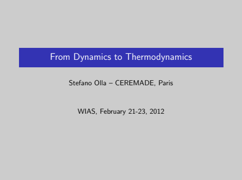
From Dynamics to Thermodynamics

Stefano Olla – CEREMADE, Paris

WIAS, February 21-23, 2012



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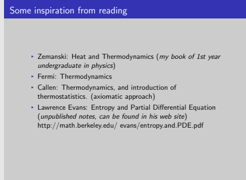
Some inspiration from reading

- Zemanski: Heat and Thermodynamics (*my book of 1st year undergraduate in physics*)
- Fermi: Thermodynamics
- Callen: Thermodynamics, and introduction of thermostatistics. (axiomatic approach)
- Lawrence Evans: Entropy and Partial Differential Equation (*unpublished notes, can be found in his web site*) http://math.berkeley.edu/ evans/entropy.and.PDE.pdf



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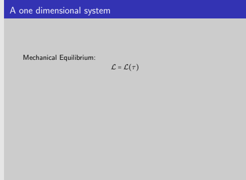
A one dimensional system

Mechanical Equilibrium:

$$\mathcal{L} = \mathcal{L}(\tau)$$



A one dimensional system
Mechanical Equilibrium:
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Draw picture bar, L, τ etc.

If a system A remains in equilibrium when isolated and placed in thermal contact first with system B and then with system C, the equilibrium of B and C will not be disturbed when they are placed in contact with each other.

Here *"remains in equilibrium"* means that $\mathcal{L}(\tau)$ does not change. We also use here the concept of *isolated system* and *thermal contact*, that require respectively the notion of adiabatic wall and conductive wall. The system A and B are separated by an *adiabatic wall* if they can have different equilibrium relation between $\mathcal{L}$ and $\mathcal{T}$. They are separated by a *conductive wall* if the must have the same equilibrium relation.

One could see all these as circular definition, in fact all this is equivalent as postulating the existence of adiabatic and diathermic (thermally conductive) walls that are defined as devices that have the above properties. From all this we obtain the existence of the parameter θ that we call temperature (see in Zemanski a very detailed discussion of this

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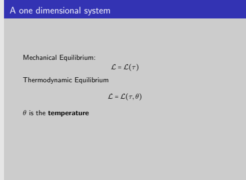
Thermodynamic Equilibrium

$$\mathcal{L} = \mathcal{L}(\tau, \theta)$$

θ is the **temperature**



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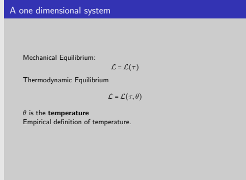

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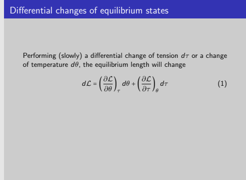
Differential changes of equilibrium states

Performing (slowly) a differential change of tension $d\tau$ or a change of temperature $d\theta$, the equilibrium length will change

$$d\mathcal{L} = \left(\frac{\partial \mathcal{L}}{\partial \theta}\right)_{\tau} d\theta + \left(\frac{\partial \mathcal{L}}{\partial \tau}\right)_{\theta} d\tau \qquad (1)$$



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One of the main issues in discussing foundations of thermodynamics is the physical meaning of these differential changes of *equilibrium* states. In principle, as we actually change the tension of the cable, the system will go into a sequence of non-equilibrium states before to relax to the new equilibrium. But, quoting Zemanski, *thermodynamics does not attempt to deal with any problem involving the rate at which the process takes place.* And, always quoting Zemanski:
Every infinitesimal in thermodynamics must satisfy the requirement that it represents a change in a quantity which is small with respect to the quantity itself and large in comparison with the effect produced by the behavior of few molecules.

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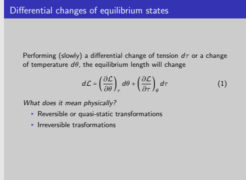
What does it mean physically?

- Reversible or quasi-static transformations
- Irreversible trasformations



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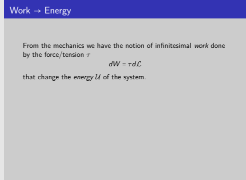

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So positive work, $dW > 0$, means the external force *tau* has done work nto the system and that energy of the system is increased.

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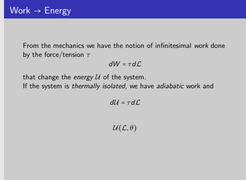

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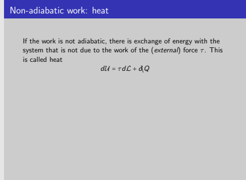
Non-adiabatic work: heat

If the work is not adiabatic, there is exchange of energy with the system that is not due to the work of the (*external*) force τ. This is called heat

$$d\mathcal{U} = \tau d\mathcal{L} + \text{đ}Q$$



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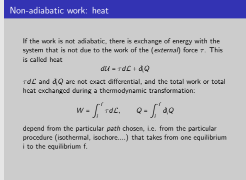

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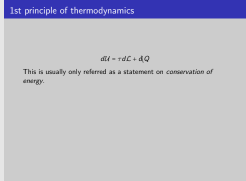

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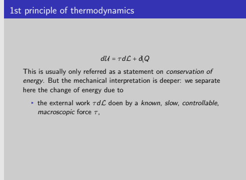

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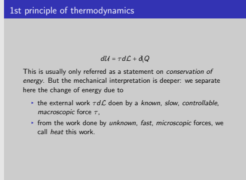

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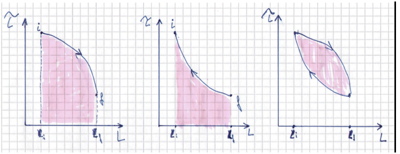
Thermodynamic transformations and Cycles

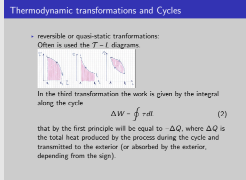
- reversible or quasi-static tranformations:
  Often is used the $\mathcal{T} - L$ diagrams.



In the third transformation the work is given by the integral along the cycle

$$\Delta W = \oint \tau dL \qquad (2)$$

that by the first principle will be equal to $-\Delta Q$, where ΔQ is the total heat produced by the process during the cycle and transmitted to the exterior (or absorbed by the exterior, depending from the sign).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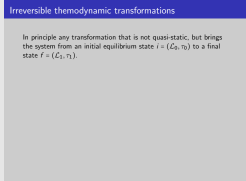
We can represent a finite thermodynamic transformation by integration along path of the differential forms defined above. Each choice of a path defines a different *thermodynamic process* or *quasi static* transformation. Depending on the type of transformation it may be interesting to make a different choice of the coordinates to represent it graphically. The first diagram on the left describe a quasi-static transformation for lenght L_i to L_f. If this is happening for example as a free expansion means that the tension $\mathcal{T}$ is decreasing, but it could be increasing if instead $\mathcal{T}$ is pulling with respect the mechanical equilibrium. The second diagram represent a compression from L_f to L_i, and the third a so called *cycle*, returning to the original state. The shaded area represent the work done during the transformation (taken with the negative sign in the second diagram).

Irreversible themodynamic transformations

In principle any transformation that is not quasi-static, but brings the system from an initial equilibrium state $i = (\mathcal{L}_0, \tau_0)$ to a final state $f = (\mathcal{L}_1, \tau_1)$.



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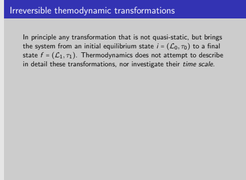

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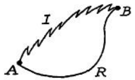
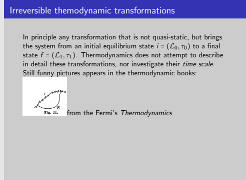


Fig. 11. from the Fermi's *Thermodynamics*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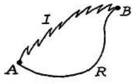

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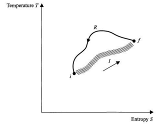
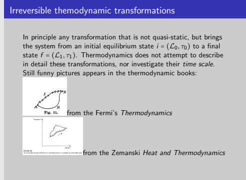


FIGURE 8-8
An irreversible process followed by a reversible process to complete an irreversible cycle. from the Zemanski *Heat and Thermodynamics*

From dynamics to thermodynamics
└─Thermodynamic crash course
 └─Irreversible themodynamic transformations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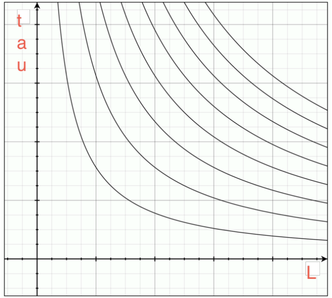
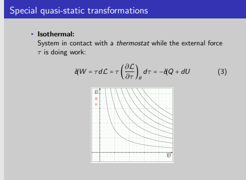
Special quasi-static transformations

- **Isothermal:**
  System in contact with a *thermostat* while the external force τ is doing work:

$$\text{đ}W = \tau d\mathcal{L} = \tau \left(\frac{\partial \mathcal{L}}{\partial \tau}\right)_\theta d\tau = -\text{đ}Q + dU \tag{3}$$

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While a force perform work on the system, this is in contact with a *thermostat*, a **huge** system in equilibrium at a given temperature θ, so big that the exchange of heat with our elastic does not perturb the equilibrium state of the thermostat. Ideally a thermostat is an infinite system. During a isothermal transformation only the length $\mathcal{L}$ changes as effect of the change of the tension $d\mathcal{T}$, and the infinitesimal exchanges of heat and work are related by (**??**).
The isothermal transformations defines isothermal lines parametrized by the temperature (each temperature defines an isothermal line in the $\tau - \mathcal{L}$ plane.

Special quasi–static Transformations

- **Adiabatic:** $\text{đ}Q = 0$.

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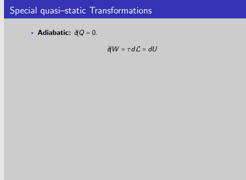

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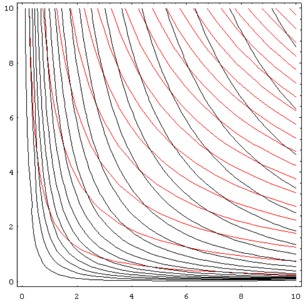
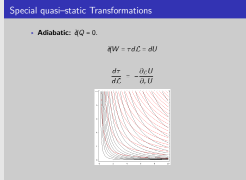
$$\frac{d\tau}{d\mathcal{L}} = -\frac{\partial_{\mathcal{L}} U}{\partial_{\tau} U}$$



2012-03-18

From dynamics to thermodynamics
└Thermodynamic crash course
└Special quasi–static Transformations



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- **Isocore**: Thermodynamic transformation at fixed length $\mathcal{L}$. Consequently $đW = 0$, no work if perfomed to or by the system, and
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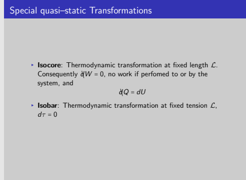

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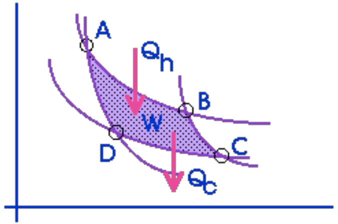
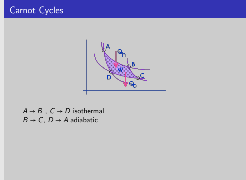
Carnot Cycles



$A \to B$, $C \to D$ isothermal
$B \to C$, $D \to A$ adiabatic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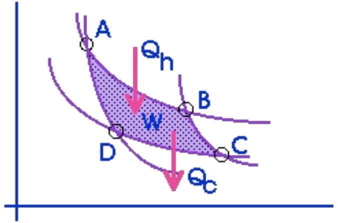

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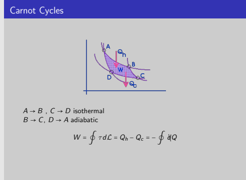
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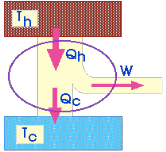

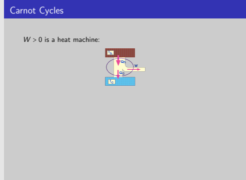

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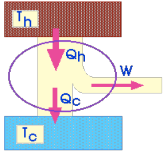

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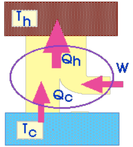

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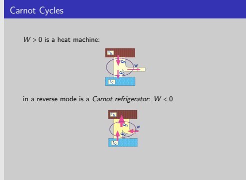
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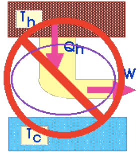
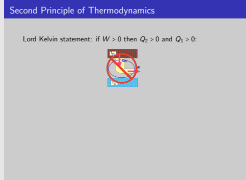
Second Principle of Thermodynamics

Lord Kelvin statement: if $W > 0$ then $Q_2 > 0$ and $Q_1 > 0$:

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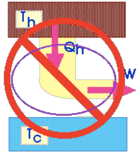
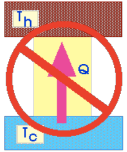
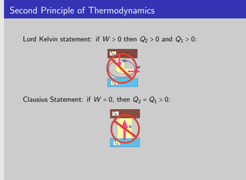


Clausius Statement: if $W = 0$, then $Q_2 = Q_1 > 0$:

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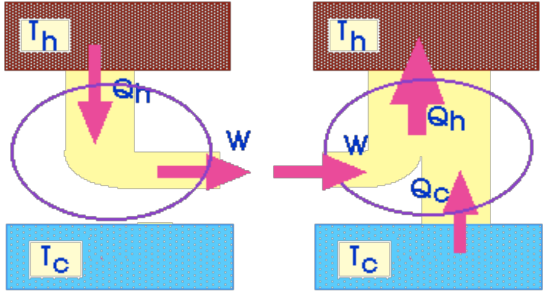
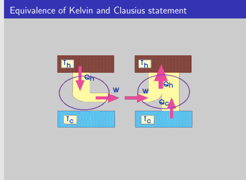
Equivalence of Kelvin and Clausius statement



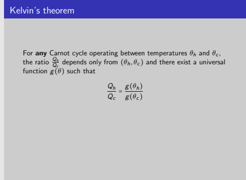

Equivalence of Kelvin and Clausius statement

if Kelvin statement is not true, we would contradict Clausius, we could use a perfectly efficient carnot machine to make work on another reversible Carnot machine and obtain just transfer of heat from cold to warm.

Kelvin's theorem

For **any** Carnot cycle operating between temperatures θ_h and θ_c, the ratio $\frac{Q_h}{Q_c}$ depends only from (θ_h, θ_c) and there exist a universal function $g(\theta)$ such that

$$\frac{Q_h}{Q_c} = \frac{g(\theta_h)}{g(\theta_c)}$$



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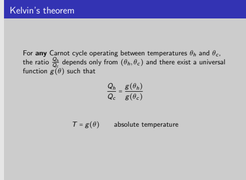

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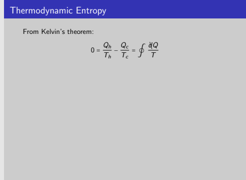
From Kelvin's theorem:

$$0 = \frac{Q_h}{T_h} - \frac{Q_c}{T_c} = \oint \frac{\text{đ}Q}{T}$$



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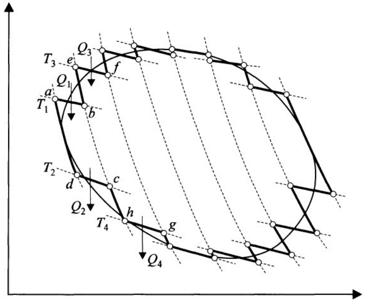

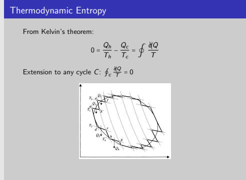
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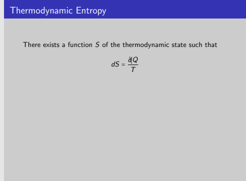

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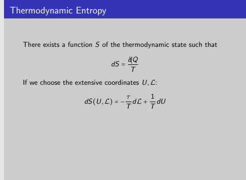

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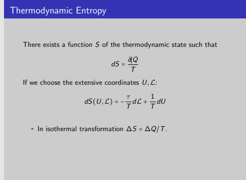

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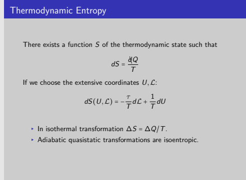

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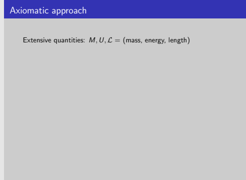
Extensive quantities: $M, U, \mathcal{L} =$ (mass, energy, length)



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We can proceed differently and make a more mathematical set-up of the thermodynamics with an axiomatic approach where the extensive quantities $U, \mathcal{L}$ are taken as basic thermodynamic coordinates to identify an equilibrium state and entropy is assumed as a state function satisfying certain properties.
It is convenient in this context to add another macroscopic extensive parameter $M > 0$ that represent the *mass* of the system. This function S contains all the informatuon about the *thermodynamics* of the system.

One can proceed in inverse way as before and construct Carnot cycles and deduce Kelvin or the equivalent Clausius statement of the second law.

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There exist an open cone set $\Gamma \subset \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R}$, and $(M, U, \mathcal{L}) \in \Gamma$.
There exists a C^1–function

$$S(M, U, \mathcal{L}) : \Gamma \to \mathbb{R}$$

such that

- S is concave,
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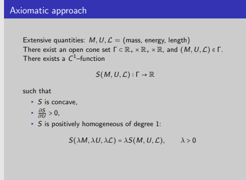

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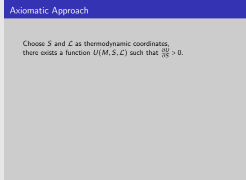

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$$T = \frac{\partial U}{\partial S} \qquad \text{temperature}$$

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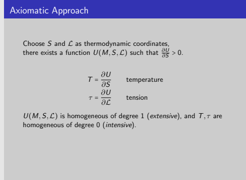
$U(M,S,\mathcal{L})$ is homogeneous of degree 1 (*extensive*), and T,τ are homogeneous of degree 0 (*intensive*).



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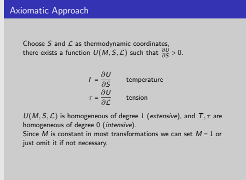

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Irreversible Transformations

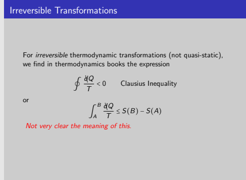
For *irreversible* thermodynamic transformations (not quasi-static), we find in thermodynamics books the expression

$$\oint \frac{\text{đ}Q}{T} < 0 \qquad \text{Clausius Inequality}$$

or

$$\int_A^B \frac{\text{đ}Q}{T} \leq S(B) - S(A)$$

Not very clear the meaning of this.



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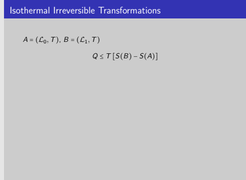
Of course there is a huge literature on this, see Evans notes for a short review.

Isothermal Irreversible Transformations

$$A = (\mathcal{L}_0, T), \; B = (\mathcal{L}_1, T)$$

$$Q \leq T\,[S(B) - S(A)]$$



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For an isothermal transformation, it is more clear what it means that it is irreversible. The system it is always in contact to a thermostat at temperature T and during the transformation it exchange the heat Q with it. Going from the state A to the state B, this implies that A and B are at the same temperature. It is convenient here to use $(\mathcal{L}, T)$ as thermodynamic coordinates

This is an upper bound of the amount of heat that can be exchanged during any quasi static isothermal transformation.this is a limit about the amount of work that can be obtained from such transformation. It is then interesting to define the *free energy* $F(\mathcal{L}, T)$ as

Isothermal Irreversible Transformations

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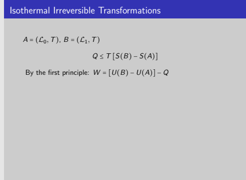
By the first principle: $W = [U(B) - U(A)] - Q$



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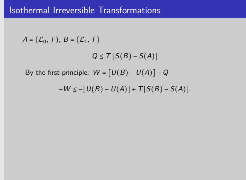

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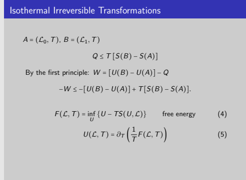

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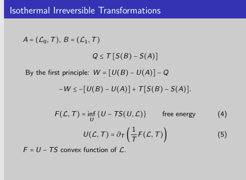

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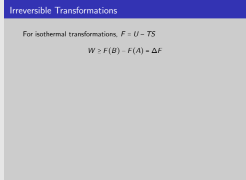

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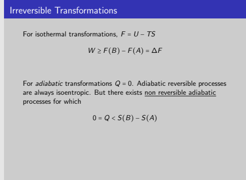

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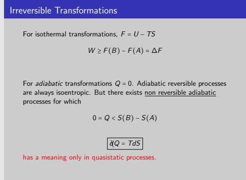

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Extended thermodynamics

Two systems: $(M_1, U_1, \mathcal{L}_1)$, $(M_2, U_2, \mathcal{L}_2)$.
If attached they are **not in equilibrium**.
We can define the total entropy as

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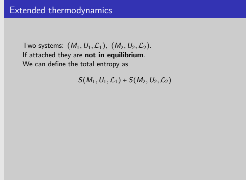

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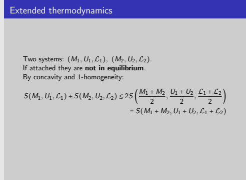

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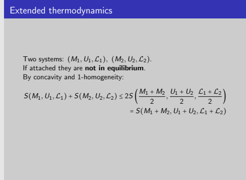

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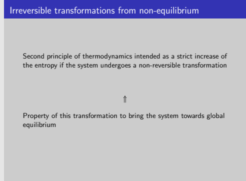
Irreversible transformations from non-equilibrium

Second principle of thermodynamics intended as a strict increase of the entropy if the system undergoes a non-reversible transformation

$$\Uparrow$$

Property of this transformation to bring the system towards global equilibrium



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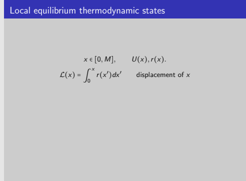

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By successive partition, we can go to a continuous description where at each material point x is associated a system in equilibrium at energy $U(x)$ and lenght (stretch) $r(x)$

Usual thermodynamics does not worry about time scales where the thermodynamic processes happens. But in the extended thermodynamics we can consider time evolutions of these profiles (typically evolving following some partial differential equations). The actual time scale in which these evolution occurs with respect to the microscopic dynamivcs of the atoms, will be the subject of the hydrodynamic limits that we will study in the later chapters.

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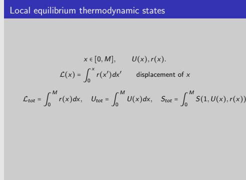

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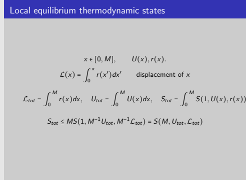

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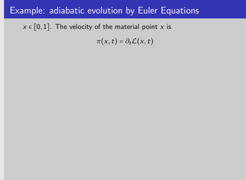

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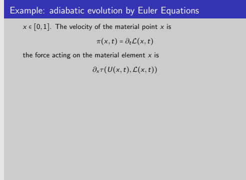

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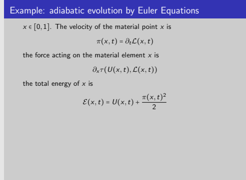

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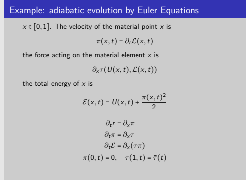

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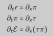

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In the smooth regime the evolution is isoentropic in the sense...
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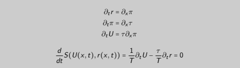

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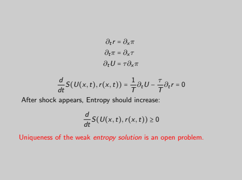

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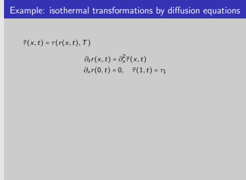
Example: isothermal transformations by diffusion equations

$$\bar{\tau}(x,t) = \tau(r(x,t), T)$$

$$\begin{aligned} \partial_t r(x,t) &= \partial_x^2 \bar{\tau}(x,t) \\ \partial_x r(0,t) &= 0, \quad \bar{\tau}(1,t) = \tau_1 \end{aligned}$$



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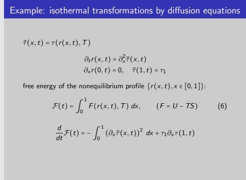

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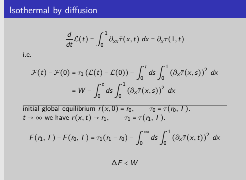

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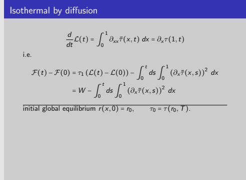

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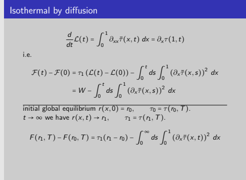

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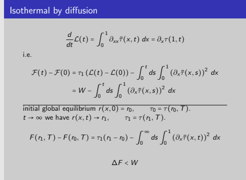

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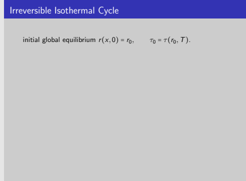

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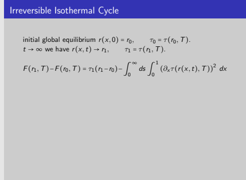

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$r(x,0) = r_1, \qquad \tau_1 = \tau(r_1, T)$,
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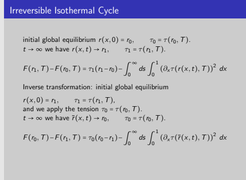

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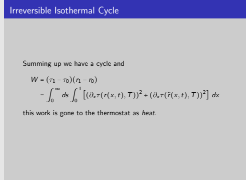

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Reversible quasi static isothermal transformation

Pull slowly: $\bar{\tau}(t)$ smooth and $\bar{\tau}(0) = \tau_0$, $\bar{\tau}(1) = \tau_1$

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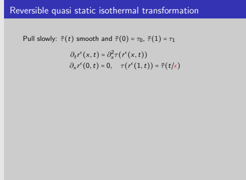

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In order to obtain the reversible (quasi static) transformation, we need to push or pool very slowly, with a tension $\bar{\tau}(t/\epsilon)$ with $\bar{\tau}$ that goes smoothly from τ_0 to τ_1.

then we have to wait an infinite time in this diffusive time scale, then still rescale time to slow down, and we obtain the reversible transformation where work done is equal to the change in free energy!

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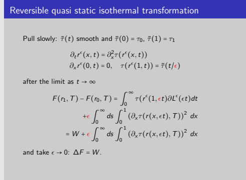

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Local Central Limit Theorem

Theorem

$\nu(d\mathbf{x})$ centered probability on $\mathbb{R}^r$, $\sigma^2 < \infty$
$\phi(\mathbf{k})$ its characteristic function,

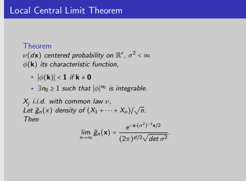
- $|\phi(\mathbf{k})| < \mathbf{1}$ *if* $\mathbf{k} \neq \mathbf{0}$
- $\exists n_0 \geq 1$ *such that* $|\phi|^{n_0}$ *is integrable.*

X_j i.i.d. with common law ν,
Let $\tilde{g}_n(x)$ density of $(X_1 + \cdots + X_n)/\sqrt{n}$.
Then

$$\lim_{n\to\infty} \tilde{g}_n(\mathbf{x}) = \frac{e^{-\mathbf{x}\cdot(\sigma^2)^{-1}\mathbf{x}/2}}{(2\pi)^{d/2}\sqrt{\det \sigma^2}}.$$

2012-03-18

From dynamics to thermodynamics
└Statistical Mechanics
  └preliminaries: the art of tilting
    └Local Central Limit Theorem



Local Central Limit Theorem

Theorem
$\nu(d\mathbf{x})$ centered probability on $\mathbb{R}^r$, $\sigma^2 < \infty$
$\phi(\mathbf{k})$ its characteristic function,
- $|\phi(\mathbf{k})| < \mathbf{1}$ if $\mathbf{k} \neq \mathbf{0}$
- $\exists n_0 \geq 1$ such that $|\phi|^{n_0}$ is integrable.

X_j i.i.d. with common law ν,
Let $\tilde{g}_n(x)$ density of $(X_1 + \cdots + X_n)/\sqrt{n}$.
Then
$$\lim_{n\to\infty} \tilde{g}_n(\mathbf{x}) = \frac{e^{-\mathbf{x}\cdot(\sigma^2)^{-1}\mathbf{x}/2}}{(2\pi)^{d/2}\sqrt{\det \sigma^2}}.$$

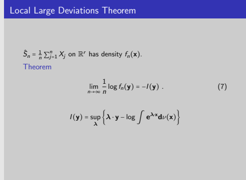
Local Large Deviations Theorem

$\hat{S}_n = \frac{1}{n}\sum_{j=1}^{n} X_j$ on $\mathbb{R}^r$ has density $f_n(\mathbf{x})$.

Theorem

$$\lim_{n\to\infty} \frac{1}{n} \log f_n(\mathbf{y}) = -I(\mathbf{y}) \ . \tag{7}$$

$$I(\mathbf{y}) = \sup_{\boldsymbol{\lambda}} \left\{ \boldsymbol{\lambda}\cdot\mathbf{y} - \log \int \mathbf{e}^{\boldsymbol{\lambda}\cdot\mathbf{x}} \mathbf{d}\nu(\mathbf{x}) \right\}$$



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Proof.

$$f_n(x,y) = \frac{e^{n(x+y)\lambda}}{M(\lambda)^n} f_n(x+y) = e^{n(I(y)+\lambda x)} f_n(x+y)$$

It follows that

$$f_n(y) = e^{-nI(y)} f_n(0,y)$$

☐

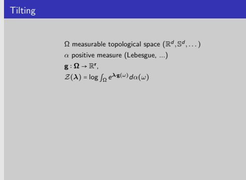
Tilting

Ω measurable topological space $(\mathbb{R}^d, \mathbb{S}^d, \dots)$

α positive measure (Lebesgue, ...)

$\mathbf{g} : \boldsymbol{\Omega} \to \mathbb{R}^{\mathbf{r}}$,

$\mathcal{Z}(\boldsymbol{\lambda}) = \log \int_\Omega e^{\boldsymbol{\lambda}\cdot\mathbf{g}(\omega)} d\alpha(\omega)$



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$\mathcal{Z}(\boldsymbol{\lambda})$ is convex and lower semicontinuous (it maybe not continuous). Again strict convexity follows by assuming that every component of $\mathbf{g}$ is not constant. Furthermore $\mathcal{D}_{\mathcal{Z}}$ is convex.

The Fenchel-Legendre transform is now defined by

With respect to $\alpha_{\boldsymbol{\lambda}}$, $\mathbf{g}$ can be seen as a vector valued random variable with average $\nabla\mathcal{Z}(\boldsymbol{\lambda})$ and covariance matrix $\mathrm{Hess}\mathcal{Z}(\boldsymbol{\lambda}) = \nabla^2\mathcal{Z}(\boldsymbol{\lambda})$. Also now $\mathrm{Hess}\mathcal{Z}(\boldsymbol{\lambda}) > 0$ just because $\mathbf{g}$ is not constant.

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$$\bar{\mathbf{x}} = \nabla\mathcal{Z}(\bar{\boldsymbol{\lambda}})$$
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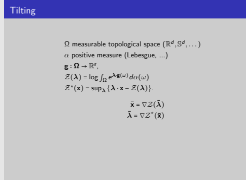

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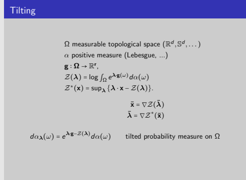
$d\alpha_{\boldsymbol{\lambda}}(\omega) = e^{\boldsymbol{\lambda}\cdot\mathbf{g} - \mathcal{Z}(\boldsymbol{\lambda})} d\alpha(\omega)$ tilted probability measure on Ω



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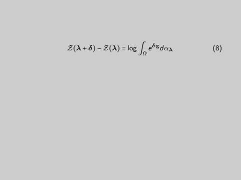
$$\mathcal{Z}(\boldsymbol{\lambda}+\boldsymbol{\delta}) - \mathcal{Z}(\boldsymbol{\lambda}) = \log \int_{\Omega} e^{\boldsymbol{\delta}\cdot\mathbf{g}} d\alpha_{\boldsymbol{\lambda}} \tag{8}$$



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In particular notice that the rate function $I_{\boldsymbol{\lambda}}(\mathbf{x})$ corresponding to the tilted measure $\alpha_{\boldsymbol{\lambda}}$ is given by

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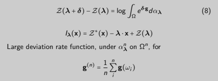
$$I_{\boldsymbol{\lambda}}(\mathbf{x}) = \mathcal{Z}^*(\mathbf{x}) - \boldsymbol{\lambda}\cdot\mathbf{x} + \mathcal{Z}(\boldsymbol{\lambda})$$

Large deviation rate function, under $\alpha_{\boldsymbol{\lambda}}^n$ on Ω^n, for

$$\mathbf{g}^{(n)} = \frac{1}{n}\sum_i^n \mathbf{g}(\omega_i)$$



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Conditioning

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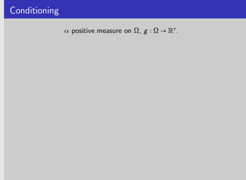

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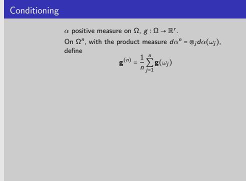
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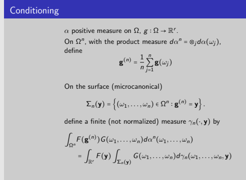
On the surface (microcanonical)

$$\Sigma_n(\mathbf{y}) = \left\{ (\omega_1, \dots, \omega_n) \in \Omega^n : \mathbf{g}^{(n)} = \mathbf{y} \right\}.$$

define a finite (not normalized) measure $\gamma_n(\cdot, \mathbf{y})$ by

$$\int_{\Omega^n} F(\mathbf{g}^{(n)}) G(\omega_1, \dots, \omega_n) d\alpha^n(\omega_1, \dots, \omega_n)$$

$$= \int_{\mathbb{R}^r} F(\mathbf{y}) \int_{\Sigma_n(\mathbf{y})} G(\omega_1, \dots, \omega_n) d\gamma_n(\omega_1, \dots, \omega_n, \mathbf{y})$$



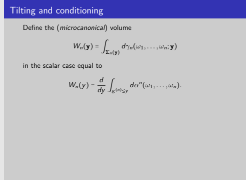
Tilting and conditioning

Define the (*microcanonical*) volume

$$W_n(\mathbf{y}) = \int_{\Sigma_n(\mathbf{y})} d\gamma_n(\omega_1, \dots, \omega_n; \mathbf{y})$$

in the scalar case equal to

$$W_n(y) = \frac{d}{dy} \int_{g^{(n)} \le y} d\alpha^n(\omega_1, \dots, \omega_n).$$



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Under $\alpha^n_{\boldsymbol{\lambda}}$, $\mathbf{g}^{(n)} = \sum_j g(\omega_j)/n$ has probability density

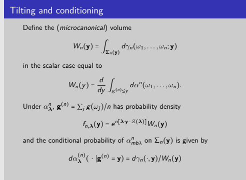
$$f_{n,\boldsymbol{\lambda}}(\mathbf{y}) = e^{n[\boldsymbol{\lambda} \cdot \mathbf{y} - \mathcal{Z}(\boldsymbol{\lambda})]} W_n(\mathbf{y})$$

and the conditional probability of $\alpha^n_{mb\lambda}$ on $\Sigma_n(\mathbf{y})$ is given by

$$d\alpha^{(n)}_{\boldsymbol{\lambda}}(\,\cdot\,|\mathbf{g}^{(n)} = \mathbf{y}) = d\gamma_n(\cdot, \mathbf{y})/W_n(\mathbf{y})$$

2012-03-18

From dynamics to thermodynamics
└Statistical Mechanics
  └preliminaries: the art of tilting
    └Tilting and conditioning



Boltzmann formula

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that imply

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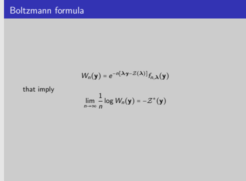

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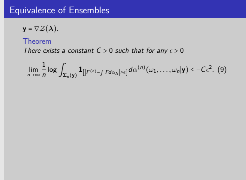
Equivalence of Ensembles

$\mathbf{y} = \nabla \mathcal{Z}(\boldsymbol{\lambda}).$

Theorem

There exists a constant $C > 0$ *such that for any* $\epsilon > 0$

$$\lim_{n\to\infty}\frac{1}{n}\log\int_{\Sigma_n(\mathbf{y})}\mathbf{1}_{[|F^{(n)}-\int F d\alpha_{\boldsymbol{\lambda}}|\ge\epsilon]}d\alpha^{(n)}(\omega_1,\dots,\omega_n|\mathbf{y}) \le -C\epsilon^2. \tag{9}$$



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Along these line, with a bit more work one can prove the following convergence on conditional measure to the unconditioned oneThis include the so-called Poincare lemma (even though Poncare had nothing to do with this statement, that goes back to Maxwell): Choose $\Omega = \mathbb{R}$ and $g(x) = x^2$. The uniform measure on the n-dimensional sphere with radius $\sqrt{n}$ converges, in terms of the finite dimensional distributions, to the product of gaussian measures $e^{-x_i^2/2}/\sqrt{2\pi}$.

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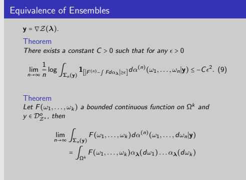
Theorem

Let $F(\omega_1, \dots, \omega_k)$ a bounded continuous function on Ω^k and $y \in \mathcal{D}^o_{\mathcal{Z}^*}$, then

$$\begin{aligned}\lim_{n\to\infty} \int_{\Sigma_n(\mathbf{y})} & F(\omega_1, \dots, \omega_k) d\alpha^{(n)}(\omega_1, \dots, d\omega_n | \mathbf{y}) \\ &= \int_{\Omega^k} F(\omega_1, \dots, \omega_k) \alpha_{\boldsymbol{\lambda}}(d\omega_1) \dots \alpha_{\boldsymbol{\lambda}}(d\omega_k)\end{aligned}$$



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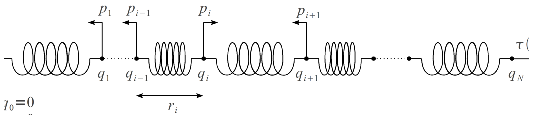
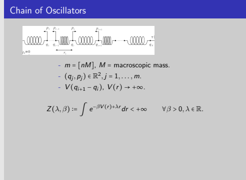
Chain of Oscillators



- $m = [nM]$, M = macroscopic mass.
- $(q_j, p_j) \in \mathbb{R}^2, j = 1, \dots, m.$
- $V(q_{i+1} - q_i)$, $V(r) \to +\infty.$

$$Z(\lambda, \beta) := \int e^{-\beta V(r) + \lambda r} dr < +\infty \qquad \forall \beta > 0, \lambda \in \mathbb{R}.$$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We study a system of $m = [nM]$ anharmonic oscillators, where $M > 0$ is a positive parameter corresponding to the macroscopic mass of the total system. The particles are denoted by $j = 1, \dots m$. We denote with $q_j, j = 1, \dots, m$ their positions, and with p_j the corresponding momentum (which is equal to its velocity since we assume that all particles have mass 1). We consider first the system attached to a *wall*, and we set $q_0 = 0, p_0 = 0$. Between each pair of consecutive particles $(i, i+1)$ there is an anharmonic spring described by its potential energy $V(q_{i+1} - q_i)$. We assume V is a positive smooth function such that $V(r) \to +\infty$ as $|r| \to \infty$ and such that It is convenient to work with interparticle distance as coordinates, rather than absolute particle position, so we define $\{r_j = q_j - q_{j-1} - a, \ j = 1, \dots, m\}$.

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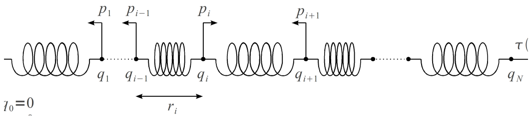

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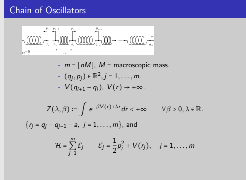
$$\mathcal{H} = \sum_{j=1}^{m} \mathcal{E}_j \qquad \mathcal{E}_j = \frac{1}{2} p_j^2 + V(r_j), \quad j = 1, \dots, m$$



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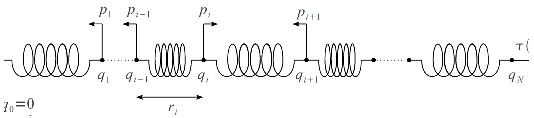

Isobar Dynamics:

$$
\begin{aligned}
\dot r_j(t) &= p_j(t) - p_{j-1}(t), \qquad j = 1, \dots, m,\\
\dot p_j(t) &= V'(r_{j+1}(t)) - V'(r_j(t)), \qquad j = 1, \dots, m-1,\\
\dot p_m(t) &= \tau - V'(r_m(t)),
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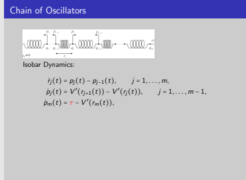

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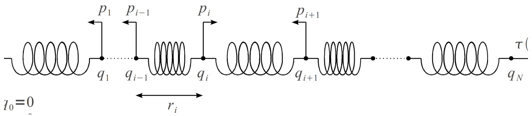
At the other end of the chain we apply a constant force $\tau \in \mathbb{R}$ on the particle n (tension). The position of the particle m is given by $q_n = \sum_{j=1}^m r_j$. We consider the isobar Hamiltonian dynamics:

Chain of Oscillators



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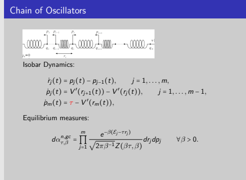
$$\begin{aligned}\dot r_j(t) &= p_j(t) - p_{j-1}(t), \qquad j = 1,\dots,m,\\ \dot p_j(t) &= V'(r_{j+1}(t)) - V'(r_j(t)), \qquad j = 1,\dots,m-1,\\ \dot p_m(t) &= \tau - V'(r_m(t)),\end{aligned}$$

Equilibrium measures:

$$d\alpha^{n,gc}_{\tau,\beta} = \prod_{j=1}^{m} \frac{e^{-\beta(\mathcal{E}_j - \tau r_j)}}{\sqrt{2\pi\beta^{-1}}Z(\beta\tau,\beta)} dr_j dp_j \qquad \forall \beta > 0.$$



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Microcanonical surface: $M > 0, U > 0, \mathcal{L} \in \mathbb{R}$,

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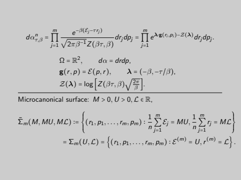

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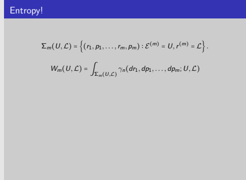

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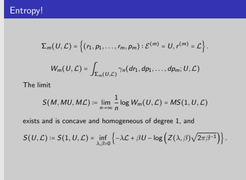

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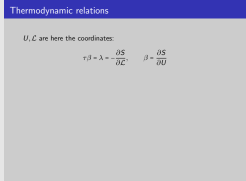
Thermodynamic relations

$U, \mathcal{L}$ are here the coordinates:

$$\tau\beta = \lambda = -\frac{\partial S}{\partial \mathcal{L}}, \qquad \beta = \frac{\partial S}{\partial U}$$



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They can be inverted:

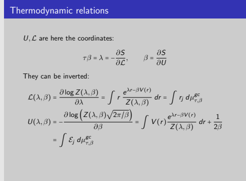
$$\mathcal{L}(\lambda,\beta) = \frac{\partial \log Z(\lambda,\beta)}{\partial \lambda} = \int r \, \frac{e^{\lambda r - \beta V(r)}}{Z(\lambda,\beta)} \, dr = \int r_j \, d\mu^{gc}_{\tau,\beta}$$

$$U(\lambda,\beta) = -\frac{\partial \log\left(Z(\lambda,\beta)\sqrt{2\pi/\beta}\right)}{\partial \beta} = \int V(r) \frac{e^{\lambda r - \beta V(r)}}{Z(\lambda,\beta)} \, dr + \frac{1}{2\beta}$$

$$= \int \mathcal{E}_j \, d\mu^{gc}_{\tau,\beta}$$

2012-03-18

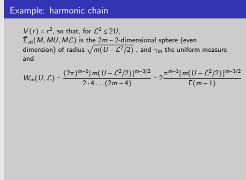
From dynamics to thermodynamics
└Statistical Mechanics
  └The microscopic model: chain of anharmonic oscillators
    └Thermodynamic relations



Example: harmonic chain

$V(r) = r^2$, so that, for $\mathcal{L}^2 \leq 2U$,
$\tilde{\Sigma}_m(M, MU, M\mathcal{L})$ is the $2m-2$-dimensional sphere (even dimension) of radius $\sqrt{m(U - \mathcal{L}^2/2)}$, and γ_m the uniform measure and

$$W_m(U, \mathcal{L}) = \frac{(2\pi)^{m-1}[m(U-\mathcal{L}^2/2)]^{m-3/2}}{2\cdot 4 \dots (2m-4)} = 2\frac{\pi^{m-1}[m(U-\mathcal{L}^2/2)]^{m-3/2}}{\Gamma(m-1)}$$



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Entropy depends only on the temperature in the harmonic chain!
Free energy depends on the lenght only through the internal energy, so $\mathcal{L}$ is the thermodynamic force (the derivative of the free energy F with respect to the lenght $\mathcal{L}$), not influenced by temperature.

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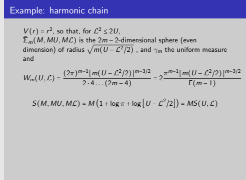

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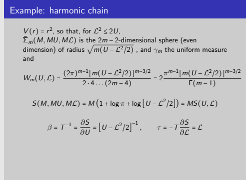

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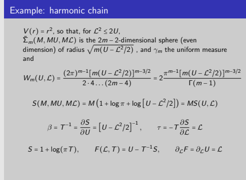

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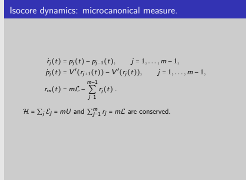

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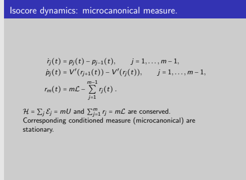

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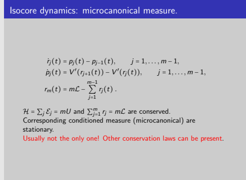

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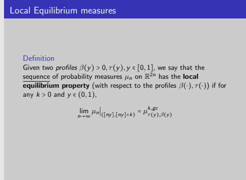
Local Equilibrium measures

Definition

Given two *profiles* $\beta(y) > 0, \tau(y), y \in [0,1]$, we say that the sequence of probability measures μ_n on $\mathbb{R}^{2n}$ has the **local equilibrium property** (with respect to the profiles $\beta(\cdot), \tau(\cdot)$) if for any $k > 0$ and $y \in (0,1)$,

$$\lim_{n\to\infty} \mu_n\big|_{([ny],[ny]+k)} = \mu^{k,gc}_{\tau(y),\beta(y)}$$



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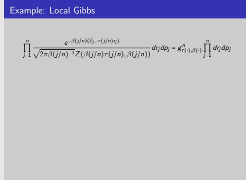
The Gibbs distributions defined in the above sections are also called equilibrium distributions for the dynamics. Studying the non-equilibrium behaviour we need the concept of local equilibrium distributions. These are probability distributions that have some asymptotic properties when the system became large ($n \to \infty$), vaguely speaking *locally* they look like Gibbs measure. We need a precise mathematical definition, that will be useful later for proving macroscopic behaviour of the system.
Sometimes we will need some weaker definition of local equilibrium (for example relaxing the pointwise convergence in y).

It is important here to understand that *local equilibrium* is a property of a *sequence* of probability measures.

Example: Local Gibbs

$$\prod_{j=1}^{n} \frac{e^{-\beta(j/n)(\mathcal{E}_j-\tau(j/n)r_j)}}{\sqrt{2\pi\beta(j/n)^{-1}}\,Z(\beta(j/n)\tau(j/n),\beta(j/n))}\, dr_j dp_j = g^n_{\tau(\cdot),\beta(\cdot)} \prod_{j=1}^{n} dr_j dp_j$$



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The most simple example of local equilibrium sequence is given by the local Gibbs measures:

Of course are local equilibrium sequence also *small order* perturbation of this sequence like

1st order corrections are very important to understand heat conduction and other phenomenaOf course we do not have a Boltzmann's formula for this entropy. The search of a Boltzmann formula out of equilibrium is a long story...

The question is: do we need a Boltzmann formula out of equilibrium?

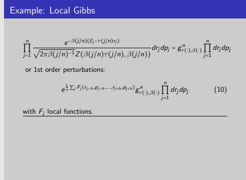
Example: Local Gibbs

$$\prod_{j=1}^{n} \frac{e^{-\beta(j/n)(\mathcal{E}_j-\tau(j/n)r_j)}}{\sqrt{2\pi\beta(j/n)^{-1}}Z(\beta(j/n)\tau(j/n),\beta(j/n))} dr_j dp_j = g^n_{\tau(\cdot),\beta(\cdot)} \prod_{j=1}^{n} dr_j dp_j$$

or 1st order perturbations:

$$e^{\frac{1}{n}\sum_j F_j(r_{j-h},p_{j-h},\dots,r_{j+h},p_{j+h})} g^n_{\tau(\cdot),\beta(\cdot)} \prod_{j=1}^{n} dr_j dp_j \tag{10}$$

with F_j local functions.



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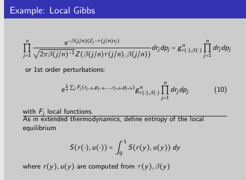

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Isothermal dynamics

Langevin thermostats in each site:

$$
\begin{aligned}
\dot{r}_j(t) &= p_j(t) - p_{j-1}(t), \qquad j = 1, \dots, n, \\
dp_j(t) &= \big(V'(r_{j+1}(t)) - V'(r_j(t))\big)\, dt - p_j(t)dt + \sqrt{\beta}dw_j(t), \\
&\qquad\qquad\qquad\qquad j = 1, \dots, n-1, \\
dp_n(t) &= \big(\tau_1 - V'(r_n(t))\big)\, dt - p_n(t)dt + \sqrt{\beta}dw_n(t)
\end{aligned}
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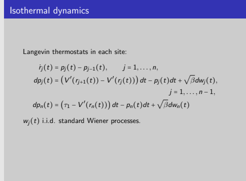
$w_j(t)$ i.i.d. standard Wiener processes.



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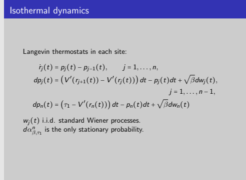
$d\alpha^n_{\beta,\tau_1}$ is the only stationary probability.



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└Statistical Mechanics
  └Isothermal dynamics
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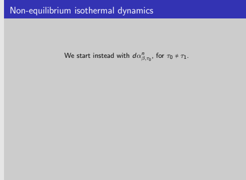

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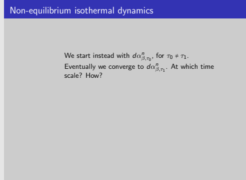

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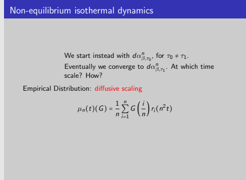

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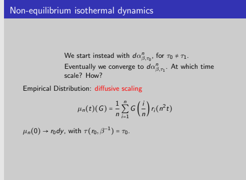

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Isothermal diffusion limit

Theorem

$$\frac{1}{n}\sum_{i=1}^{n} G\left(\frac{i}{n}\right) r_i(n^2 t) \xrightarrow[n\to\infty]{} \int_0^1 G(y) r(y,t)\, dy$$

in probability, with $r(y,t)$ *solution of*

$$\begin{aligned} &\partial_t r(y,t) = \partial_y^2 \tau(r(y,t),T) \\ &\partial_y r(0,t) = 0, \qquad \tau(r(1,t),T) = \tau_1 \end{aligned}$$

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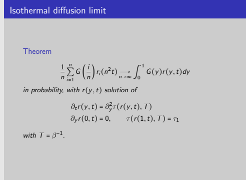

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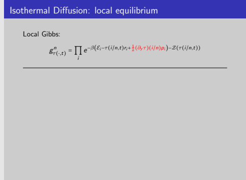
This is the isothermal non-equilibrium transformation we describe in thermodynamic before.

Isothermal Diffusion: local equilibrium

Local Gibbs:

$$g^n_{\tau(\cdot,t)} = \prod_i e^{-\beta\left(\mathcal{E}_i - \tau(i/n,t) r_i + \frac{1}{n}(\partial_y \tau)(i/n) p_i\right) - \mathcal{Z}(\tau(i/n,t))}$$



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$$L = A + S$$

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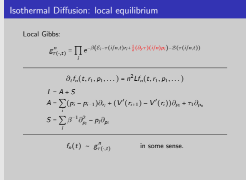
$$f_n(t) \sim g^n_{\tau(\cdot,t)} \qquad \text{in some sense.}$$



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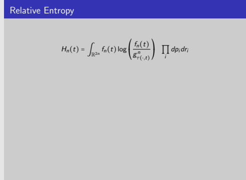
Relative Entropy

$$H_n(t) = \int_{\mathbb{R}^{2n}} f_n(t) \log\left(\frac{f_n(t)}{g^n_{\tau(\cdot,t)}}\right) \prod_i dp_i dr_i$$



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local equilibrium property in a bit weaker sense than pointwise: for any local function F of the configurations and a test function G on the macroscopic interval.

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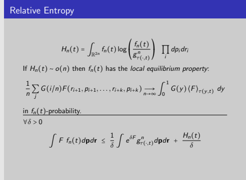
If $H_n(t) \sim o(n)$ then $f_n(t)$ has the *local equilibrium property*:

$$\frac{1}{n}\sum_j G(i/n) F(r_{i+1}, p_{i+1}, \dots, r_{i+k}, p_{i+k}) \xrightarrow[n\to\infty]{} \int_0^1 G(y) \langle F \rangle_{\tau(y,t)} \; dy$$

in $f_n(t)$-probability.

$\forall \delta > 0$

$$\int F \; f_n(t) d\mathbf{p} d\mathbf{r} \;\leq\; \frac{1}{\delta}\int e^{\delta F} g^n_{\tau(\cdot,t)} d\mathbf{p} d\mathbf{r} \;+\; \frac{H_n(t)}{\delta}$$



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Relative Entropy method

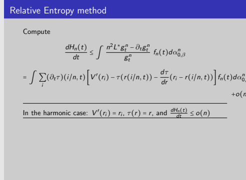
Compute

$$\frac{dH_n(t)}{dt} \le \int \frac{n^2 L^* g_t^n - \partial_t g_t^n}{g_t^n}\, f_n(t)\, d\alpha^n_{0,\beta}$$

$$= \int \sum_i (\partial_t \tau)(i/n, t)\left[V'(r_i) - \tau(r(i/n,t)) - \frac{d\tau}{dr}(r_i - r(i/n,t))\right] f_n(t)\, d\alpha^n_{0,\beta}$$

$$+ o(n)$$

In the harmonic case: $V'(r_i) = r_i$, $\tau(r) = r$, and $\frac{dH_n(t)}{dt} \le o(n)$



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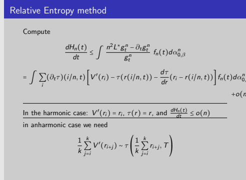
in anharmonic case we need

$$\frac{1}{k}\sum_{j=i}^{k} V'(r_{i+j}) \sim \tau\left(\frac{1}{k}\sum_{j=i}^{k} r_{i+j}, T\right)$$



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$$\frac{1}{k}\sum_{j=i}^{k} V'(r_{i+j}) \sim \tau\left(\frac{1}{k}\sum_{j=i}^{k} r_{i+j},\, T\right)$$

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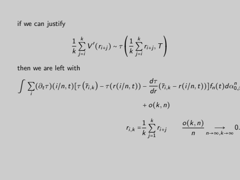
$$\int \sum_i (\partial_t \tau)(i/n,t)\left[\tau\left(\bar r_{i,k}\right) - \tau(r(i/n,t)) - \frac{d\tau}{dr}(\bar r_{i,k} - r(i/n,t))\right] f_n(t)\, d\alpha^n_{0,\beta}$$

$$+\, o(k,n)$$

$$r_{i,k} = \frac{1}{k}\sum_{j=1}^{k} r_{i+j} \qquad \frac{o(k,n)}{n} \xrightarrow[n\to\infty,k\to\infty]{} 0.$$



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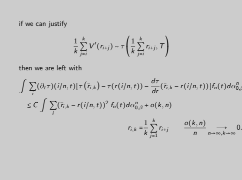

relative entropy (end)

Use again the relative entropy inequality:

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&\leq \frac{C}{\delta} \log \int e^{\delta \sum_i (\bar{r}_{i,k} - r(i/n,t))^2}\, g_n(t)\, d\alpha^n_{0,\beta} + C\frac{H_n(t)}{\delta} + o(n,k) \\
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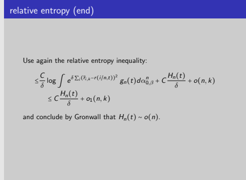
and conclude by Gronwall that $H_n(t) \sim o(n)$.



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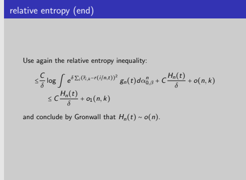


relative entropy (end)

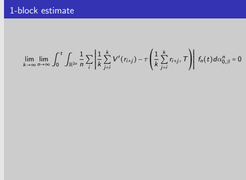
Use again the relative entropy inequality:

$$\begin{aligned}&\leq \frac{C}{\delta}\log\int e^{\delta\sum_i(\bar{r}_{i,k}-r(i/n,t))^2}\, g_n(t)\,d\alpha^n_{0,\beta} + C\frac{H_n(t)}{\delta} + o(n,k)\\ &\leq C\frac{H_n(t)}{\delta} + o_1(n,k)\end{aligned}$$

and conclude by Gronwall that $H_n(t) \sim o(n)$.

1-block estimate

$$\lim_{k\to\infty}\lim_{n\to\infty}\int_0^t\int_{\mathbb{R}^{2n}}\frac{1}{n}\sum_i\left|\frac{1}{k}\sum_{j=i}^{k}V'(r_{i+j})-\tau\left(\frac{1}{k}\sum_{j=i}^{k}r_{i+j},T\right)\right| f_n(t)d\alpha^n_{0,\beta}=0$$



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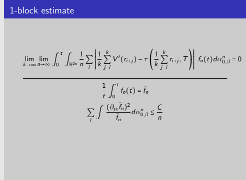
$$\frac{1}{t}\int_0^t f_n(t)=\bar{f}_n$$

$$\sum_i\int\frac{(\partial_{p_i}\bar{f}_n)^2}{\bar{f}_n}\,d\alpha^n_{0,\beta}\le\frac{C}{n}$$



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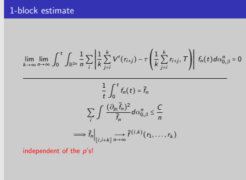
$$\Longrightarrow \bar{f}_n\Big|_{[i,i+k]}\xrightarrow[n\to\infty]{}\tilde{f}^{(i,k)}(r_1,\dots,r_k)$$

independent of the p's!



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$$\bar{f}_n\Big|_{[i,i+k]}\alpha^k_{\beta,0} \xrightarrow[n\to\infty]{} \tilde{f}^{(i,k)}\alpha^k_{\beta,0} \xrightarrow[k\to\infty]{} \nu_i$$

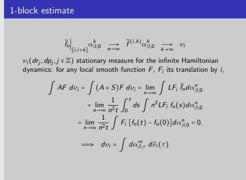
$\nu_i(dr_j, dp_j, j\in\mathbb{Z})$ stationary measure for the infinite Hamiltonian dynamics: for any local smooth function F, F_i its translation by i,

$$\begin{aligned}\int AF\, d\nu_i = \int (A+S)F\, d\nu_i &= \lim_{n\to\infty}\int LF_i\, \bar{f}_n d\alpha^n_{\beta,0}\\ &= \lim_{n\to\infty}\frac{1}{n^2 t}\int_0^t ds\int n^2 LF_i\, f_n(s)d\alpha^n_{\beta,0}\\ &= \lim_{n\to\infty}\frac{1}{n^2 t}\int F_i\,[f_n(t)-f_n(0)]d\alpha^n_{\beta,0} = 0.\end{aligned}$$

$$\Longrightarrow \quad d\nu_i = \int d\alpha^\infty_{\beta,\tau}\, d\tilde{\nu}_i(\tau)$$

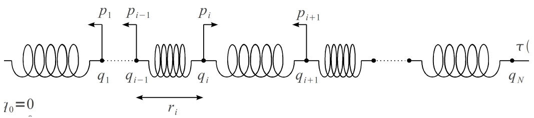
2012-03-18

From dynamics to thermodynamics
└Statistical Mechanics
  └Isothermal dynamics
    └1-block estimate



This argument shows that just from the presence of the thermostats (noisy), the local distributions are maxwellian on the velocities with the right temperature, and in the positions is a convex combinations of Gibbs of different tensions τ. The hard part is to show that this convex combination is a delta on the right one given by the solution of the macroscopic equation.

Adiabatic dynamics



Balistic dynamics:

$$
\begin{aligned}
\dot r_j(t) &= p_j(t) - p_{j-1}(t), \qquad j = 1, \dots, n,\\
dp_j(t) &= \big(V'(r_{j+1}(t)) - V'(r_j(t))\big)\, dt, \qquad\qquad j = 1, \dots, n-1,\\
dp_n(t) &= \big(\tau_1 - V'(r_n(t))\big)\, dt
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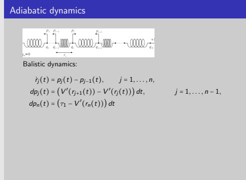
2012-03-18

From dynamics to thermodynamics
- Statistical Mechanics
  - Adiabatic dynamics
    - Adiabatic dynamics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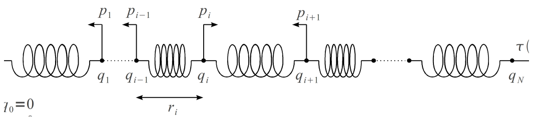

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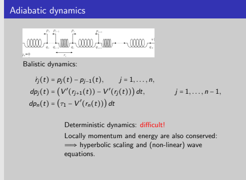
Deterministic dynamics: difficult!

Locally momentum and energy are also conserved: $\Longrightarrow$ hyperbolic scaling and (non-linear) wave equations.

2012-03-18

From dynamics to thermodynamics
└Statistical Mechanics
 └Adiabatic dynamics
  └Adiabatic dynamics



Hyperbolic Adiabatic Dynamics

3 conserved quantities:

stretch $\mathcal{R}_n(t)[G] = \frac{1}{n}\sum_i G(i/n)r_i(nt)$

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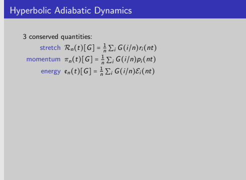

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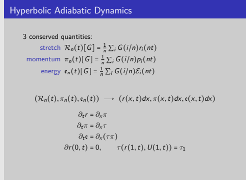

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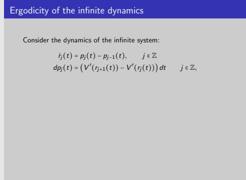
Ergodicity of the infinite dynamics

Consider the dynamics of the infinite system:

$$\begin{aligned} \dot r_j(t) &= p_j(t) - p_{j-1}(t), \qquad j \in \mathbb{Z} \\ dp_j(t) &= \big(V'(r_{j+1}(t)) - V'(r_j(t))\big)\, dt \qquad j \in \mathbb{Z}, \end{aligned}$$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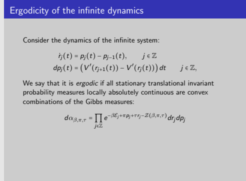

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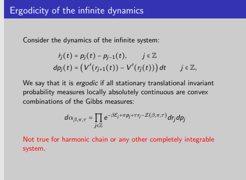

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Theorem (Fritz, Funaki, Lebowitz, 1993)

if $d\nu$ *is a (regular) translation invariant probability on* $(\mathbb{R}^2)^{\mathbb{Z}}$ *stationary for the infinite dynamics and such that*

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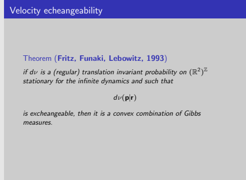

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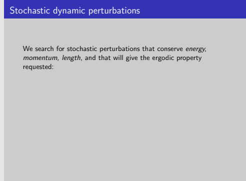
So it should be the collision mechanism due to the non-linearities of the dynamics, to induce this excheangeability properties of the stationary measures.

This ergodic property seems too difficult to be proven for determnistic dynamics, but this theorem suggest what a stochastic perturbation should do in order to garantier the ergodicity of the infinite dynamics.

Stochastic dynamic perturbations

We search for stochastic perturbations that conserve *energy*, *momentum*, *length*, and that will give the ergodic property requested:



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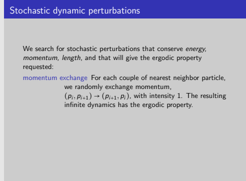
2012-03-18

From dynamics to thermodynamics
└Statistical Mechanics
  └Adiabatic dynamics
    └Stochastic dynamic perturbations



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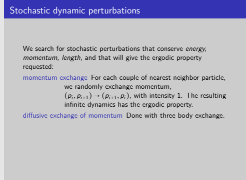

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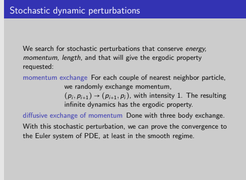

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If $V(r) = \frac{r^2}{2}$, we have $\tau(\mathcal{L}, U) = \mathcal{L}$, and the system became

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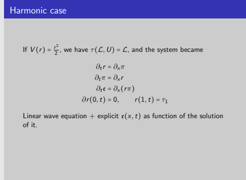
Linear wave equation + explicit $\mathfrak{e}(x,t)$ as function of the solution of it.



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In the harmonic case there is no dissipation in the hyperbolic time scale, the equation itself will not converge to *equilibrium*.
But we know that the stochastic mechanism makes the dynamics ergodic and eventually the system will converge to equilibrium, but not in the hyperbolic scale.

Observe that the coherent evolution of the energy in the equation is due to the stochastic mechanism. Otherwise energies of each mode will be conserved.

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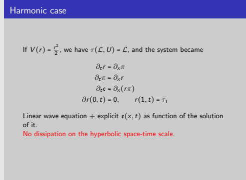

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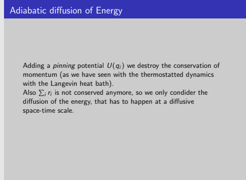
Adiabatic diffusion of Energy

Adding a *pinning* potential $U(q_i)$ we destroy the conservation of momentum (as we have seen with the thermostatted dynamics with the Langevin heat bath).
Also $\sum_i r_i$ is not conserved anymore, so we only condider the diffusion of the energy, that has to happen at a diffusive space-time scale.



Adiabatic diffusion of Energy

Adding a *pinning* potential $U(q_i)$ we destroy the conservation of momentum (as we have seen with the thermostatted dynamics with the Langevin heat bath).
Also $\sum_i r_i$ is not conserved anymore, so we only condider the diffusion of the energy, that has to happen at a diffusive space-time scale.

Chain of Anharmonic oscillators

$p_i, q_i \in \mathbb{R}$, $i \in \Lambda$, $|\Lambda| = N$ or $\Lambda = \mathbb{Z}$.

$$\begin{aligned} \mathcal{H} &= \sum_i \left[\frac{p_i^2}{2} + V(q_i - q_{i-1}) + U(q_j) \right] \\ &= \sum_i e_i \end{aligned}$$

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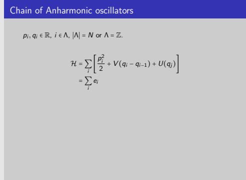
From dynamics to thermodynamics
└Statistical Mechanics
  └Adiabatic dynamics
    └Chain of Anharmonic oscillators



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From dynamics to thermodynamics
- Statistical Mechanics
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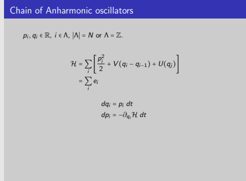

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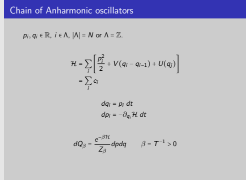

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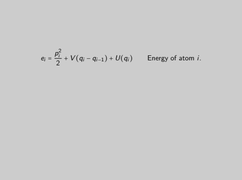

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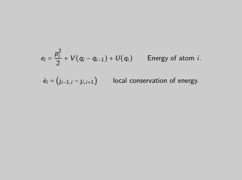

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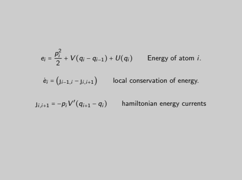
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Non-stationary behavior

We would like to prove that

$$\frac{1}{N}\sum_i G(i/N)e_i(N^2 t) \xrightarrow[N\to\infty]{} \int G(y)u(t,y)dy$$

with $u(t,y)$ solution of the nonlinear heat equation:

$$\partial_t u = \partial_y \mathcal{D}(u)\partial_y u$$

with the thermal conductivity defined by the *Green-Kubo formula*:

$$\mathcal{D}(u) = \chi_\beta^{-1}\sum_{i\in\mathbb{Z}}\int_0^\infty \left\langle \mathsf{j}_{i,i+1}(t)\mathsf{j}_{0,1}(0)\right\rangle_\beta \, dt \ , \qquad \beta = \beta(u)$$

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From dynamics to thermodynamics
- Statistical Mechanics
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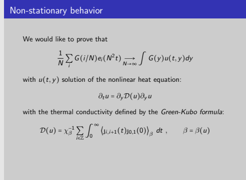
    - Non-stationary behavior



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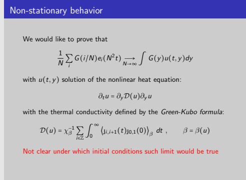

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Equilibrium Fluctuations: Linear response

Here is a theorem that has a clear and precise mathematical statement:

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From dynamics to thermodynamics
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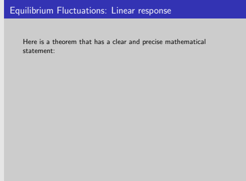
    └Adiabatic dynamics
      └Equilibrium Fluctuations: Linear response



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  └Adiabatic dynamics
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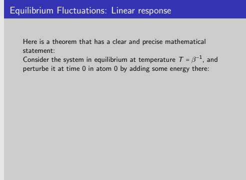
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We want to study the time evolution of

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From dynamics to thermodynamics
- Statistical Mechanics
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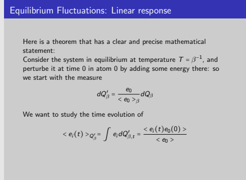

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$$\boxed{\mathcal{D} = \frac{\kappa}{\beta^2 \chi(\beta)} = \frac{< e_0 >_\beta}{\chi(\beta)} \lim_{t \to \infty} \frac{1}{t} \sum_{i \in \mathbb{Z}} i^2 < e_i(t) >_{Q'_\beta}}$$

with $\chi(\beta) = \sum_i (< e_i e_0 >_\beta - < e_i >_\beta < e_0 >_\beta)$.

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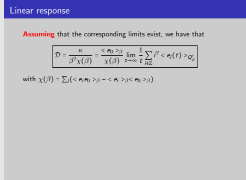

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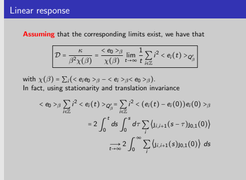

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Linearized heat equation

Define

$$C(i,j,t) =< e_i(t)e_j(0) >_\beta \; - \bar{e}^2$$

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From dynamics to thermodynamics
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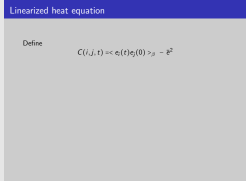
      Linearized heat equation



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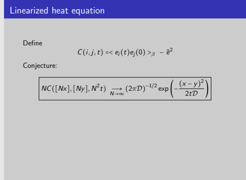

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From dynamics to thermodynamics
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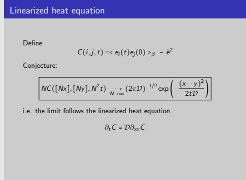

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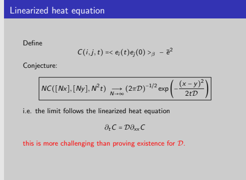

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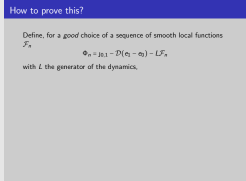

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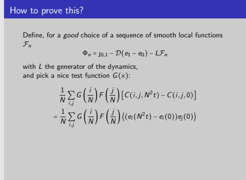

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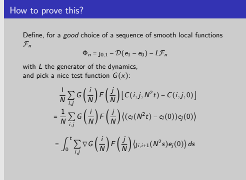

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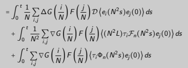
$$\begin{aligned} &\frac{1}{N}\sum_{i,j} G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right)\left[C(i,j,N^2t) - C(i,j,0)\right] \\ =&\frac{1}{N}\sum_{i,j} G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right)\left\langle (e_i(N^2t) - e_i(0))e_j(0)\right\rangle \\ =&\int_0^t \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right)\left\langle j_{i,i+1}(N^2s)e_j(0)\right\rangle ds \end{aligned}$$

$$
\begin{aligned}
&= \int_0^t \frac{1}{N} \sum_{i,j} \Delta G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \mathcal{D}\left\langle e_i(N^2 s) e_j(0)\right\rangle ds \\
&\quad + \int_0^t \frac{1}{N^2} \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \left\langle (N^2 L)\tau_i \mathcal{F}_n(N^2 s) e_j(0)\right\rangle ds \\
&\quad + \int_0^t \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \left\langle \tau_i \Phi_n(N^2 s) e_j(0)\right\rangle ds
\end{aligned}
$$



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$$

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\begin{aligned}
&\sim \int_0^t \frac{1}{N}\sum_{i,j}\Delta G\left(\frac{i}{N}\right)F\left(\frac{j}{N}\right)\mathcal{D}NC(i,j,N^2 t)ds \\
&\quad + \frac{1}{N^2}\sum_{i,j}\nabla G\left(\frac{i}{N}\right)F\left(\frac{j}{N}\right)\left\langle \tau_i(\mathcal{F}_n(N^2 t)-\mathcal{F}_n(0))e_j(0)\right\rangle ds \\
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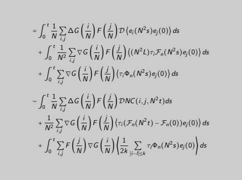
2012-03-18

From dynamics to thermodynamics
└Statistical Mechanics
  └Adiabatic dynamics



$$\Phi_n = j_{0,1} - \mathcal{D}(e_1 - e_0) - LF_n$$

$$\hat{\Phi}_{n,k} = \frac{1}{2k} \sum_{|j| \le k} \tau_j \Phi_n$$

By Schwarz we can bound the square of the last term by

$$\|F\|^2 \bar{e}^2 \left\langle \left(\int_0^t N \sum_i G'\left(\frac{i}{N}\right) \tau_i \hat{\Phi}_{n,k}(N^2 s) ds \right)^2 \right\rangle$$

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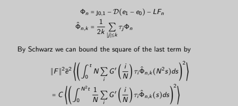

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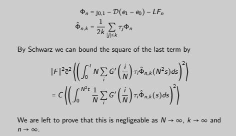

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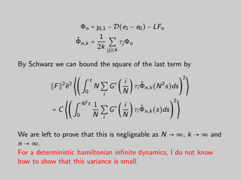
From dynamics to thermodynamics
└Statistical Mechanics
 └Adiabatic dynamics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Varadhan's Non Gradient methods.

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From dynamics to thermodynamics
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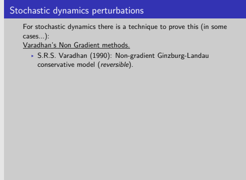

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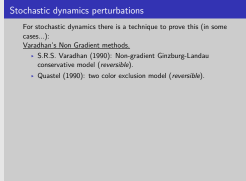

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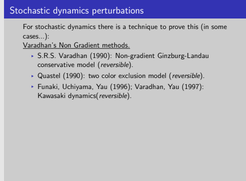

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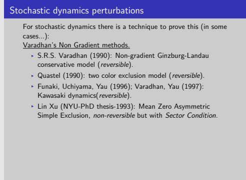

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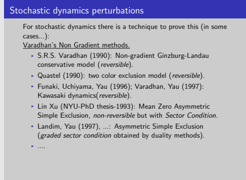

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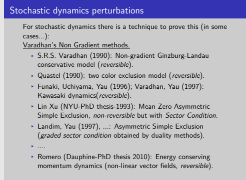

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How can the space-time variance be small?

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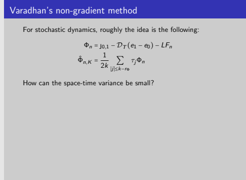
From dynamics to thermodynamics
- Statistical Mechanics
  - Adiabatic dynamics
    - Varadhan's non-gradient method



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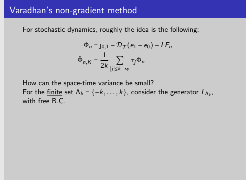

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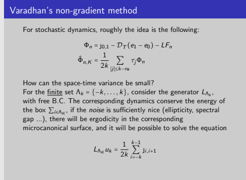
$$L_{\Lambda_K} u_k = \frac{1}{2k} \sum_{i=-k}^{k-1} j_{i,i+1}$$



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  └Statistical Mechanics
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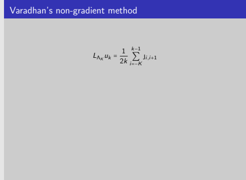
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going back to the full generator of the infinite dynamics:

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It is the boundary term $(L - L_{\Lambda_k})u_k$ that gives origin to the gradient $\mathcal{D}_T(e_k - e_{-k})$, in the proper limit.

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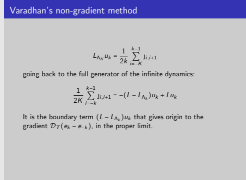

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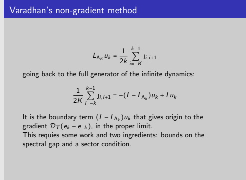
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Chain un unpinned anharmonic oscillators with conservative noise

Joint work with *Makiko Sasada* (Keio University, Tokyo).
Take $U = 0$ (unpinned), and

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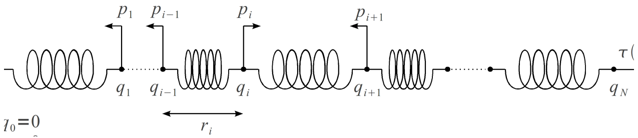

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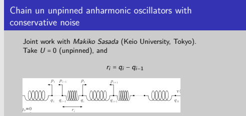
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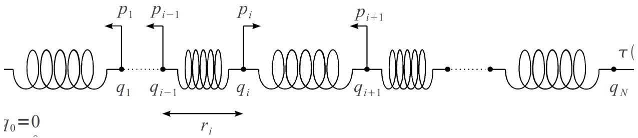

Equilibrium measure are product:

$$dQ_\beta = \prod_i \frac{e^{-\beta(p_i^2/2+V(r_i))}}{Z_\beta} dp_i dr_i \qquad \beta = T^{-1} > 0$$

$V \in \mathcal{C}^2$, $0 < C_- \le V''(r) \le C_+ < +\infty$.

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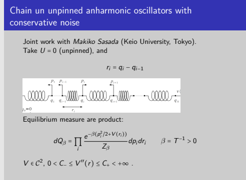
From dynamics to thermodynamics
└Statistical Mechanics
  └Adiabatic dynamics
    └Chain un unpinned anharmonic oscillators with conservative noise



Energy Conserving Noise

We use the vector fields tangent to the microcanonical surface:

$$
\begin{aligned}
Y_{i,j} &= p_i \partial_{r_j} - V'(r_j)\partial_{p_i}, \\
X_i &= Y_{i,i}
\end{aligned}
$$

The Hamiltonian vector field is

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A = \sum_i (p_i - p_{i-1})\partial_{r_i} - V'(r_i)(\partial_{p_i} - \partial_{p_{i-1}}) = \sum_i (X_i - Y_{i-1,i})
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└Statistical Mechanics
  └Adiabatic dynamics
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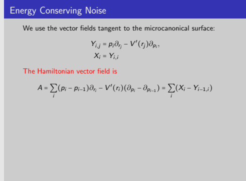

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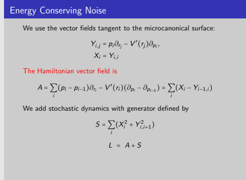
We add stochastic dynamics with generator defined by

$$S = \sum_i (X_i^2 + Y_{i,i+1}^2)$$

$$L = A + S$$



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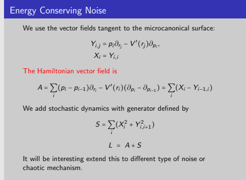
From dynamics to thermodynamics
└Statistical Mechanics
  └Adiabatic dynamics
    └Energy Conserving Noise



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NON GRADIENT CURRENTS

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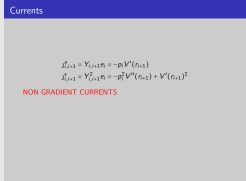
From dynamics to thermodynamics
- Statistical Mechanics
  - Adiabatic dynamics
    - Currents



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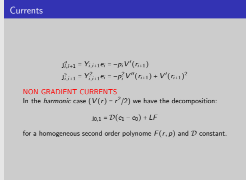

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$$\hat{\Phi}_{n,K} = \frac{1}{2K} \sum_{|j| \leq K} \tau_j \Phi_n$$

By a general inequality valid for all Markov processes:

$$\left\langle \left(\int_0^t N \sum_j G'(i/N) \tau_i \hat{\Phi}_{n,K}(N^2 s) ds \right)^2 \right\rangle$$
$$\leq Ct \left\langle \sum_i G'(i/N) \tau_i \hat{\Phi}_{n,K}, (-S)^{-1} \sum_i G'(i/N) \tau_i \hat{\Phi}_{n,K} \right\rangle$$
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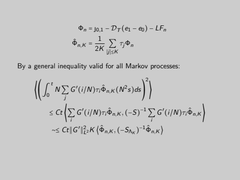
From dynamics to thermodynamics
└Statistical Mechanics
 └Adiabatic dynamics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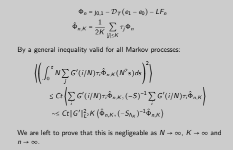
We are left to prove that this is negligeable as $N \to \infty$, $K \to \infty$ and $n \to \infty$.



Microcanonical variance

$< \cdot >_{K,E}$: microcanonical expectation on the energy shell

$$\Sigma_{K,E} = \left\{ (r_1, p_1, \dots, r_K, p_K) : \sum_{i=1}^{K} e_i = KE \right\}$$

Hypothesis on $V \Longrightarrow$ connected surface.

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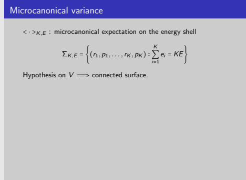
- From dynamics to thermodynamics
  - Statistical Mechanics
    - Adiabatic dynamics
      - Microcanonical variance



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From dynamics to thermodynamics
- Statistical Mechanics
  - Adiabatic dynamics
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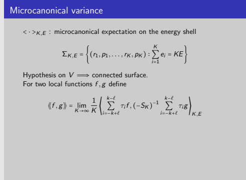
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└Statistical Mechanics
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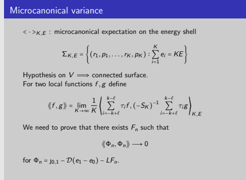

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variational formulas

Let $\Phi = X_0 F + Y_{0,1} G$, for some local F, G, then

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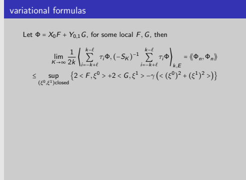

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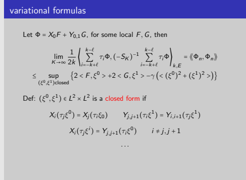
$$\dots$$



exact forms

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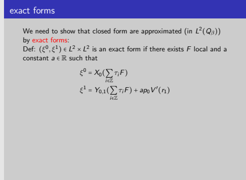

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This is proven by a careful construction, integrating the form

$$\{\xi_j^m, j = 1, \dots, K, m = 0, 1\}$$

on the microcanonical surface $\Sigma_{E,K}$, that has the same cohomology of the 2K-sphere, and controlling the boundary conditions as $K \to \infty$, with the spectral gap on S_K.

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From dynamics to thermodynamics
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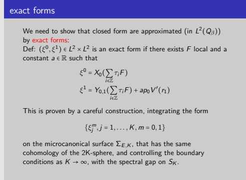
　└Adiabatic dynamics
　　└exact forms



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Ingredients to prove this:

- Spectral gap bound for S_K: $SG(S_K) \geq CK^{-2}$.
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i.e. for any smooth local f such that $< f >_{K,E} = 0$

$$< f^2 >_{K,E} \leq \; C_1 \sum_{i=1}^{K} \left\langle (X_i f)^2 \right\rangle_{K,E} + C_2 K^2 \sum_{i=1}^{K-1} \left\langle (Y_{i,i+1} f)^2 \right\rangle_{K,E}$$

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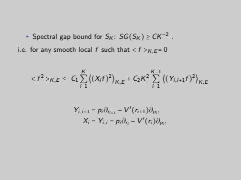

Sector Condition

For any i decompose $f = f_{i,odd} + f_{i,even}$

$$f_{i,odd}(p) = \frac{1}{2}\left(f(p^{(i)}) - f(p)\right), \qquad f_{i,even}(p) = \frac{1}{2}\left(f(p^{(i)}) + f(p)\right),$$

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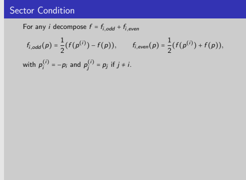

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$$\langle vAu \rangle = \sum_i \left\langle v(X_i - Y_{i-1,i})u \right\rangle$$

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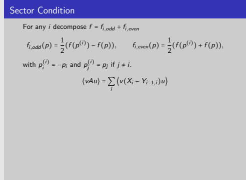
From dynamics to thermodynamics
  Statistical Mechanics
    Adiabatic dynamics
      Sector Condition



Sector Condition

For any i decompose $f = f_{i,odd} + f_{i,even}$

$$f_{i,odd}(p) = \frac{1}{2}\left(f(p^{(i)}) - f(p)\right), \qquad f_{i,even}(p) = \frac{1}{2}\left(f(p^{(i)}) + f(p)\right),$$

with $p_i^{(i)} = -p_i$ and $p_j^{(i)} = p_j$ if $j \neq i$.

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\langle vX_i u \rangle &= \left\langle v_{i,odd} X_i u_{i,even} \right\rangle + \left\langle v_{i,even} X_i u_{i,odd} \right\rangle \\
&= \left\langle v_{i,odd} X_i u_{i,even} \right\rangle - \left\langle u_{i,odd} X_i v_{i,even} \right\rangle \\
&\leq \left\langle v_{i,odd}^2 \right\rangle^{1/2} \left\langle (X_i u_{i,even})^2 \right\rangle^{1/2} + \left\langle u_{i,odd}^2 \right\rangle^{1/2} \left\langle (X_i v_{i,even})^2 \right\rangle^{1/2} \\
&\leq C \left\langle (X_i v)^2 \right\rangle^{1/2} \left\langle (X_i u)^2 \right\rangle^{1/2} + \left\langle (X_i u)^2 \right\rangle^{1/2} \left\langle (X_i v)^2 \right\rangle^{1/2}
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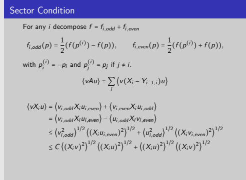
From dynamics to thermodynamics
- Statistical Mechanics
  - Adiabatic dynamics
    - Sector Condition



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and similarly for $< vY_{i-1,i}u >$.

$\Longrightarrow \quad |\langle vAu \rangle| \leq C \langle v(-S)v \rangle \langle u(-S)u \rangle.$

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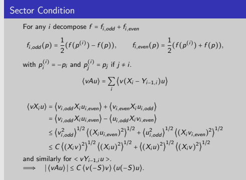
└─Statistical Mechanics
  └─Adiabatic dynamics
    └─Sector Condition



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equilibrium fluctuations

Equivalently we can express the result in term of the fluctuation field

$$Y^N = \frac{1}{\sqrt{N}} \sum_i \delta_{i/N} \left\{ e_i(0) - e \right\}$$

It converges in law to a delta correlated centered gaussian field Y

$$\mathbb{E}\left[Y(F) Y(G) \right] = \chi \int F(y) G(y) dy$$

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From dynamics to thermodynamics
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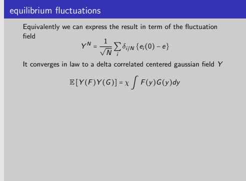

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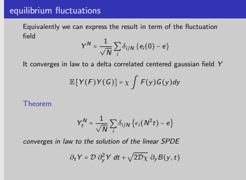

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proof of spectral gap bound

start with the martingale decomposition:

$$\mathcal{G}_k = \sigma\left\{e_1, \dots, e_k, p_{k+1}, r_{k+1}, \dots, p_L, r_L\right\}$$

$$f_k := E[f|\mathcal{G}_k], \qquad f_L = f_L(e_1, \cdots, e_L)$$

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From dynamics to thermodynamics
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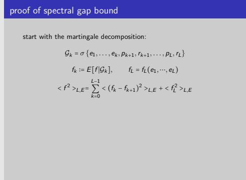
  - Adiabatic dynamics
    - proof of spectral gap bound



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each X_k^2 has his uniform spectral gap in the corresponding microcanonical surface ($X_k e_k = 0$):

$$< f^2 >_{L,E} \leq C \sum_{k=0}^{L-1} < (X_{k+1} f_k)^2 >_{L,E} + < f_L^2 >_{L,E}$$

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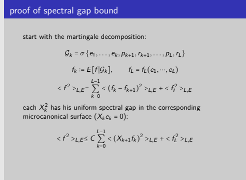

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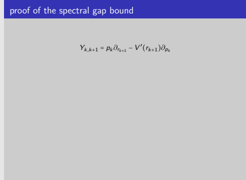

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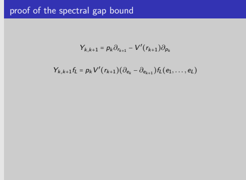

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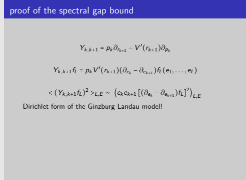
Dirichlet form of the Ginzburg Landau model!



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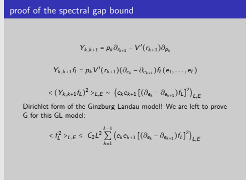

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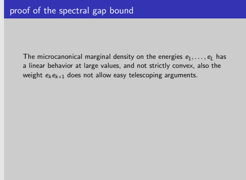

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Caputo approach + a smart telescoping + the elementary inequality

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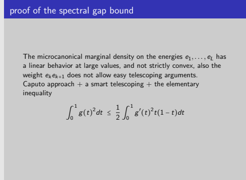

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