, econophysics, etc. (talk to P. Jensen), computer science, *e.g.* combinatorial optimisation.

Frustrated magnets (talk to P. Holdsworth).

Quantum phase transitions (talk to D. Carpentier, P. Degiovanni, A. Fedorenko, P. Holdsworth, E. Orignac, T. Roscilde).

Exact results in low d classical and quantum integrable models (talk to F. Delduc, M. Magro, J-M Maillet).

Part 2.

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Discussion

- A few variables ruled by Newton dynamics : dynamical systems (talk to F. Bouchet, B. Castaing, K. Gawedzki).
- 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 (talk to S. Ciliberto, K. Gawedzki, S. Joubaud, A. Petrosyan).

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

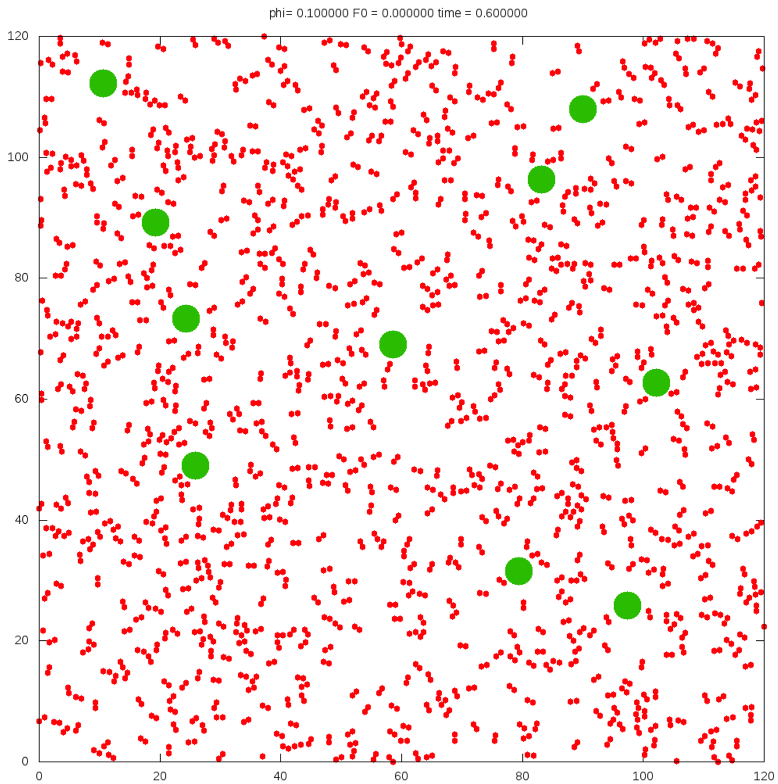
the system size, $\boxed{\lim_{N\gg 1} t_{eq}(N) \gg t}$

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

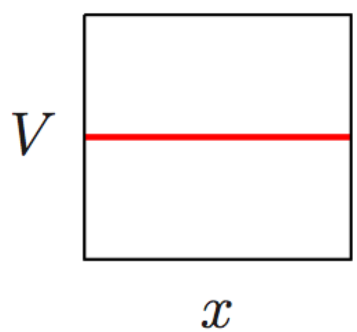
Markov normal diffusion

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 $\boxed{\text{equipartition}}$ for the velocity variable

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

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



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

$$\boxed{D = k_B T/\gamma_o} \qquad \text{diffusion constant.}$$

The particle is out of equilibrium !

Stochastic dynamics

Open systems

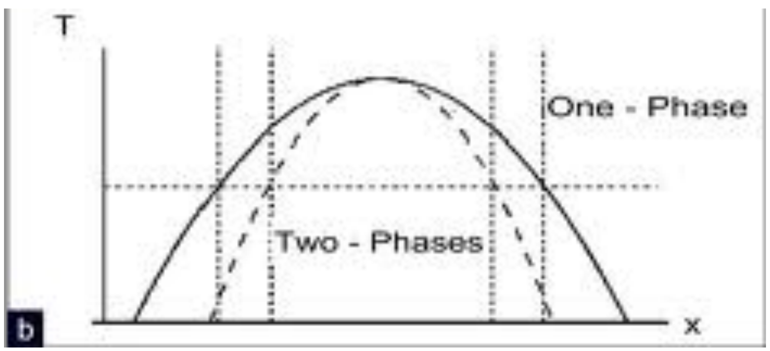
- Stochastic equation, noise, fluctuations Stochastic calculus
- Dissipation, breakdown of time-reversal invariance, irreversibility.
- Similar equations are proposed as phenomenological equations for the evolution of more complex systems, even macroscopic ones, coupled to even larger environments that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

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

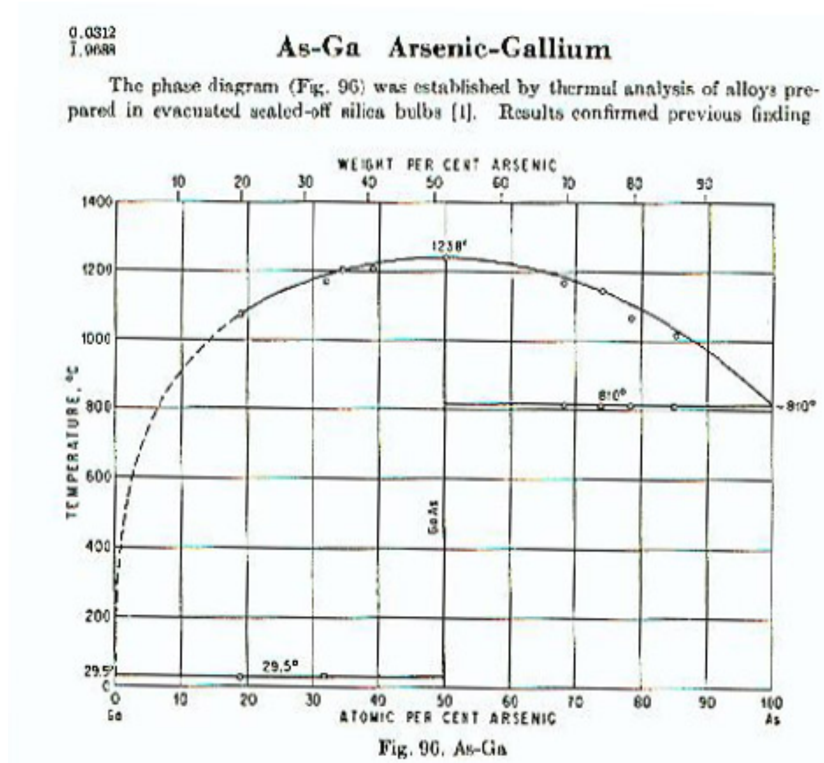
Effective Langevin equation: time is present, no usual thermodynamics.

Demixing transitions

Two species ● and ●, repulsive interactions between them.



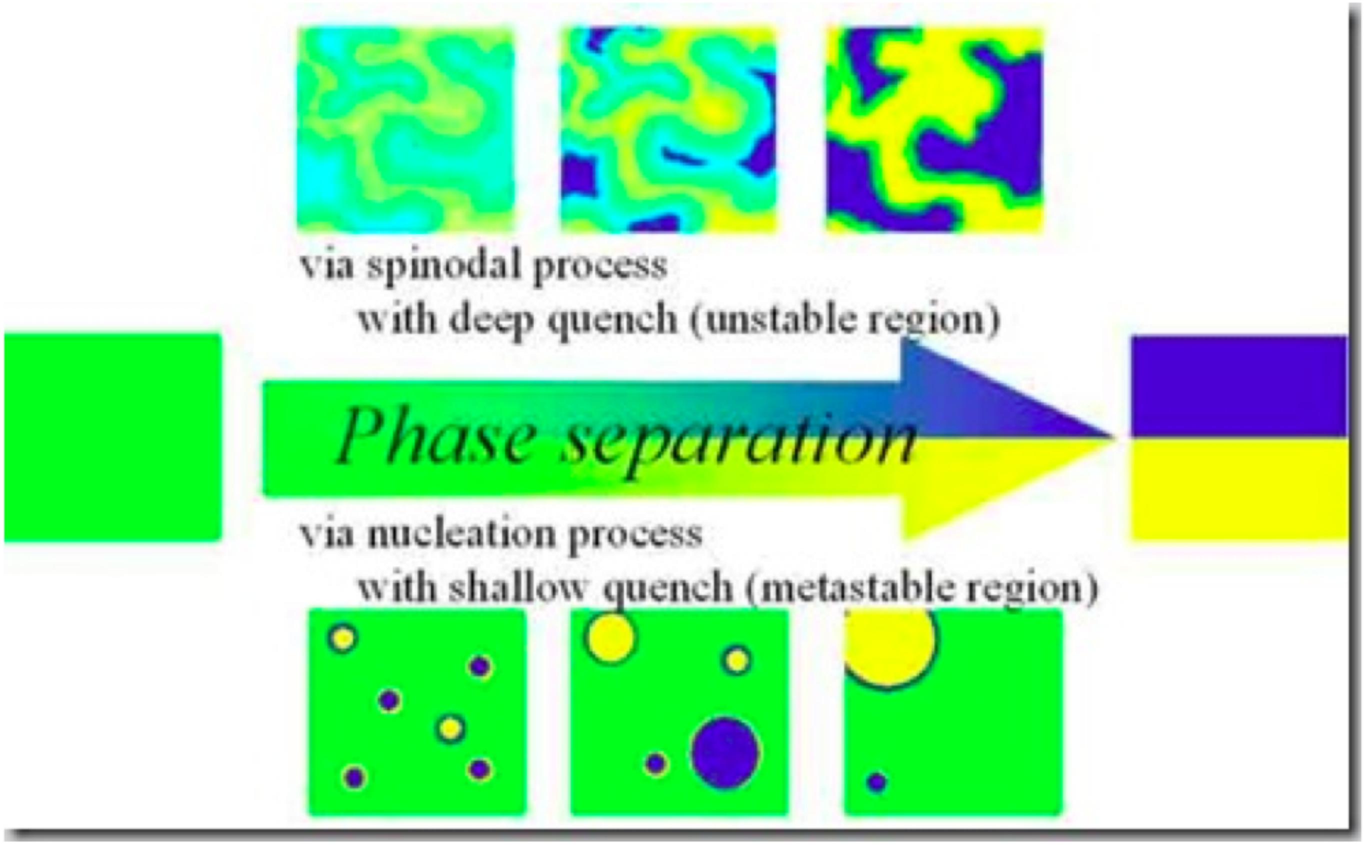
Sketch



Experimental phase diagram

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

Phase separation



Modelled with an effective Langevin equation on a scalar field $\phi(\vec{x}, t)$: that is close to zero in the mixed green phase, and takes two opposite values in the yellow and blue configurations.

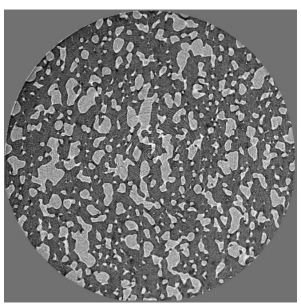
Phase ordering kinetics

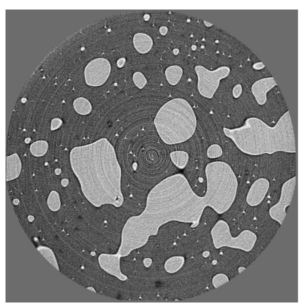
Are these quench dynamics fast processes ? Can we simply forget what happens during the transient, t_{eq}, and focus on the subsequent *equilibrium* behaviour ?

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

Vortex dynamics

Quenched 3d xy model

M. Kobayashi & LFC

Vortex dynamics

3d xy model - reconnection

M. Kobayashi & LFC

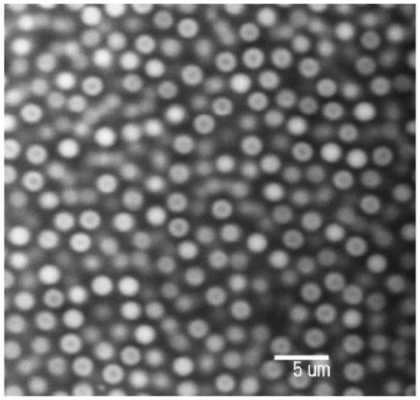
Every-day life glasses

- 3000 BC Glass discovered in the Middle East. LUXURIOUS OBJECTS.
- 1st century BC Blowpipe discovered on the Phoenician coast. Glass manufacturing flourished in the Roman empire. EVERYDAY-LIFE USE.
- By the time of the Crusades glass manufacture had been revived in Venice. CRISTALLO
- After 1890, the engineering of glass as a material developed very fast everywhere.

What do glasses look like ?

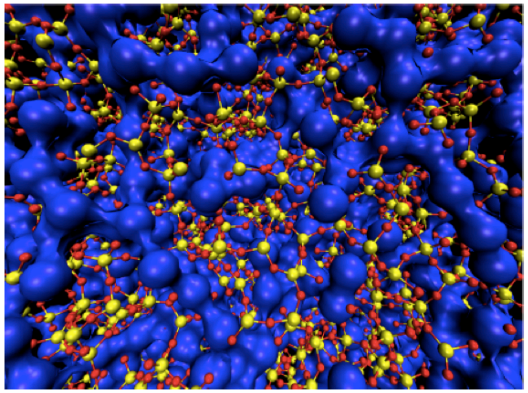
Experiments

Granular matter

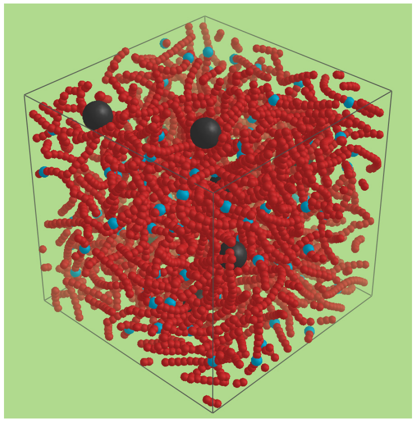


Confocal microscopy - colloids

Simulation



Molecular (Sodium Silicate)



Polymer melt

Structural glasses

Characteristics

- Selected variables (molecules, colloidal particles, vortices or polymers in the pictures) are coupled to their surroundings (other kinds of molecules, water, etc.) that act as thermal baths in equilibrium.
- The interactions each variable feels are typically in competition, e.g. Lennard-Jones potential, implying frustration.
- Each variable feels a different set of forces, heterogeneity and this is time-dependent. Sometimes one talks about **self-generated disorder**.

They continue to evolve in time, e.g. $\langle V \rangle = f(t)$

but one does not see any spatial structure developing.

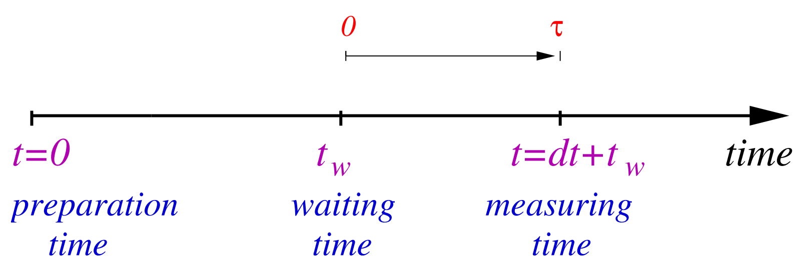
What is the mechanism for relaxation ?

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 and Be'er, 13

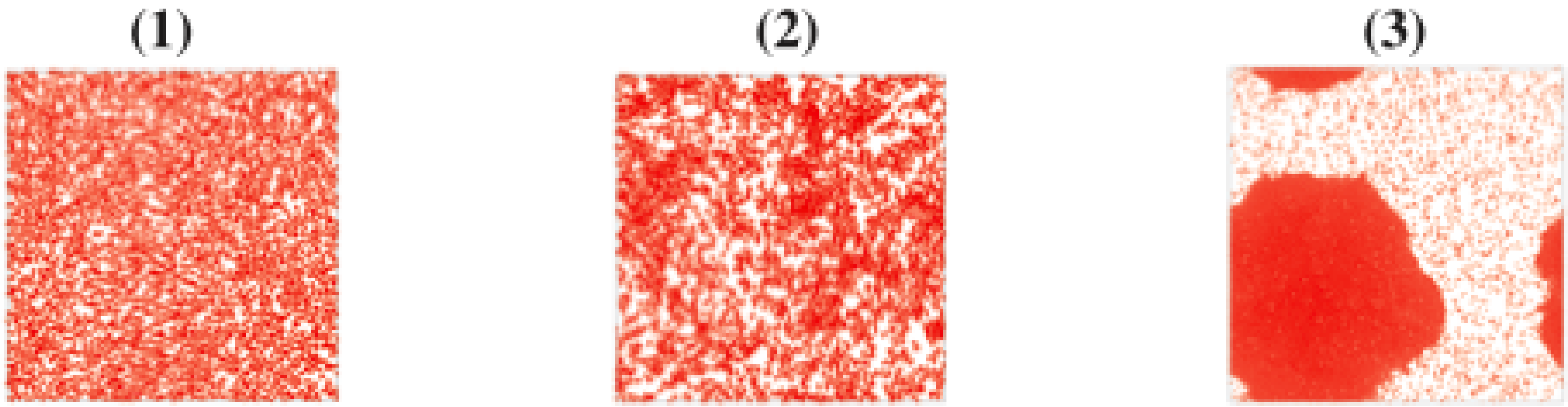
Active dumbbells

Molecular dynamics

Active dumbbells

Phase segregation

Fixed density and fixed activity.



$T = 0.5$	$T = 0.05$	$T = 0.01$
Mixed	Large density fluctuations	Segregation dense-gas

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

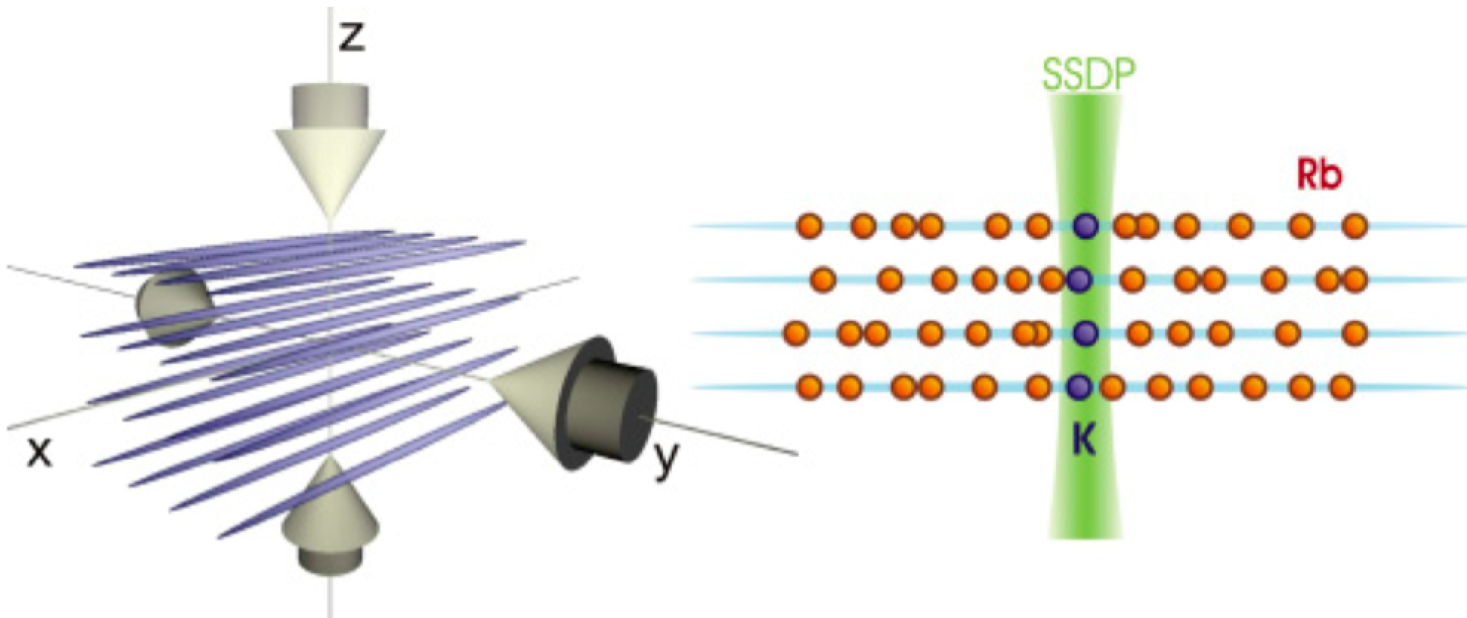
Active dumbbells

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)

$T \simeq 350$ nK

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

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

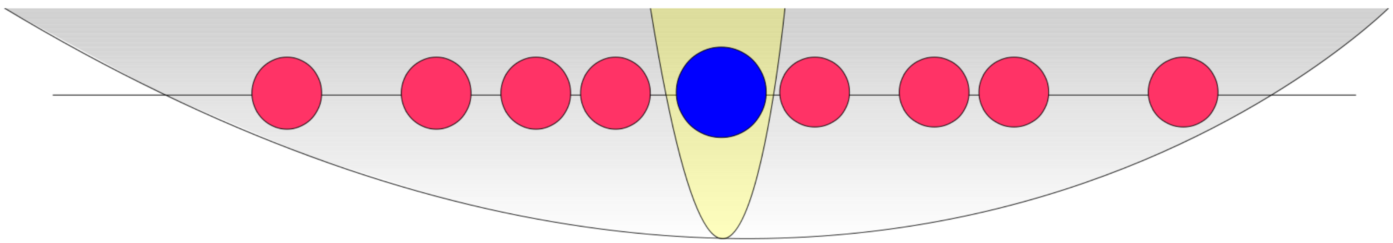
all confined in one dimensional tubes

Catani *et al.* 12 (Firenze)

Experiment

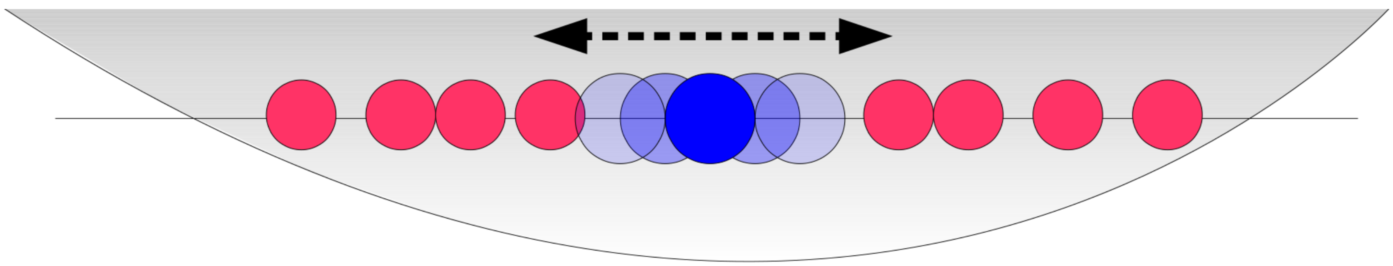
Sketch

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

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

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

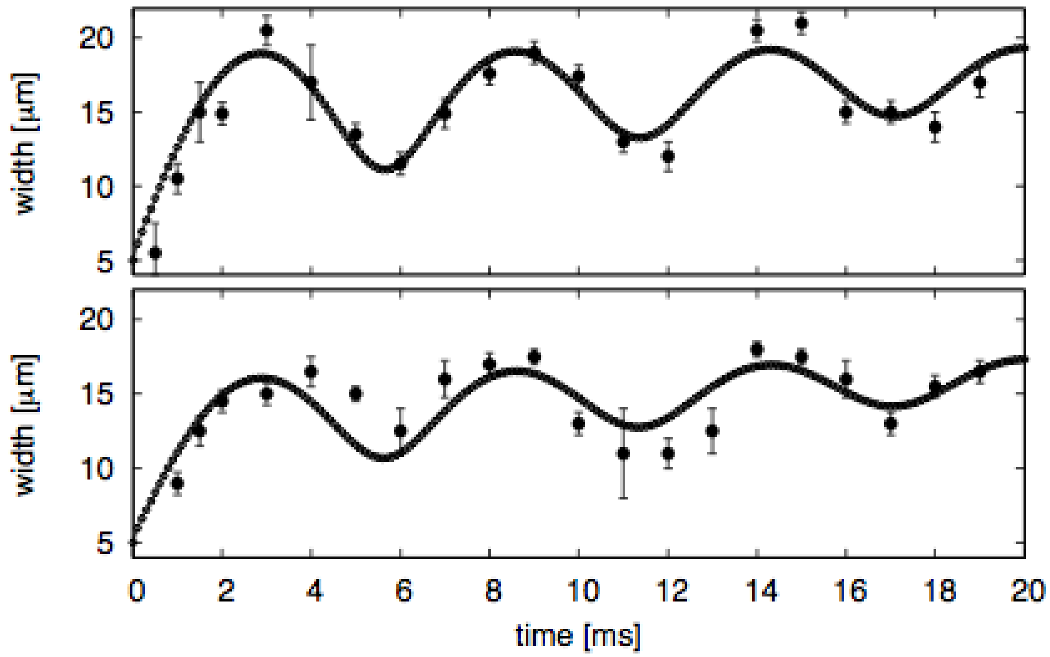
At time $t_0 = 0$ the impurity is released, the laser blade is switched-off and the atom only feels the *wide* confining harmonic potential $\boxed{\kappa_0 \longrightarrow \kappa}$ as well as the bath made by the other species.

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 $\lim_{t\to\infty}\langle x^2(t)\rangle \to k_BT/\kappa$:

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

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 ?

- Fluctuation theorems, work relations.

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

- Effective temperatures.

LFC, Kurchan, Peliti...

- Stochastic thermodynamics

Sekimoto, Maes, Seifert...

(Talk to S. Ciliberto, K. Gawedzki, S. Joubaud, A. Naert, A. Petrosyan.)