.

Large scale stochastic dynamics

August 26 – September 1, 2007

Oberwolfach, Germany

Macroscopic description of non equilibrium stationary states and fluctuations

Joint work with:

L. Bertini, D. Gabrielli, G. Jona-Lasinio, C. Landim.

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Outline

A) Macroscopic theory

1. description of thermod. systems out of equil.,
2. *local equilibrium* (0-th principle of therm.),
3. *stat. state* & *hydrod. eq.*: (1-st principle),
4. *free energy functional* (2-nd principle),
5. *Hamilton-Jacobi eq.* for the free energy,
6. study of the *long range correlations*.

B) Microscopic models

1. definition of *stochastic lattice gases* (examples: SEP, ZR, KMP),
2. local equilibrium,
3. stationary state and hydrodynamic equation,
4. large deviations and free energy functional,
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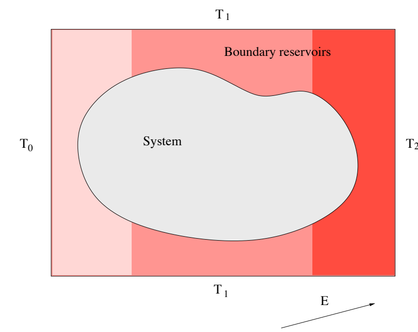
Description of thermodynamic systems out of equilibrium

We consider a macroscopic system in a domain $V \subset \mathbb{R}^d$,

in contact with boundary reservoirs. It is *macr. described* if we know the macroscopic variables in each point:

$$\rho_1(u), \dots, \rho_s(u)\,, \;\; u \in V$$



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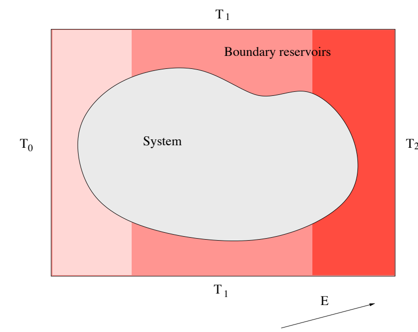
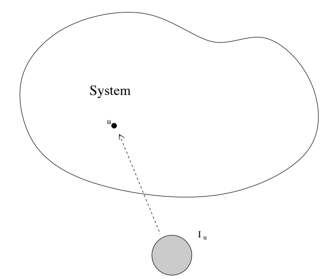


Local equilibrium: given $u \in V$ and a region $u \in I_u \subset V$

s.t. $\epsilon^d |V| \ << \ |I_u| \ << \ |V|$, the macr. variables ρ_i are approximately constant in I_u:

$$\rho(v) \ \simeq \ \rho(u)\,, \ \forall v \in I_u$$



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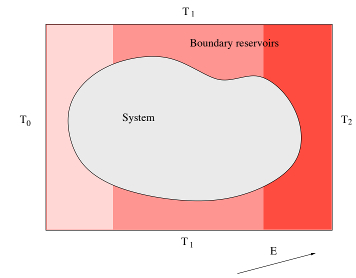

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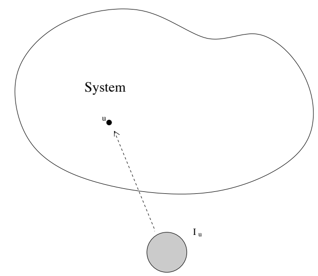

Hydrodynamic eqn: at macr times $\Delta\tau >> \Delta t$, the density evolves smoothly among local equilibrium profiles: $\rho = \rho(\tau, u)$. It is solution of the *hydrodynamic equation*. For conservative diffusive systems:

$$\partial_\tau \rho(\tau,u) + \nabla_u \cdot \underbrace{\Big(-\frac{1}{2}D(\rho)\nabla_u\rho(\tau,u) + \chi(\rho)E(u)\Big)}_{J(\tau,u):\quad \text{macr. current}} = 0$$

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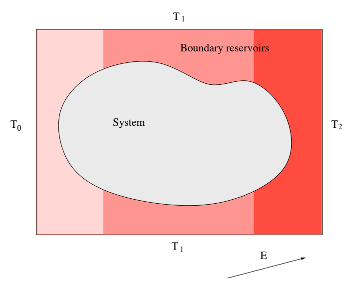

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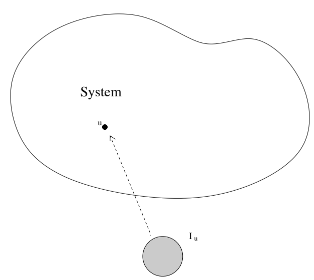

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Stationary state: far from phase transitions, the hydrodynamic eq. has a unique stationary solution $\bar{\rho}$, s.t.

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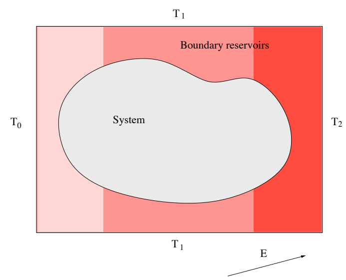

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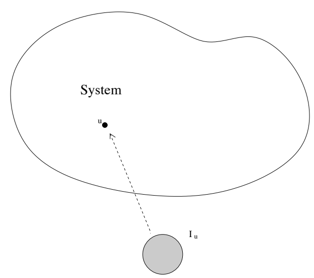

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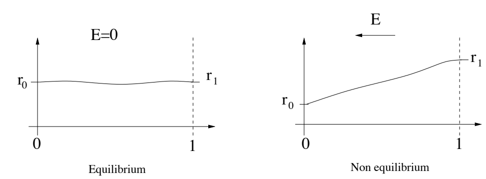

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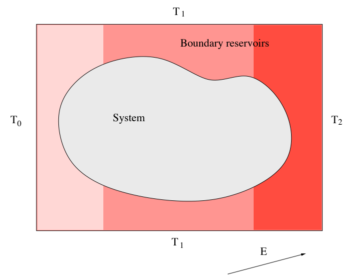

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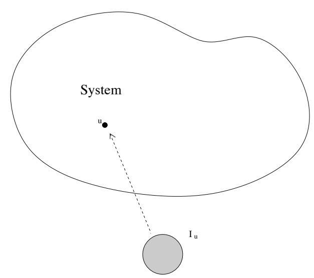

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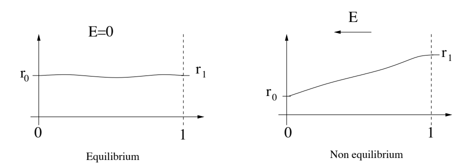
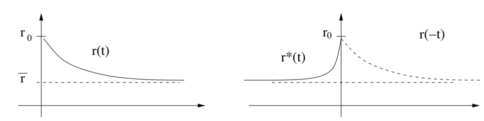


A system is macroscopically reversible if, for every $\rho_0(u)$,

$$\rho^*(\tau,u) = \rho(-\tau,u)$$

where $\rho(\tau)$ is solution of the hydrodyn. eq. with initial cond. ρ_0, and $\rho^*(\tau,u)$ is the evolution of minimal "cost" which produces the fluctuation ρ_0.



We have: $E = 0, \lambda_0 = \text{cost.} \implies \text{macr.rev.} \implies \text{macr.equil.}$

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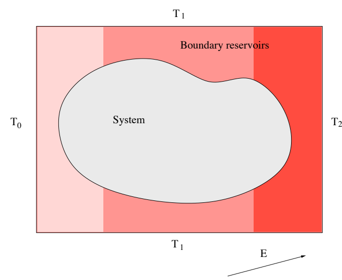

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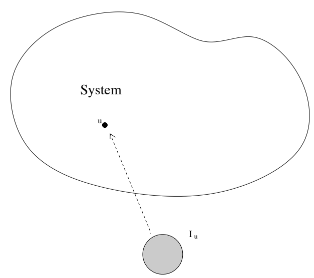

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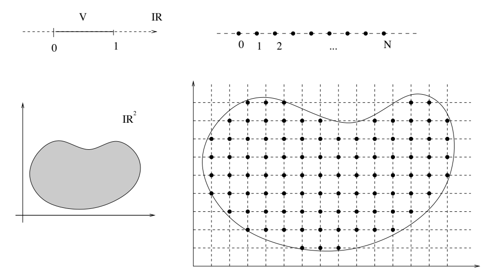
Microscopic models: stochastic lattice gases

Lattice: fix $V \subset \mathbb{R}^d$, $N \in \mathbb{N}$ and take $V_N := (N \cdot V) \cap \mathbb{Z}^d$

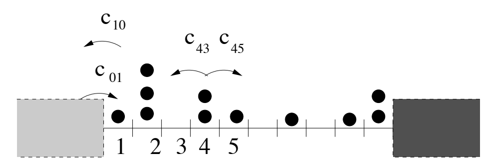


Configuration space: fix $X \subset \mathbb{N}$ and take $\mathcal{H} := X^{V_N}$.

A *configuration* is $\eta = (\eta_x)_{x \in V_N}$, $\eta_x = \#\{\text{particles at } x\}$.

Ex: $X = \{0,1\} \rightarrow$"fermions" , $X = \mathbb{N} \rightarrow$"bosons".

Stochastic dynamics:



$P_t(\eta, \eta') = e^{tL}(\eta, \eta')$, where the *generator* L is defined by

$$Lf(\eta) = \frac{1}{2} \sum_{\substack{(x,y)\,|\,|x-y|=1 \\ \{x,y\}\cap V_N \neq \emptyset}} c_{xy}(\eta)\big(f(\sigma^{xy}\eta) - f(\eta)\big)$$

where $(\sigma^{xy}\eta)_x = \eta_x - 1$, $(\sigma^{xy}\eta)_y = \eta_y + 1$, $(\sigma^{xy}\eta)_z = \eta_z$ if $z \neq x, y$

A state μ is a prob. on X^{V_N}. Time evolution: $\mu_t = e^{tL}\mu_0$.

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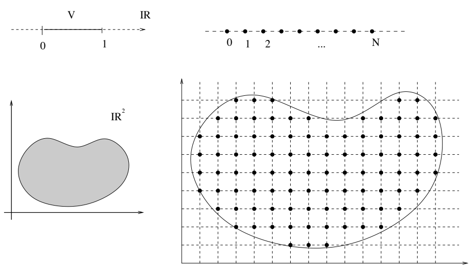

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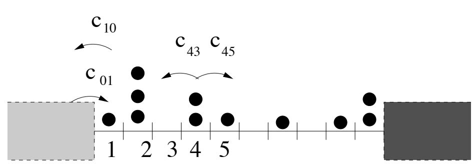

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Equilibrium models. the detailed balance condition holds:

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$H : X^{V_N} \rightarrow \mathbb{R}$: Hamilt. funct., $\lambda_0 \in \mathbb{R}$: chemical potent.

Models out of equilibrium.

1) chemical potential non constant, $\lambda_0 \mapsto \lambda_0(y/N)$.

2) non zero (weak) external field $E : V \rightarrow \mathbb{R}^d$; new rates

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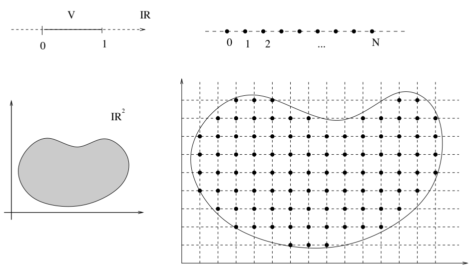

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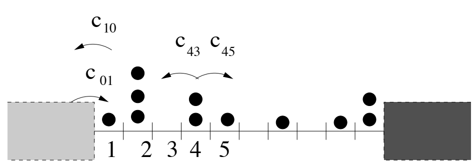

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Equilibrium models: $\mu_{eq}(\eta) \propto e^{-H(\eta) + \lambda_0 \sum_x \eta_x}$

Non equilibrium models: the stat. state $\bar{\mu}$ is not known

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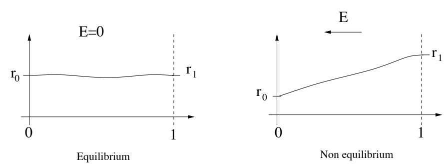

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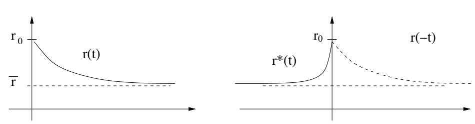

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Equilibrium models: $\mu_{eq}(\eta) \propto e^{-H(\eta) + \lambda_0 \sum_x \eta_x}$

Non equilibrium models: the stat. state $\bar{\mu}$ is not known

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Stationary state: far from phase transitions, the hydrodynamic eq. has a unique stationary solution $\bar{\rho}$, s.t.

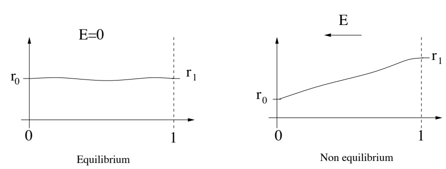
$$\nabla_u \bar{J}(u) = \nabla_u \cdot \left(\frac{1}{2} D(\bar{\rho}) \nabla_u \bar{\rho}(\tau, u) - \chi(\bar{\rho}) E(u)\right) = 0$$

and every solution $\rho(\tau, u)$ evolves towards the stat. solution:

$$\lim_{\tau \to \infty} \rho(\tau, u) = \bar{\rho}(u)$$

Macroscopic equilibrium and reversibility

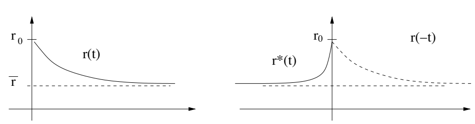
A system is in macroscopic equilibrium if $\bar{J}(u) = 0$.



A system is macroscopically reversible if, for every $\rho_0(u)$,

$$\rho^*(\tau, u) = \rho(-\tau, u)$$

where $\rho(\tau)$ is solution of the hydrodyn. eq. with initial cond. ρ_0, and $\rho^*(\tau, u)$ is the evolution of minimal "cost" which produces the fluctuation ρ_0.



We have: $E = 0, \lambda_0 = \text{cost.} \implies$ macr.rev. $\implies$ macr.equil.

Equilibrium models. the detailed balance condition holds:

$$c^0_{xy}(\eta) = e^{-[H(\sigma^{xy}\eta) - H(\eta)]} c^0_{yx}(\sigma^{xy}\eta) \text{ if } x, y \in V_N$$

$$c^0_{xy}(\eta) = e^{-[H(\sigma^{xy}\eta) - H(\eta)] - \lambda_0} c^0_{yx}(\sigma^{xy}\eta) \text{ if } x \in V_N, y \notin V_N$$

$H : X^{V_N} \to \mathbb{R}$: Hamilt. funct., $\lambda_0 \in \mathbb{R}$: chemical potent.

Models out of equilibrium.

1) chemical potential non constant, $\lambda_0 \mapsto \lambda_0(y/N)$.

2) non zero (weak) external field $E : V \to \mathbb{R}^d$; new rates

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The adjoint generator is given by $\bar{\mu}(f \cdot Lg) = \bar{\mu}(g \cdot L^* f)$. It is the generator of the time reversed process:

$$\mathbb{P}_{\bar{\mu}}(\eta(0) = \xi_1, \eta(T) = \xi_2) = \mathbb{P}^*_{\bar{\mu}}(\eta(-T) = \xi_2, \eta(0) = \xi_1)$$

The model is microscopically reversible if $L^* = L$.

Obvious remark:

micr. reversibility is *equivalent* to micr. equilibrium.

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Local equilibrium and hydrodynamic equation

Definition. The empirical measure is a random variable $\pi^N : X^{V_N} \to \mathcal{M}_+(V)$ given by

$$\pi^N(\eta; du) = \frac{1}{N} \sum_{x \in V_N} \eta_x \delta_{x/N}(du)$$

Hypothesis. We *assume* that the initial state μ^N_0 is in local equilibrium w.r.t. $\rho_0(u)$, i.e. we have a law of large numbers

$$\pi^N(\eta, du) \xrightarrow[\mu^N_0]{N\to\infty} \rho_0(u)du$$

In particular, the stat. state $\bar{\mu}$ should satisfy the local equilibrium w.r.t. the stationary density profile $\bar{\rho}$.

"Theorem". We let the system evolve. For every macroscopic time $\tau > 0$ local equilibrium holds:

$$\pi^N(\eta, du) \xrightarrow[\mu^N_{N^2\tau}]{N\to\infty} \rho(\tau, u)du$$

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Thermodynamic functionals: free energy

In equilibrium statistical mechanics, the free energy $F(\rho)$ is defined by the *Boltzmann-Einstein* relation

$$P(\rho \simeq r) \propto e^{-\epsilon^{-d}\Delta F(r)/KT}$$

We generalize to *local* fluctuations of the density; this defines the free energy functional $\mathcal{F}(\rho)$ for system out of equilibrium:

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Main difference between equilibrium and non equilibrium:

- in equilibrium $\mathcal{F}$ is a local functional, i.e.

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- out of equilibrium, *typically* $\mathcal{F}$ is a non local functional. Hence we can have long range density correlations.

Conclusion: second principle of thermodynamics:

1. $\mathcal{F}(\rho(u)) \geq 0$ and $\mathcal{F}(\rho(u)) = 0$ iff $\rho = \bar{\rho}$,
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A. Static large deviations

"**Theorem**" If η is distributed with $\bar{\mu}^N$, then:

$$\bar{\mu}^N(\pi^N(\eta, du) \simeq \rho(u)du, u \in V) \overset{N\to\infty}{\sim} e^{-N\mathcal{F}(\rho)}$$

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B. Dynamical large deviations

"Theorem"

$$\mathbb{P}_{\bar\mu^N}\Big(\begin{matrix}\pi^N(\eta_{N^2\tau},du) \simeq \hat\rho(\tau,u)du \\ u \in V, \tau \in [0,T]\end{matrix}\Big) \overset{N\to\infty}{\sim} e^{-N(\mathcal{F}(\hat\rho(0)) + J_{[0,T]}(\hat\rho))}$$

Two contributions to the rate function:

- $\mathcal{F}(\hat\rho(0))$ = "cost" of observing $\hat\rho_0$ at time $\tau = 0$;
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Free energy for equilibrium models

Partition function: $Z_N(\lambda) = \sum_{\eta\in X^{V_N}} e^{-H(\eta)+\lambda_0\sum_x \eta_x}$
pressure: $p_0(\lambda) = \lim_{N\to\infty} \frac{1}{|V_N|}\log Z_N(\lambda)$
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Explicit examples: ZR & ASEP

1. Zero range model $(d = 1,\ E = 0,\ \lambda_0 \neq \lambda_1)$

Lattice: $V_N = \{1 \dots N\}$; conf. space: $\mathbb{N}^{\{1\dots N\}}$; jump rates:

$$c_{x,x+1}(\eta) = g(\eta_x)\,,\ x = 1, \dots, N-1$$
$$c_{01}(\eta) = e^{\lambda_0}\,,\ c_{N,N-1}(\eta) = e^{\lambda_1}$$

Invariant measure: prod. measure $\bar{\mu}(\eta) = \prod_{x=1\dots N-1} \mu_x(\eta_x)$

with marginals

$$\mu_x(\eta_x = k) = \frac{1}{Z(\bar{\phi}(x))} \frac{\bar{\phi}(x)^k}{g(k)!}$$

where $\bar{\phi}(x) = e^{\lambda_0} + \frac{x}{N}(e^{\lambda_1} - e^{\lambda_0})$, and $Z(\phi) = \sum_{k\in\mathbb{N}} \frac{\phi^k}{g(k)!}$.

Hydrodynamic equation (with external field E):

$$\partial_\tau \rho = \frac{1}{2}\Delta\phi(\rho) - \nabla(\phi(\rho)E)$$

where $\phi = R^{-1}$ and $R(\varphi) = \frac{1}{Z(\varphi)} \sum_{k\in\mathbb{N}} \frac{k\varphi^k}{g(k)!}$.

Diffusion coefficient: $D(\rho) = \phi'(\rho)$; mobility: $\chi(\rho) = \phi(\rho)$.

Free energy functional:

$$\mathcal{F}(\rho) = \int_0^1 \left(\rho(u) \log \frac{\phi(\rho(u))}{\bar{\phi}(u)} - \log \frac{Z(\phi(\rho(u)))}{Z(\bar{\phi}(u))}\right) du$$

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2. Simple exclusion model $(d = 1,\ E \neq 0,\ \lambda_0 \neq \lambda_1)$

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Invariant measure, $\bar{\mu}$, exists and is unique (not a product measure).

Hydrodynamic equation:

$$\partial_\tau \rho = \frac{1}{2}\Delta\rho - \nabla(\rho(1-\rho)E)$$

Hence, diffusion coefficient: $D(\rho) = 1$, mobility: $\chi(\rho) = \rho(1-\rho)$.

Free energy functional: non local, expressed in terms of a variational problem

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Generalized Onsager-Machlup principle

Recall: direct process $\mathbb{P}_{st}$ and "adjoint" process $\mathbb{P}^*_{st}$ are related by time reversal

$$\mathbb{P}^*_{st}(\eta_t, t \in [0,T]) = \mathbb{P}_{st}(\eta_{-t}, t \in [-T, 0])$$

Assume: dynamical large deviations for $\mathbb{P}$ & $\mathbb{P}^*$. Hence

$$\mathbb{P}_{st}\begin{pmatrix} \pi^N(\eta_{N^2\tau}) \simeq \hat{\rho}(\tau)du \\ \tau \in [T_1, T_2] \end{pmatrix} \sim e^{-N(\mathcal{F}(\hat{\rho}(T_1)) + J_{[T_1,T_2]}(\hat{\rho}))}$$

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Choose $T_1 = -\infty$, $T_2 = 0$ and $\hat{\rho}$ s.t. $\hat{\rho}(-\infty) = \bar{\rho}$, $\hat{\rho}(0) = \rho$. Comparing the exponents

$$J_{(-\infty,0]}(\hat{\rho}) = \mathcal{F}(\rho_0) + J^*_{[0,\infty)}(\theta \circ \hat{\rho})$$

Conclusions:

- Generalized Onsager-Machlup principle: the evolution $\hat{\rho}(\tau)$ which minimizes the "cost" function $J_{(-\infty,0]}(\hat{\rho})$, is $\rho^*(-\tau, u)$.

  Hence: macroscopically reversibility $\equiv$ direct and adjoint hydrodynamic eq's coincide.

- $\mathcal{F}(\rho) = \inf_{\hat{\rho} \,|\, \hat{\rho}(-\infty)=\bar{\rho}, \hat{\rho}(0)=\rho} J_{(-\infty,0]}(\hat{\rho})$

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$$\mathbb{P}^*_{st}\begin{pmatrix} \pi^N(\eta_{N^2\tau}) \simeq \hat\rho(-\tau)du \\ \tau \in [-T_2, -T_1] \end{pmatrix} \sim e^{-N(\mathcal{F}(\hat\rho(T_2)) + J^*_{[-T_2,-T_1]}(\theta\circ\hat\rho))}$$

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$$J_{(-\infty,0]}(\hat\rho) = \mathcal{F}(\rho_0) + J^*_{[0,\infty)}(\theta \circ \hat\rho)$$

Conclusions:

- Generalized Onsager-Machlup principle: the evolution $\hat\rho(\tau)$ which minimizes the "cost" function $J_{(-\infty,0]}(\hat\rho)$, is $\rho^*(-\tau, u)$.

  Hence: macroscopically reversibility $\equiv$ direct and adjoint hydrodynamic eq's coincide.
- $\mathcal{F}(\rho) = \inf_{\hat\rho \mid \hat\rho(-\infty)=\bar\rho, \hat\rho(0)=\rho} J_{(-\infty,0]}(\hat\rho)$

Hamilton-Jacobi equation

Recall: the dyn. rate funct. $J_{[T_1,T_2]}(\hat\rho) = \int_{T_1}^{T_2} d\tau \mathcal{L}(\rho, \partial_\tau\rho)$ where

$$\mathcal{L}(\rho, \partial_\tau\rho) = \Big\langle \nabla^{-1}(\partial_\tau\rho - \mathcal{D}(\rho)), \chi^{-1}(\rho)\nabla^{-1}(\partial_\tau\rho - \mathcal{D}(\rho)) \Big\rangle$$

and $\mathcal{D}(\rho) = \frac{1}{2}D(\rho)\nabla\rho - \chi(\rho)E$ = RHS of the hydr.eq.

The free energy $\mathcal{F}(\rho) = \inf_{\hat\rho} \mathcal{L}(\hat\rho, \partial_\tau\hat\rho)$ is the "action".

Hence $\mathcal{F}$ solves the Hamilton-Jacobi equation:

$$\mathcal{H}\Big(\rho, \frac{\delta\mathcal{F}}{\delta\rho}\Big) = 0$$

where $\mathcal{H}$ is the Hamiltonian

$$\mathcal{H}(\rho, H) = \Big\langle \nabla H, \frac{1}{2}\chi(\rho)\nabla H - \mathcal{D}(\rho) \Big\rangle$$

Selection criterion:

$\mathcal{F}$ is the maximal solution of the Hamilton-Jacobi eq., namely

$$\mathcal{F}(\rho) \geq V(\rho)$$

for all $V(\rho)$ solutions of the H-J equation s.t. $V(\bar\rho) = 0$.

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"Proof" of the selection criterion.

$$\begin{aligned}
\mathcal{F}(\rho) &= J_{(-\infty,0]}(\hat\rho) \ \big(\text{at the min. } \hat\rho \text{ s.t. } \hat\rho(-\infty)=\bar\rho,\ \hat\rho(0)=\rho\big) \\
&= \frac{1}{2}\int_{-\infty}^{0} d\tau \langle \nabla H, \chi(\hat\rho)\nabla H\rangle \ \big(\text{where } H \text{ is s.t. } \partial_\tau\hat\rho = \mathcal{D}(\hat\rho) - \nabla\chi(\hat\rho)\nabla H\big) \\
&= \frac{1}{2}\int_{-\infty}^{0} d\tau\, \underbrace{\langle \nabla(H - \frac{\delta V}{\delta\rho}), \chi(\hat\rho)\nabla(H - \frac{\delta V}{\delta\rho})\rangle}_{\geq 0} \\
&\quad + \int_{-\infty}^{0} d\tau \langle \nabla\frac{\delta V}{\delta\rho}, \chi(\hat\rho)\nabla H\rangle \\
&\quad - \frac{1}{2}\int_{-\infty}^{0} d\tau \underbrace{\langle \nabla\frac{\delta V}{\delta\rho}, \chi(\hat\rho)\nabla\frac{\delta V}{\delta\rho}\rangle}_{\text{by H-J eq. } = \langle \nabla\frac{\delta V}{\delta\rho}, \mathcal{D}(\hat\rho)\rangle} \\
&\geq \int_{-\infty}^{0} d\tau \langle \frac{\delta V}{\delta\rho}, \underbrace{\mathcal{D}(\hat\rho) - \nabla\chi(\hat\rho)\nabla H}_{\partial_\tau\hat\rho}\rangle \\
&= \int_{-\infty}^{0} d\tau \langle \frac{\delta V}{\delta\rho}, \partial_\tau\hat\rho\rangle = \int_{-\infty}^{0} d\tau \frac{d}{d\tau} V(\hat\rho) \\
&= V(\underbrace{\hat\rho(0)}_{\rho}) - V(\underbrace{\hat\rho(-\infty)}_{\bar\rho}) = V(\rho)
\end{aligned}$$

□

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Application of H-J equation to long range correlations

The macr. density correlation function $C(u, v)$, $u, v \in V$, is

$$C^{-1}(u, v) = \frac{\delta \mathcal{F}}{\delta \rho(u) \delta \rho(v)}$$

- for equilibrium models, $\mathcal{F}$ is a local functional, hence there are NO long range correlations.
- for models out of equilibrium, in general $\mathcal{F}$ is non local and there can be long range correlations.

It is convenient to introduce the pressure functional

$$\mathcal{G}(h) = \sup_\rho \Big\{ \langle h, \rho \rangle - \mathcal{F}(\rho) \Big\}$$

By Legendre duality, the relation between C and $\mathcal{F}$ gives

$$\frac{\delta \mathcal{G}}{\delta h} \simeq \bar{\rho} + Ch + o(h)$$

and the H-J equation becomes

$$\mathcal{H}\Big(\frac{\delta \mathcal{G}}{\delta h}, h\Big) = 0$$

for all functions $h : V \to \mathbb{R}$ such that $h|_{\partial V} = 0$.

Next: we make the change of variable

$$C(x, y) = C_{eq}(x)\delta(x - y) + B(x, y)$$

where $C_{eq}(x) = D^{-1}(\bar{\rho}(x))\chi(\bar{\rho}(x))$ (Einstein formula), and we expand up to order h^2.

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Conclusion: equation for B

$$\mathcal{L}^{\dagger} B(x, y) = \alpha(x) \delta(x - y)$$

where $\mathcal{L}^{\dagger}$ is the adjoint w.r.t. the Lebesgue measure of the elliptic operator $\mathcal{L} = L_x + L_y$, where

$$L_x = \frac{1}{2} D_{ij}(\bar{\rho}(x)) \partial_{x_i} \partial_{x_j} + \chi'_{ij}(\bar{\rho}(x)) E_j(x) \partial_{x_i}$$

and

$$\alpha(x) = \partial_{x_i} (\chi'_{ij}(\bar{\rho}(x)) D^{-1}_{jk}(\bar{\rho}(x)) \bar{J}_k(x))$$

$\bar{J}$ is the macroscopic current in the stationary profile $\bar{\rho}$.

Observation 1

For systems in macroscopic equilibrium, for which $\bar{J} = 0$, we have $\alpha = 0$, hence $B = 0$, hence there are no long range correlations and $C(x, y) = C_{eq}(x) \delta(x - y)$.

Observation 2

Since $\mathcal{L}$ is an elliptic operator, the sign of B is determined by the sign of α:

$$\alpha(x) > 0 \forall x \quad \Longrightarrow \quad B(x, y) < 0 \forall x, y$$
$$\alpha(x) < 0 \forall x \quad \Longrightarrow \quad B(x, y) > 0 \forall x, y$$

Examples:

Z.R. model: $\chi' = D = \phi' \implies \alpha = \nabla \bar{J} = 0 \implies C = C_{eq}$

S.E.P. model: $D = 1, \chi = \rho(1 - \rho) \implies \alpha = (\nabla \bar{\rho})^2 > 0$
$\implies B(x, y) = -(\nabla \bar{\rho})^2 x(1 - y) < 0$