Entropic Hypocoercivity and Hydrodynamic Limits

Stefano Olla
CEREMADE, Université Paris-Dauphine, PSL

Supported by ANR *LSD*

Rouen, September 16, 2016

ENZA

ENZA

ENZA

ENZA

Damped dynamics

$$dq_t = p_t \; dt$$
$$dp_t = -V'(q_t) \; dt - \gamma p_t \; dt + \sqrt{2\gamma T} \; dw_t$$

Generator:

$$L = \left(p \; \partial_q - V'(q)\partial_p\right) + \gamma \left(T\partial_p^2 - p\partial_p\right) = A + \gamma S$$

Stationary (equilibrium) measure:

$$d\mu_T \;=\; \frac{e^{-(V(q)+p^2/2)/T}}{Z_T} dp \; dq$$

$$L^* \;=\; -A + \gamma S$$

Overdamped dynamics

the limit (in law)

$$q_{\gamma t} \underset{\gamma\to\infty}{\longrightarrow} \tilde{q}_t$$

solves the SDE

$$d\tilde{q}_t = -V'(\tilde{q}_t)\ dt + \sqrt{2T}\ d\tilde{w}_t$$

with symmetric generator

$$\tilde{L} = T\ \partial_q^2\ - V'(q)\ \partial_q\ =\ T\ e^{V(q)/T}\partial_q e^{-V(q)/T}\partial_q$$

$$\tilde{L}^* = \tilde{L}$$

Relative entropy evolution and Fisher information

The initial probability distribution $f_0(p,q)d\mu_T$, evolves following

$$\partial_t f_t \;=\; L^* f_t \;=\; -Af_t + \gamma S f_t$$

Relative entropy evolution and Fisher information

The initial probability distribution $f_0(p,q)d\mu_T$, evolves following

$$\partial_t f_t \;=\; L^* f_t \;=\; -Af_t + \gamma S f_t$$

Relative entropy:

$$H(f_t) = \int f_t \ln f_t \; d\mu_T$$

Relative entropy evolution and Fisher information

The initial probability distribution $f_0(p,q)d\mu_T$, evolves following

$$\partial_t f_t \;=\; L^* f_t \;=\; -Af_t + \gamma S f_t$$

Relative entropy:

$$H(f_t) = \int f_t \ln f_t \; d\mu_T$$

$$\frac{d}{dt}H(f_t) = \int \partial_t f_t \; d\mu_T - \int A f_t \ln f_t \; d\mu_T + \gamma \int S f_t \ln f_t \; d\mu_T$$

$$= -\gamma \int \frac{(\partial_p f_t)^2}{f_t} \; d\mu_T := -\gamma I_p(f_t)$$

to obtain the bound on the Fisher information (uniform in all parameters!)

$$\frac{1}{t}\int_0^t I_p(f_s)\; ds \;=\; \frac{H(f_0) - H(f_t)}{\gamma t} \;\leq\; \frac{H(f_0)}{\gamma t}$$

Relative entropy and Fisher Information for the overdamped

same calculation for the overdamped dynamics:

$$\partial_t \tilde{f}_t \;=\; \tilde{L}^* \tilde{f}_t$$

$$\frac{d}{dt} H(\tilde{f}_t) = -\int \frac{(\partial_q \tilde{f}_t)^2}{\tilde{f}_t}\, d\mu_T := -I_q(\tilde{f}_t)$$

that gives the bound on the Fisher information for the q's

$$\frac{1}{t}\int_0^t I_q(\tilde{f}_s)\, ds \;\leq\; \frac{H(\tilde{f}_0)}{t}$$

Can we obtain the same bound for the damped dynamics?

Skew Fisher information

Choose $a, b, c > 0$, s.t. $b^2 < ac$, define the Skew Fisher information:

$$I(f_t) = \; a I_p(f_t) + c I_q(f_t) + 2b \int \frac{(\partial_p f_t)(\partial_q f_t)}{f_t} \, d\mu_T > 0$$

Skew Fisher information

Choose $a, b, c > 0$, s.t. $b^2 < ac$, define the Skew Fisher information:

$$I(f_t) = \; a I_p(f_t) + c I_q(f_t) + 2b \int \frac{(\partial_p f_t)(\partial_q f_t)}{f_t} \, d\mu_T > 0$$

After a *long* calculation:

$$\frac{d}{dt}\left[H(f_t) + I(f_t)\right] \leq -\lambda I(f_t),$$

with $\lambda > 0$ depending only on γ and $\|V''\|_\infty$ (or hessian $\|\partial_q^2 V\|_\infty$).

Skew Fisher information

Choose $a, b, c > 0$, s.t. $b^2 < ac$, define the Skew Fisher information:

$$I(f_t) = \; aI_p(f_t) + cI_q(f_t) + 2b \int \frac{(\partial_p f_t)(\partial_q f_t)}{f_t} \, d\mu_T > 0$$

After a *long* calculation:

$$\frac{d}{dt}\left[H(f_t) + I(f_t)\right] \leq -\lambda I(f_t),$$

with $\lambda > 0$ depending only on γ and $\|V''\|_\infty$ (or hessian $\|\partial_q^2 V\|_\infty$).

$$\begin{aligned} \frac{1}{t}\int_0^t I_q(f_s)ds \; &\leq \; C\frac{1}{t}\int_0^t I(f_s)ds \\ &\leq \; \frac{C}{\lambda t}\left(H(f_0) + I(f_0)\right) \end{aligned}$$

Details of calculations

$$g_t = \sqrt{f}_t, \qquad \partial_t g_t = -Ag_t + \gamma S g_t + \gamma \frac{|\partial_p g_t|^2}{g_t}$$

$$\frac{d}{dt}\int |\partial_p g_t|^2 \, d\mu = 2\int \partial_p g_t \cdot \partial_q g_t \, d\mu - 2\gamma \int |\partial_p g_t|^2 \, d\mu$$
$$-\gamma \int \left(\partial_p^2 g_t - g^{-1}(\partial_p g_t)^2\right)^2 d\mu$$

Details of calculations

$$g_t = \sqrt{f}_t, \qquad \partial_t g_t = -Ag_t + \gamma S g_t + \gamma \frac{|\partial_p g_t|^2}{g_t}$$

$$\frac{d}{dt}\int |\partial_p g_t|^2 \, d\mu = 2\int \partial_p g_t \cdot \partial_q g_t \, d\mu - 2\gamma \int |\partial_p g_t|^2 \, d\mu$$
$$-\gamma \int \left(\partial_p^2 g_t - g^{-1}(\partial_p g_t)^2\right)^2 d\mu$$

$$\frac{d}{dt}\int |\partial_q g_t|^2 \, d\mu = 2\int \partial_p g_t (\partial_q^2 V) \partial_q g_t \, d\mu$$
$$-\gamma \int \left(\partial_p \partial_q g_t - g^{-1}(\partial_p g_t)(\partial_q g_t)\right)^2 d\mu$$

Details of calculations

$$g_t = \sqrt{f}_t, \qquad \partial_t g_t = -Ag_t + \gamma S g_t + \gamma \frac{|\partial_p g_t|^2}{g_t}$$

$$\frac{d}{dt}\int |\partial_p g_t|^2 \, d\mu = 2\int \partial_p g_t \cdot \partial_q g_t \, d\mu - 2\gamma \int |\partial_p g_t|^2 \, d\mu$$
$$-\gamma \int \left(\partial_p^2 g_t - g^{-1}(\partial_p g_t)^2\right)^2 d\mu$$

$$\frac{d}{dt}\int |\partial_q g_t|^2 \, d\mu = 2\int \partial_p g_t (\partial_q^2 V)\partial_q g_t \, d\mu$$
$$-\gamma \int \left(\partial_p \partial_q g_t - g^{-1}(\partial_p g_t)(\partial_q g_t)\right)^2 d\mu$$

$$\frac{d}{dt} 2\int (\partial_p g_t)(\partial_q g_t) \, d\mu = -2\int |\partial_q g_t|^2 \, d\mu$$
$$+2\int \left((\partial_p g_t)^2 \cdot (\partial_q^2 V) \; - 2\gamma(\partial_p g_t)(\partial_q g_t)\right) \, d\mu$$
$$-2\gamma \int \left(\partial_p^2 g_t - g^{-1}(\partial_p g_t)^2\right)\left(\partial_p \partial_q g_t - g^{-1}(\partial_p g_t)(\partial_q g_t)\right) d\mu$$

Some remarks

- Bounds independent of the *dimensions*.

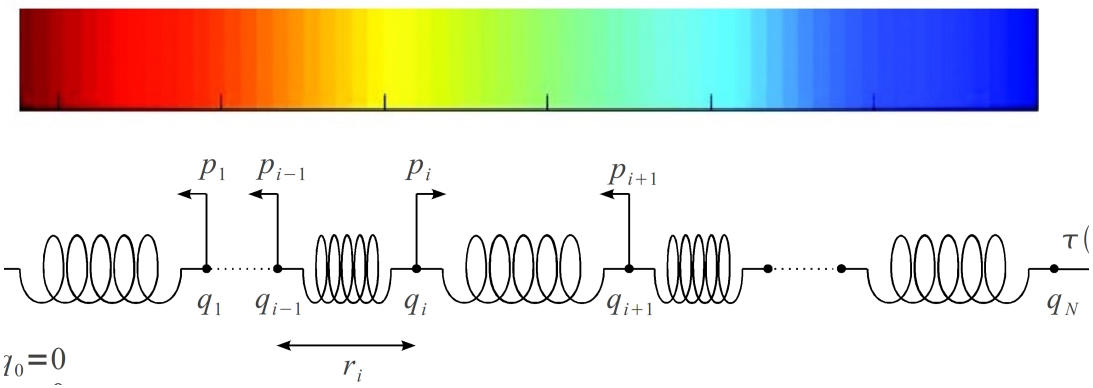
Some remarks

- Bounds independent of the *dimensions*.
- the bound is stable for perturbations of the dynamics.

Some remarks

- Bounds independent of the *dimensions*.
- the bound is stable for perturbations of the dynamics.
- Villani (Memoirs AMS 2009) introduced *entropic hypocoercivity*.

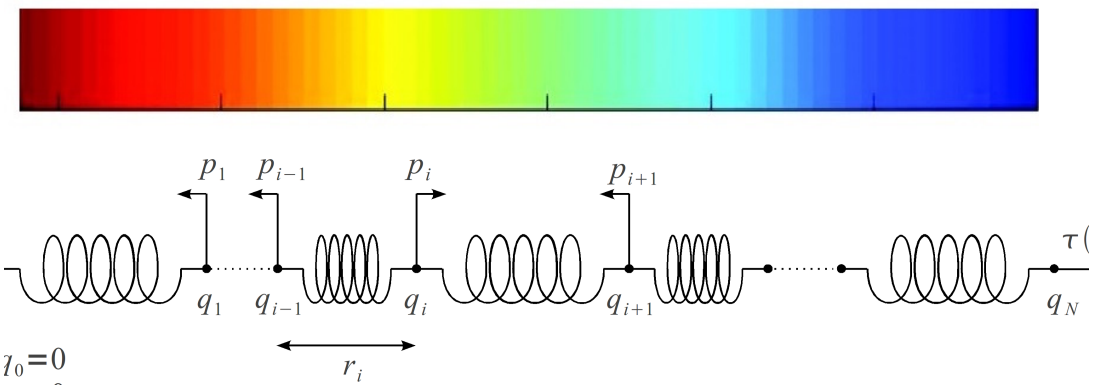
Anharmonic Chain in a temperature gradient



Consider and anharmonic chain on n atoms, n very big, in contact of a termostated damping environment with non-constant temperature $T(j/n)$, with a tension (force) $\bar{\tau}(t/n^2)$ changing slowly in time:

$$
\begin{aligned}
\dot{q}_j(t) &= p_j(t), \qquad j = 1, \dots, n, \\
dp_j(t) &= \big(V'(q_{j+1} - q_j) - V'(q_{j+1} - q_j)\big)\, dt \\
&\qquad - \gamma p_j(t) dt + \sqrt{2\gamma T(j/n)}\, dw_j(t), \qquad j = 1, \dots, n-1, \\
dp_N(t) &= \big(\bar{\tau}(t/n^2) - V'(q_n - q_{n-1}))\big)\, dt - \gamma p_n(t) dt + \sqrt{2\gamma T(1)}\, dw_n(t)
\end{aligned}
$$

Anharmonic Chain in a temperature gradient



Consider and anharmonic chain on n atoms, n very big, in contact of a termostated damping environment with non-constant temperature $T(j/n)$, with a tension (force) $\bar{\tau}(t/n^2)$ changing slowly in time:

$$\dot{q}_j(t) = n^2 p_j(t), \qquad j = 1, \dots, n,$$

$$dp_j(t) = n^2 \left(V'(q_{j+1} - q_j) - V'(q_{j+1} - q_j) \right) dt$$
$$- n^2 \gamma p_j(t) dt + n\sqrt{2\gamma T(j/n)}\, dw_j(t), \qquad j = 1, \dots, n-1,$$

$$dp_n(t) = n^2 \left(\bar{\tau}(t) - V'(q_n - q_{n-1}) \right) \right) dt - n^2 \gamma p_n(t) dt + n\sqrt{2\gamma T(1)}\, dw_n(t)$$

Stationary measures

As $n \to \infty$, the *slow* locally conserved quantity is the *volume*, i.e. the sum of the interparticle distances

$$\sum_i r_i, \qquad r_i = q_i - q_{i-1}$$

If temperature $T(y) = T$ and tension $\bar{\tau}(t) = \tau$ are constant, the equilibrium stationary measures are

$$d\mu_{T,\tau} = \prod_j e^{-T^{-1}[p_j^2/2 + V(r_j) - \tau r_j] - \mathcal{G}(\tau,T)} dr_j dp_j$$

The equilibrium tension is

$$\tau = \frac{\int V'(r_1) e^{-T^{-1}(V(r_1) - \tau r_1)} dr_1}{\int e^{-T^{-1}(V(r_1) - \tau r_1)} dr_1}$$

Stationary measures

As $n \to \infty$, the *slow* locally conserved quantity is the *volume*, i.e. the sum of the interparticle distances

$$\sum_i r_i, \qquad r_i = q_i - q_{i-1}$$

If temperature $T(y) = T$ and tension $\bar{\tau}(t) = \tau$ are constant, the equilibrium stationary measures are

$$d\mu_{T,\tau} = \prod_j e^{-T^{-1}[p_j^2/2 + V(r_j) - \tau r_j] - \mathcal{G}(\tau,T)} dr_j dp_j$$

The equilibrium tension is

$$\tau = \frac{\int V'(r_1) e^{-T^{-1}(V(r_1) - \tau r_1)} dr_1}{\int e^{-T^{-1}(V(r_1) - \tau r_1)} dr_1}$$

When $T(y)$ is not constant, stationary measure is not explicit, and is a non-equilibrium stationary measure (energy flows into the system from the hot to the cold parts.

Hydrodynamic limit

In material coordinate $y \in [0,1]$:

$$\frac{1}{n}\sum_j G\left(j/n\right) r_j(t) \underset{n\to\infty}{\longrightarrow} \int_0^1 G(y) r(y,t)\, dy$$

$$\partial_t r(y,t) = \frac{1}{\gamma}\partial_y^2 \tau(r(y,t), T(y))$$

$$\tau(r(1,t), T(1)) = \bar{\tau}(t),$$
$$\partial_y \tau(r(y,t), T(y))|_{y=0} = 0.$$

Overdamped Dynamics: Ginzburg-Landau model

The corresponding overdamped dynamics ($q_j(\gamma t) \to \tilde{q}_j(t)$, as $\gamma \to \infty$) is

$$
\begin{aligned}
d\tilde{q}_j(t) &= \big(V'(\tilde{q}_{j+1} - \tilde{q}_j) - V'(\tilde{q}_{j+1} - \tilde{q}_j)\big)\, dt \\
&\qquad + \sqrt{2T(j/n)}\, dw_j(t), \qquad j = 1, \dots, n-1, \\
d\tilde{q}_n(t) &= \big(\bar{\tau}(t/n^2) - V'(\tilde{q}_n - \tilde{q}_{n-1}))\big)\, dt + \sqrt{2T(1)}\, dw_n(t)
\end{aligned}
$$

For T constant and periodic boundary conditions, this is the **Ginzburg-Landau** model studied by *Guo-Papanicolaou-Varadhan* (CMP 2007), with relative entropy and Fisher informations bounds.

Previous results

- S.O., SRS Varadhan, HL for interacting Orstein-Uhlenbeck diffusion, CMP 1991. (Special tricks in $d = 1$.)
- C. Tremoulet, HL for interacting Orstein-Uhlenbeck particles, SPA 2002. The Yau's relative entropy method worked here because the stationary measures where of *equilibrium*.

Previous results

- S.O., SRS Varadhan, HL for interacting Orstein-Uhlenbeck diffusion, CMP 1991. (Special tricks in $d = 1$.)
- C. Tremoulet, HL for interacting Orstein-Uhlenbeck particles, SPA 2002. The Yau's relative entropy method worked here because the stationary measures where of *equilibrium*.

When a gradient of temperature is present, Yau's relative entropy method does not work: a big term of order n appears in the derivative of the relative entropy, related to the entropy production of the stationary states.
Entropic hypocoercivity provides the extension of the GPV techniques to this case.

Idea of the Proof

Why we need a bound on $I_q(t)$?

$$\frac{d}{dt}\left(\frac{1}{n}\sum_j G\left(j/n\right) r_j(t)\right) \sim \sum_j G'\left(j/n\right) p_j(t) + O(1/n)$$

$$\sim \frac{1}{n}\sum_j G''\left(j/n\right) V'(r_j(t)) \; + O(1/n)$$

$$= \frac{1}{n}\sum_j G''\left(j/n\right)\left(\frac{1}{2k}\sum_{|i-j|<k} V'(r_j(t))\right) + O'(k/n)$$

Idea of the Proof

Why we need a bound on $I_q(t)$?

$$\frac{d}{dt}\left(\frac{1}{n}\sum_j G(j/n)\, r_j(t)\right) \sim \sum_j G'(j/n)\, p_j(t) + O(1/n)$$

$$\sim \frac{1}{n}\sum_j G''(j/n)\, V'(r_j(t)) \; + O(1/n)$$

$$= \frac{1}{n}\sum_j G''(j/n)\left(\frac{1}{2k}\sum_{|i-j|<k} V'(r_j(t))\right) + O'(k/n)$$

main point is

$$\frac{1}{n}\sum_j G''(j/n)\,\tau\left(\frac{1}{2k}\sum_{|i-j|<k} r_j(t), T(j/n)\right) + O'(k/n)$$

as $N \to \infty$, $k = \epsilon N$, then $\epsilon \to 0$.

Local equilibrum by Fisher Informations

This can be achieved with the bound

$$\int_0^t ds \sum_{i=1}^n \int \frac{(\partial_{q_i} f_s)^2}{f_s} d\mu_{T(\cdot),0} \leq \frac{C}{n}$$

where the reference measure is the inhomogeneous Gibbs measure:

$$d\mu_{T(\cdot),0} = \prod_j e^{-T^{-1}(j/n)[p_j^2/2+V(r_j)]-\mathcal{G}(0,T(j/n))} dr_j dp_j$$

and f_s is the density wrt to $d\mu_{T(\cdot),0}$.

If $T(\cdot)$ is not constant, $d\mu_{T(\cdot),0}$ is NOT the stationary distribution!

Relative entropy

Typically

$$H_n(0) = \int f_0 \ln f_0 d\mu_{T(\cdot),0} \leq Cn$$

and since noise acts only on p's

$$\frac{d}{dt} H_n(t) = -\gamma n^2 \sum_{i=1}^{n} T(j/n) \int \frac{(\partial_{p_i} f_t)^2}{f_t} d\mu_{T(\cdot),0} + O(n)$$

Relative entropy

Typically

$$H_n(0) = \int f_0 \ln f_0 d\mu_{T(\cdot),0} \leq Cn$$

and since noise acts only on p's

$$\frac{d}{dt} H_n(t) = -\gamma n^2 \sum_{i=1}^{n} T(j/n) \int \frac{(\partial_{p_i} f_t)^2}{f_t} d\mu_{T(\cdot),0} + O(n)$$

$$\int_0^t ds \sum_{i=1}^{n} T(j/n) \int \frac{(\partial_{p_i} f_s)^2}{f_s} d\mu_{T(\cdot),0} \leq \frac{H_n(0)}{\gamma n^2} \leq \frac{C}{\gamma n}$$

Hypocoercive Fisher information

By the use of

$$I_n(t) = \sum_{i=1}^{n} T\left(\frac{j}{n}\right) \int \frac{\left[(\partial_{p_i} + \partial_{q_i}) f_t\right]^2}{f_t} d\mu_{T(\cdot),0}$$

$$\frac{d}{dt} I_n(t) = -\lambda n^2 I_n(t) + Cn$$

that implies $I_n(t) \leq \frac{C}{n}$ and consequently

$$\int_0^t ds \sum_{i=1}^{n} T\left(\frac{j}{n}\right) \int \frac{(\partial_{q_i} f_s)^2}{f_s} d\mu_{T(\cdot),0} \ \leq \ \frac{C}{n}$$

and the 1-block, 2-block estimates follows.

Possible extensions and open problems

- Viscosity depending on the distances between the nearest neighbor particles

$$\gamma = \gamma_i = \gamma(q_{i+1} - q_{i-1})$$

non-gradient dynamics. It shpould be possible to extend Varadhan's non-gradient techniques to this case, with the help of Hyporcoercivity.

Possible extensions and open problems

- Viscosity depending on the distances between the nearest neighbor particles

$$\gamma = \gamma_i = \gamma(q_{i+1} - q_{i-1})$$

  non-gradient dynamics. It shpould be possible to extend Varadhan's non-gradient techniques to this case, with the help of Hyporcoercivity.

- Open Problem: Poissonian noise, like thermalization by random independent renewal of velocities with gaussian distributed velocities with variance T_i:

$$Sf(q,p) = \sum_i \int \left(f(q,\tilde{p}^i) - f(q,p)\right) e^{-\tilde{p}_i^2/2T_i}\, d\tilde{p}_i$$

Possible extensions and open problems

- Viscosity depending on the distances between the nearest neighbor particles

$$\gamma = \gamma_i = \gamma(q_{i+1} - q_{i-1})$$

  non-gradient dynamics. It shpould be possible to extend Varadhan's non-gradient techniques to this case, with the help of Hyporcoercivity.

- Open Problem: Poissonian noise, like thermalization by random independent renewal of velocities with gaussian distributed velocities with variance T_i:

$$Sf(q,p) = \sum_i \int \left(f(q,\tilde{p}^i) - f(q,p)\right) e^{-\tilde{p}_i^2/2T_i}\, d\tilde{p}_i$$

- Noise with conservation laws (momentum, energy)

Non-Equilibrium Thermodynamics

We can use this results to construct *isothermal* transformations for *non-equilibrium thermodynamics*.

Non-Equilibrium Thermodynamics

We can use this results to construct *isothermal* transformations for *non-equilibrium thermodynamics*.
In usual (equilibrium) thermodynamics, equilibrium states are characterised by *temperature* and *tension*. Isothermal transformations connect two **equilibrium** states of same temperature T and different tensions τ_0, τ_1. This is done by changing the applied tension and keeping the system in contact with a heat bath at temperature T.

Non-Equilibrium Thermodynamics

We can use this results to construct *isothermal* transformations for *non-equilibrium thermodynamics*.
In usual (equilibrium) thermodynamics, equilibrium states are characterised by *temperature* and *tension*. Isothermal transformations connect two **equilibrium** states of same temperature T and different tensions τ_0, τ_1. This is done by changing the applied tension and keeping the system in contact with a heat bath at temperature T.
The 1st law says that

$$U(\tau_1) - U(\tau_0) = W + Q$$

–W work done during the trasformation
–Q heat (energy) exchanged with the thermostats

Non-Equilibrium Thermodynamics

Here we want to construct thermodynamic trasformations that connect two different *stationary non–equilibrium states*.
In this context a stationary state is characterized bay a value of tension τ_0, and a profile of temperatures $T(y), y \in [0,1]$.

Non-Equilibrium Thermodynamics

Here we want to construct thermodynamic trasformations that connect two different *stationary non–equilibrium states*.
In this context a stationary state is characterized bay a value of tension τ_0, and a profile of temperatures $T(y), y \in [0,1]$.
We keep $T(y)$ constant and we change the tension, performing work on the system.

Macroscopic Stationary State

$$\partial_t r(y,t) = \gamma^{-1}\partial_y^2 \tau(r(y,t), T(y))$$
$$\tau(r(1,t), T(1)) = \bar{\tau}(t),$$
$$\partial_y \tau(r(y,t), T(y))|_{y=0} = 0.$$

For $\tau(t) = \tau_0$ has the stationary profile $r_0(y)$ solution of:

$$\tau(r_0(y), T(y)) = \tau_0$$

Macroscopic Stationary State

$$\partial_t r(y,t) = \gamma^{-1}\partial_y^2 \tau(r(y,t), T(y))$$
$$\tau(r(1,t), T(1)) = \bar{\tau}(t),$$
$$\partial_y \tau(r(y,t), T(y))|_{y=0} = 0.$$

For $\tau(t) = \tau_0$ has the stationary profile $r_0(y)$ solution of:

$$\tau(r_0(y), T(y)) = \tau_0$$

Changing tension to $\tau(t) = \tau_1$ for $t > t_1$, it relaxes as $t \to \infty$, to the new stationary profile $r_1(y)$, solution of $\tau(r_1(y), T(y)) = \tau_1$.

Macroscopic Stationary State

$$\partial_t r(y,t) = \gamma^{-1}\partial_y^2 \tau(r(y,t), T(y))$$
$$\tau(r(1,t), T(1)) = \bar{\tau}(t),$$
$$\partial_y \tau(r(y,t), T(y))|_{y=0} = 0.$$

For $\tau(t) = \tau_0$ has the stationary profile $r_0(y)$ solution of:

$$\tau(r_0(y), T(y)) = \tau_0$$

Changing tension to $\tau(t) = \tau_1$ for $t > t_1$, it relaxes as $t \to \infty$, to the new stationary profile $r_1(y)$, solution of $\tau(r_1(y), T(y)) = \tau_1$.

In the equilibrium case, $T(y) = T$ constant, this is the irreversible isothermal thermodynamic trasformation.

Excess heat

Internal energy (average per particle):

$$U_n = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{p_i^2}{2} + V(r_i) \right)$$

Excess heat

Internal energy (average per particle):

$$U_n = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{p_i^2}{2} + V(r_i)\right)$$

$$U_n(t) - U_n(0) = W_n(t) + Q_n(t)$$

the work done is

$$W_n(t) = \frac{1}{n}\int_0^t \bar{\tau}(s)dq_n(s) = n\int_0^t \bar{\tau}(s)p_n(s)ds$$

and the energy exchanged with the thermostats is

$$Q_n(t) = \gamma\, n\sum_{j=1}^{n}\int_0^t \left(p_j^2(s) - T_j\right)ds + \sum_{j=1}^{n}\sqrt{2\gamma T_j}\int_0^t p_j(s)dw_i(s).$$

Excess Heat

A consequence of the hydrodynamic limit is the macroscopic work converges:

$$\lim_{n\to\infty} \mathcal{W}_n(t) = \int_0^t \bar{\tau}(s)\, d\mathcal{L}(s)$$

where $\mathcal{L}(t) = \int_0^1 r(x,t)dx = \lim_{n\to\infty} \frac{q_n(t)}{n}$, the total macroscopic length at time t.

Excess Heat

A consequence of the hydrodynamic limit is the macroscopic work converges:

$$\lim_{n\to\infty} \mathcal{W}_n(t) = \int_0^t \bar{\tau}(s) d\mathcal{L}(s)$$

where $\mathcal{L}(t) = \int_0^1 r(x,t)dx = \lim_{n\to\infty} \frac{q_n(t)}{n}$, the total macroscopic length at time t. Local equilibrium implies that:

$$\lim_{n\to\infty} (U_n(t) - U_n(0)) = \int_0^1 [u(\tau(r(x,t), T(x)), T(x)) - u(\tau_0, T(x))]\, dx$$

where $u(\tau, T)$ is the average energy for $\mu_{T,\tau}$, i.e.

$$u(\tau, T) = \int \mathcal{E}_1 d\mu^1_{\tau,T} = \frac{T}{2} + \int V(r) e^{-(V(r)-\tau r)/T - \tilde{\mathcal{G}}(\tau,T)} dr$$

with $\tilde{\mathcal{G}}(\tau, T) = \log \int e^{-(V(r)-\tau r)/T} dr$.

Excess Heat

After the limit $t \to \infty$ the macroscopic equation will reach the stationary state at tension τ_1, so that $u(\tau(r(x,t), T(x)), T(x)) \to u(\tau_1, T(x))$ and the difference of energies will became

$$\int_0^1 (u(\tau_1, T(x)) - u(\tau_0, T(x)))\, dx = \int_0^{+\infty} \bar{\tau}(s) d\mathcal{L}(s) ds + Q = \mathcal{W} + Q$$

This is the 1st principle.

Notice that $Q = \lim_{t\to\infty} \lim_n Q_n(t)$, is a deterministic quantity that we identify with *Heat*.

Free Energy, Clausius inequality

$$\mathcal{F}(r, T) = \sup_{\tau} \{\tau r - \mathcal{G}(\tau, T)\}$$

Free Energy, Clausius inequality

$$\mathcal{F}(r,T) = \sup_{\tau} \{\tau r - \mathcal{G}(\tau,T)\}$$

$$\widetilde{\mathcal{F}}(t) = \int_0^1 \mathcal{F}(r(x,t),T(x))dx$$

$$\widetilde{\mathcal{F}}_{ss}(\tau) = \int_0^1 \mathcal{F}(r_{ss,\tau}(x),T(x))dx$$

Free Energy, Clausius inequality

$$\mathcal{F}(r,T) = \sup_{\tau} \{\tau r - \mathcal{G}(\tau,T)\}$$

$$\widetilde{\mathcal{F}}(t) = \int_0^1 \mathcal{F}(r(x,t),T(x))dx$$

$$\widetilde{\mathcal{F}}_{ss}(\tau) = \int_0^1 \mathcal{F}(r_{ss,\tau}(x),T(x))dx$$

A straightforward calculation gives

$$\widetilde{\mathcal{F}}(t) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W}(t) - \gamma^{-1}\int_0^t ds \int_0^1 \left[\partial_x \tau(r(x,s),T(x))\right]^2 dx$$

after $t \to \infty$ this gives

$$\widetilde{\mathcal{F}}(\tau_1) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W} - \gamma^{-1}\int_0^\infty ds \int_0^1 \left[\partial_x \tau(r(x,s),T(x))\right]^2 dx$$

$$\geq \mathcal{W} \qquad \text{Clausius inequality}$$

Quasi-static limit: reversible isothermal trasformation

Very slow change of tension: $\bar{\tau}(\epsilon t)$
Then $\tilde{r}^\varepsilon(x,t) = r(x, \varepsilon^{-1} t)$ satisfies

$$\begin{cases} \partial_t \tilde{r}^\varepsilon(x,t) = \frac{1}{\epsilon\gamma} \partial_x^2 \tau(\tilde{r}^\varepsilon(x,t), T(x)) \qquad \text{for} \qquad x \in [0,1] \\ \partial_x \tau(\tilde{r}^\varepsilon(t,x), T(x))|_{x=0} = 0, \quad \tau(\tilde{r}^\varepsilon(t,x), T(x))|_{x=1} = \bar{\tau}(t), \quad t > 0 \\ \tau(\tilde{r}^\varepsilon(0,x), T(x)) = \tau_0, \quad x \in [0,1] \end{cases}$$

Quasi-static limit: reversible isothermal trasformation

Very slow change of tension: $\bar{\tau}(\epsilon t)$
Then $\tilde{r}^\varepsilon(x,t) = r(x, \varepsilon^{-1} t)$ satisfies

$$\begin{cases} \partial_t \tilde{r}^\varepsilon(x,t) = \frac{1}{\epsilon\gamma} \partial_x^2 \tau(\tilde{r}^\varepsilon(x,t), T(x)) \qquad \text{for} \qquad x \in [0,1] \\ \partial_x \tau(\tilde{r}^\varepsilon(t,x), T(x))|_{x=0} = 0, \quad \tau(\tilde{r}^\varepsilon(t,x), T(x))|_{x=1} = \bar{\tau}(t), \quad t > 0 \\ \tau(\tilde{r}^\varepsilon(0,x), T(x)) = \tau_0, \quad x \in [0,1] \end{cases}$$

$$\widetilde{\mathcal{F}}_{ss}(\tau_1) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W}^\varepsilon - \frac{1}{\epsilon\gamma} \int_0^{+\infty} dt \int_0^1 (\partial_x \tau(\tilde{r}^\varepsilon(x,t), T(x)))^2 \, dx$$

$$\xrightarrow[\varepsilon \to 0]{} \mathcal{W} \qquad \text{Clausius equality}$$

Quasi-static limit: reversible isothermal trasformation

Very slow change of tension: $\bar{\tau}(\epsilon t)$
Then $\tilde{r}^\varepsilon(x,t) = r(x, \varepsilon^{-1} t)$ satisfies

$$\begin{cases} \partial_t \tilde{r}^\varepsilon(x,t) = \frac{1}{\epsilon\gamma}\partial_x^2 \tau(\tilde{r}^\varepsilon(x,t), T(x)) \qquad \text{for} \qquad x \in [0,1] \\ \partial_x \tau(\tilde{r}^\varepsilon(t,x), T(x))|_{x=0} = 0, \quad \tau(\tilde{r}^\varepsilon(t,x), T(x))|_{x=1} = \bar{\tau}(t), \quad t > 0 \\ \tau(\tilde{r}^\varepsilon(0,x), T(x)) = \tau_0, \quad x \in [0,1] \end{cases}$$

$$\widetilde{\mathcal{F}}_{ss}(\tau_1) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W}^\varepsilon - \frac{1}{\epsilon\gamma}\int_0^{+\infty} dt \int_0^1 (\partial_x \tau(\tilde{r}^\varepsilon(x,t), T(x)))^2 \, dx$$

$$\xrightarrow[\varepsilon \to 0]{} \mathcal{W} \qquad \text{Clausius equality}$$

$$Q = \int_0^1 T(x) \left(S(r_{ss}(x,\tau_1), u_{ss}(x,\tau_1)) - S(r_{ss}(x,\tau_0), u_{ss}(x,\tau_0)) \right) dx$$

For the equilibrium: $Q = T\Delta S$.

Quasistatic Hydrodynamic limit

With Anna De Masi (JSP–2015).
This is a direct quasistatic limit. For $\alpha > 0$:

$$
\begin{aligned}
\dot{q}_j(t) &= n^{2+\alpha} p_j(t), \qquad j = 1, \dots, n, \\
dp_j(t) &= n^{2+\alpha} \left(V'(q_{j+1} - q_j) - V'(q_{j+1} - q_j) \right) dt \\
&\qquad - n^{2+\alpha} \gamma p_j(t) dt + n\sqrt{2\gamma T(j/n)} dw_j(t), \qquad j = 1, \dots, n-1, \\
dp_n(t) &= n^{2+\alpha} \left(\bar{\tau}(t) - V'(q_n - q_{n-1})) \right) dt \\
&\qquad - n^{2+\alpha} \gamma p_n(t) dt + n\sqrt{2\gamma T(1)} dw_n(t)
\end{aligned}
$$

Quasistatic Hydrodynamic limit

$$\frac{1}{n}\sum_j G\left(j/n\right) r_j(t) \underset{n\to\infty}{\longrightarrow} \int_0^1 G(y) r(y,t)\, dy$$

where $r(y,t)$ is the solution of the quasistatic equation

$$\tau(r(y,t), T(y)) = \bar{\tau}(t), \qquad y \in [0,1],\ t \geq 0$$

Quasistatic Hydrodynamics limit: thermodynamics

$$U_n(t) - U_n(0) = W_n(t) + Q_n(t)$$

the work done is

$$W_n(t) = \frac{1}{n}\int_0^t \bar{\tau}(s)dq_n(s) = n^{1+\alpha}\int_0^t \bar{\tau}(s)p_n(s)ds$$

$$Q_n(t) = \gamma\, n^{1+\alpha}\sum_{j=1}^n \int_0^t \left(p_j^2(s) - T_j\right) ds + n^{\alpha/2}\sum_{j=1}^n \sqrt{2\gamma T_j}\int_0^t p_j(s)dw_i(s).$$

Quasistatic Hydrodynamics limit: thermodynamics

$$U_n(t) - U_n(0) = W_n(t) + Q_n(t)$$

the work done is

$$W_n(t) = \frac{1}{n}\int_0^t \bar{\tau}(s)dq_n(s) = n^{1+\alpha}\int_0^t \bar{\tau}(s)p_n(s)ds$$

$$Q_n(t) = \gamma\, n^{1+\alpha}\sum_{j=1}^n \int_0^t \left(p_j^2(s) - T_j\right)ds + n^{\alpha/2}\sum_{j=1}^n \sqrt{2\gamma T_j}\int_0^t p_j(s)dw_i(s).$$

$$W_n(t) \to W(t) = \int_0^t \bar{\tau}(s)dL(s), \qquad L(t) = \int_0^1 r(y,t)dy.$$

$$Q_n(t) \to Q(t) = \int_0^1 \left[u(\bar{\tau}(t), T(y)) - u(\bar{\tau}(0), T(y))\right]dy - W(t)$$

Quasistatic Hydrodynamics limit: thermodynamics

$$\widetilde{\mathcal{F}}(t) = \int_0^1 \mathcal{F}(r(y,t), T(y))dy$$

A straightforward calculation gives directly the Clausius equality:

$$\widetilde{\mathcal{F}}(t) - \widetilde{\mathcal{F}}(0) = \int_0^t ds \int_0^1 dy \bar{\tau}(s)\partial_s r(y,s) = \int_0^t \bar{\tau}(s) d\mathcal{L}(s) = \mathcal{W}(t)$$

Quasistatic Hydrodynamics limit: thermodynamics

$$\widetilde{\mathcal{F}}(t) = \int_0^1 \mathcal{F}(r(y,t), T(y))dy$$

A straightforward calculation gives directly the Clausius equality:

$$\widetilde{\mathcal{F}}(t) - \widetilde{\mathcal{F}}(0) = \int_0^t ds \int_0^1 dy \bar{\tau}(s)\partial_s r(y,s) = \int_0^t \bar{\tau}(s) d\mathcal{L}(s) = \mathcal{W}(t)$$

and the relation of the (excess) heat in quasi static transformations

$$\int_0^1 dy T(y) \left(S(r(y,t), u(y,t)) - S(r(y,0), u(y,0))\right) = Q(t)$$

that for T constant is the familiar quasistatic relation:

$$\frac{dS}{dt} = \frac{1}{T}\frac{dQ}{dt}$$

Large Deviation for the Stationary Measure

For fixed tension τ, let $\mu^{\tau}_{n,ss}$ the corresponding stationary measure. A formal computation (not rigorous) gives, for a deviation to $r(u), u \in [0,1]$:

$$\frac{1}{n} \log \mu^{\tau}_{n,ss} \left(\frac{1}{n} \sum_i r_j \delta_{i/n} \sim r(\cdot) \right) \sim - \int_0^1 \mathfrak{V}(r(y); r_{ss}(y), T(y))\, dy$$

with

$$\mathfrak{V}(r; \bar{r}, T) = \mathcal{F}(r, T) - \mathcal{F}(\bar{r}, T) - \partial_r \mathcal{F}(\bar{r}, T)(r - \bar{r}).$$

same LDF as for the corresponding local Gibbs measure, no non-local term appears here.