From dynamics to thermodynamics
From Dynamics to Thermodynamics
Sederer Olis - CEREMOD; Pers
WMX; February 22-22, 2022

From Dynamics to Thermodynamics

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Some inspiration from reading

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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 withlished notes can be found in his web site) ttp://math.berkeley.edu/ evans/entropy.and.PDE.pdf

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#### A one dimensional system

Mechanical Equilibrium:

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

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A one dimensional system

#### Draw picture bar, L, au etc.

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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 <u>adiabatic wall</u> and <u>conductive wall</u>. 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  $\theta$  that we call temperature (see in Zemanski a very detailed discussion of this

### A one dimensional system

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Thermodynamic Equilibrium

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

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 $\theta$  is the **temperature** 

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Mechanical Equilibrium:  $\mathcal{L} = \mathcal{L}(\tau)$  Thermodynamic Equilibrium  $\mathcal{L} = \mathcal{L}(\tau, \theta)$   $\theta$  is the temperature

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 $\theta$  is the **temperature** Empirical definition of temperature.

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

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

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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

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

From dynamics to thermodynamics Thermodynamic crash course Differential changes of equilibrium states Differential changes of equilibrium states

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## Work $\rightarrow$ Energy

From the mechanics we have the notion of infinitesimal work done by the force/tension  $\boldsymbol{\tau}$ 

$$dW = \tau d\mathcal{L}$$

that change the energy  $\mathcal{U}$  of the system.

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#### Work $\rightarrow$ Energy

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This permit to define the energy (called *internal energy*) as a function of the state of the system:  $\mathcal{U}(\mathcal{L}, \theta)$ . 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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### 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  $\tau$ . This is called heat

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

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

 $\tau d\mathcal{L}$  and dQ are not exact differential, and the total work or total heat exchanged during a thermodynamic transformation:

$$W = \int_{i}^{f} \tau d\mathcal{L}, \qquad Q = \int_{i}^{f} d\langle Q$$

depend from the particular *path* chosen, i.e. from the particular procedure (isothermal, isochore....) that takes from one equilibrium i to the equilibrium f.

From dynamics to thermodynamics Thermodynamic crash course Non-adiabatic work: heat

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## 1st principle of thermodynamics

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1st principle of thermodynamics

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I think this is the main conceptual point of point thermodynamics, in particular in its connection to the microscopic mechanics. This decomposition contains the **separation of scales** (time and space) between microscopic and macroscopic.

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## 1st principle of thermodynamics

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 the external work τdL doen by a known, slow, controllable, macroscopic force τ, From dynamics to thermodynamics

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└─1st principle of thermodynamics

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- the external work \(\tau d\mathcal{L}\) doen by a known, slow, controllable, macroscopic force \(\tau,\).
- from the work done by unknown, fast, microscopic forces, we call heat this work.

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## Thermodynamic transformations and Cycles

reversible or quasi-static tranformations:



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

$$\Delta W = \oint \tau dL \tag{2}$$

that by the first principle will be equal to  $-\Delta Q$ , where  $\Delta Q$  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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└──Thermodynamic transformations and Cycles



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).

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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Irreversible themodynamic transformations

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## Special quasi-static transformations

#### Isothermal:

System in contact with a *thermostat* while the external force  $\tau$  is doing work:

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



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Special quasi-static transformations

- Isothermal: System in contact with a thermostat while the external forc  $\tau$  is doing work:

 $\tilde{q}W = \tau d\mathcal{L} = \tau \left(\frac{\partial \mathcal{L}}{\partial \tau}\right)_{0} d\tau = -\tilde{q}Q + dU$  (3)



While a force perform work on the system, this is in contact with a *thermostat*, a **huge** system in equilibrium at a given temperature  $\theta$ , 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:  $\partial Q = 0$ .

 $\partial W = \tau d\mathcal{L} = dU$ 

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└──Special quasi–static Transformations

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## Special quasi-static Transformations

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Special quasi-static Transformations

Isocore: Thermodynamic transformation at fixed length L Consequently dW = 0, no work if performed to or by the dQ = dUIsobar: Thermodynamic transformation at fixed tension L

▶ **Isocore**: Thermodynamic transformation at fixed length *L*. Consequently  $\partial W = 0$ , no work if performed to or by the system, and

 $\partial Q = dU$ 

▶ **Isobar**: Thermodynamic transformation at fixed tension *L*,  $d\tau = 0$ 

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W > 0 means that has done a work W on the exterior (heat machine). W < 0 is a refrigerator.

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



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

$$W=\oint \tau d\mathcal{L}=Q_h-Q_c=-\oint dQ$$

W > 0 is a heat machine:



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W > 0 is a heat machine:



W > 0 is a heat machine:



in a reverse mode is a *Carnot refrigerator*: W < 0



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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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Second Principle of Thermodynamics

Second Principle of Thermodynamics

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



## Second Principle of Thermodynamics

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



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



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## Equivalence of Kelvin and Clausius statement



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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.

Equivalence of Kelvin and Clausius statement

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For any Carnot cycle operating between temperatures  $\theta_h$  and  $\theta_c$ , the ratio  $\frac{\sigma_h}{\sigma_c}$  depends only from  $(\theta_h, \theta_c)$  and there exist a universal function  $g(\theta)$  such that

For **any** Carnot cycle operating between temperatures  $\theta_h$  and  $\theta_c$ , the ratio  $\frac{Q_h}{Q_c}$  depends only from  $(\theta_h, \theta_c)$  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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Kelvin's theorem

For any Carnot cycle operating between temperatures  $\theta_h$  and  $\theta_c$ , the ratio  $\frac{\partial_c}{\partial_c}$  depends only from  $(\theta_h, \theta_c)$  and there exist a universal function  $g(\theta)$  such that

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

 $T = g(\theta)$  absolute temperature

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

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

 $T = g(\theta)$  absolute temperature

From Kelvin's theorem:

$$0 = \frac{Q_h}{T_h} - \frac{Q_c}{T_c} = \oint \frac{dQ}{T}$$

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Thermodynamic Entropy

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Extension to any cycle  $C: \oint_C \frac{dQ}{T} = 0$ 



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There exists a function S of the thermodynamic state such that

$$dS = \frac{\partial Q}{T}$$

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#### Thermodynamic Entropy

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There exists a function S of the thermodynamic state such that

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If we choose the extensive coordinates  $U, \mathcal{L}$ :

$$dS(U,\mathcal{L}) = -\frac{\tau}{T}d\mathcal{L} + \frac{1}{T}dU$$

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#### Thermodynamic Entropy

There exists a function S of the thermodynamic state such that  $dS = \frac{4Q}{\tau}$ If we choose the extensive coordinates U, E:  $dS(U, E) = -\frac{\tau}{\tau} dE + \frac{1}{\tau} dU$
# Thermodynamic Entropy

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• In isothermal transformation  $\Delta S = \Delta Q/T$ .

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- Adiabatic quasistatic transformations are isoentropic.

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#### Thermodynamic Entropy

There exists a function S of the thermodynamic state such that

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In isothermal transformation ΔS = ΔQ/T.
 Adiabatic quasistatic transformations are isoentropic

#### Axiomatic approach

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

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Extensive quantities: M, U, L = (mass, energy, length)

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.

#### Axiomatic approach

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

- $\frac{\partial S}{\partial U} > 0$ ,
- S is positively homogeneous of degree 1:

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 $S(\lambda M, \lambda U, \lambda \mathcal{L}) = \lambda S(M, U, \mathcal{L}), \qquad \lambda > 0$ 

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Extension an open cone set  $\Gamma \in \mathbb{R}_+ \times \mathbb{R}_- \times \mathbb{R}_-$  and  $(M, U, L) \in \Gamma$ Three exists a  $C^{1-d}$ -function  $S(M, U, L) : \Gamma \to \mathbb{R}$ such that

Axiomatic approach

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 35/30 > 0,
 S is positively homogeneous of degree 1:
 S(M M( J( )) = 3S(M (I / )) = 3 > 0)

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.

#### Axiomatic Approach

Choose S and  $\mathcal{L}$  as thermodynamic coordinates, there exists a function  $U(M, S, \mathcal{L})$  such that  $\frac{\partial U}{\partial S} > 0$ .

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$$T = \frac{\partial U}{\partial S} \qquad \text{temperature}$$
$$\tau = \frac{\partial U}{\partial \mathcal{L}} \qquad \text{tension}$$

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

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rreversible Transformations

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e find in thermodynamics books the expression  

$$\oint \frac{d^2Q}{d\tau} < 0 \quad \text{Chassius Inequality}$$

$$\int_{A}^{B} \frac{dQ}{d\tau} \leq S(B) - S(A)$$
Not very clear the managing of this.

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

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

or

$$\int_{A}^{B} \frac{\partial \langle Q}{T} \leq S(B) - S(A)$$

Not very clear the meaning of this.

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

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

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

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Isothermal Irreversible Transformations

 $A = (\mathcal{L}_0, T), B = (\mathcal{L}_1, T)$  $Q \leq T [S(B) - S(A)]$ 

└── Isothermal Irreversible Transformations

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 Qwith it. Going from the state A to the state B, this implies that A and Bare 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

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$$\begin{split} &A = (\mathcal{L}_0, T), \ B = (\mathcal{L}_1, T) \\ &Q \leq T \left[ S(B) - S(A) \right] \\ &By \ \text{the first principle:} \ W = \left[ U(B) - U(A) \right] - Q \\ &-W \leq - \left[ U(B) - U(A) \right] + T \left[ S(B) - S(A) \right]. \end{split}$$

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$$F(\mathcal{L}, T) = \inf_{U} \{ U - TS(U, \mathcal{L}) \}$$
 free energy (4)  
$$U(\mathcal{L}, T) = \partial_{T} \left( \frac{1}{T} F(\mathcal{L}, T) \right)$$
 (5)

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$$\begin{split} &A = (\mathcal{L}_0, \, T), \, B = (\mathcal{L}_1, \, T) \\ &Q \leq T \left[ S(B) - S(A) \right] \\ &By the first principle: \, W + \left[ U(B) - U(A) \right] - Q \\ &-W \leq - \left[ U(B) - U(A) \right] + T \left[ S(B) - S(A) \right] \end{split}$$

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F = U - TS convex function of  $\mathcal{L}$ .

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#### Irreversible Transformations

For isothermal transformations, F = U - TS

 $W \ge F(B) - F(A) = \Delta F$ 

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└── Irreversible Transformations

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So in a *reversible* isothermal trasformation we have equality and the work done by the system is equal to the difference of the free energy. In a non reversible one, the difference in free energy is only a bound.

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#### Irreversible Transformations

For isothermal transformations, F = U - TS

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For *adiabatic* transformations Q = 0. Adiabatic reversible processes are always isoentropic. But there exists non reversible adiabatic processes for which

0 = Q < S(B) - S(A)

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 $\partial Q = TdS$ 

has a meaning only in quasistatic processes.

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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

 $S(M_1, U_1, \mathcal{L}_1) + S(M_2, U_2, \mathcal{L}_2)$ 

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Extended thermodynamics

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A possible definition of a non-equilibrium state is to consider the system, in our case the wire, as spatially extended, and with different parts of the system in different equilibrium states. For example our wire could be constituted by two different wires, that have the same constitutive materials (i.e. they are make by the same material) and they have mass  $M_1$  and  $M_2$  respectively, but they are prepared in two different equilibrium state, parametrized by the extensive quantities:  $(U_1, \mathcal{L}_1), (U_2, \mathcal{L}_2)$ . The internal energy of the total system composed by the two wires glued together, will be  $U_1 + U_2$ , while its length will be  $\mathcal{L}_1 + \mathcal{L}_2$ . Even though the wire is not in equilibrium, we can say that also the other extensive quantities are given by the sum of the corresponding values of each constitutive part in equilibrium, i.e. in the example the entropy will be given by  $S(M_1, U_1, \mathcal{L}_1) + S(M_2, U_2, \mathcal{L}_2)$ .

If the thermodynamic evolution is governed by a dynamics conserving Energy (adiabatic) and length (isocore), and it reach global equilibrium, then the final entropy is higher than the initial sum of the two entropies.

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$$(M_1, U_1, \mathcal{L}_1)$$
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If attached they are **not in equilibrium**.  
By concavity and 1-homogeneity:

$$S(M_1, U_1, \mathcal{L}_1) + S(M_2, U_2, \mathcal{L}_2) \le 2S\left(\frac{M_1 + M_2}{2}, \frac{U_1 + U_2}{2}, \frac{\mathcal{L}_1 + \mathcal{L}_2}{2}\right)$$
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Extended thermodynamics

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

↑

Property of this transformation to bring the system towards global equilibrium

#### Local equilibrium thermodynamic states

$$x \in [0, M],$$
  $U(x), r(x).$   
 $\mathcal{L}(x) = \int_0^x r(x') dx'$  displacement of  $x$ 

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Local equilibrium thermodynamic states

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Local equilibrium thermodynamic states

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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#### Local equilibrium thermodynamic states

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$$\mathcal{L}_{tot} = \int_0^M r(x) dx, \quad U_{tot} = \int_0^M U(x) dx, \quad S_{tot} = \int_0^M S(1, U(x), r(x)) dx.$$

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Local equilibrium thermodynamic states

Local equilibrium thermodynamic states

$$\begin{split} & x \in [0,M], \qquad \mathcal{U}(x), r(x).\\ \mathcal{L}(x) - \int_0^x r(x') dx' & \text{displacement of } x\\ \mathcal{L}_{ux} = \int_0^M r(x) dx, \quad U_{ux} - \int_0^M U(x) dx, \quad S_{ux} = \int_0^M S(1,U(x), r(x)) dx \end{split}$$

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$$S_{tot} \leq MS(1, M^{-1}U_{tot}, M^{-1}\mathcal{L}_{tot}) = S(M, U_{tot}, \mathcal{L}_{tot})$$

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Local equilibrium thermodynamic states

Local equilibrium thermodynamic states

$$\begin{split} & x \in [0,M], \qquad U(x), r(x).\\ \mathcal{L}(x) - \int_0^{x^*} r(x') dx' & \text{displacement of } x\\ \mathcal{L}_{tot} = \int_0^{M} r(x) dx, \quad U_{tot} = \int_0^{M} U(x) dx, \quad S_{tot} = \int_0^{M} S(1, U(x), r(x))\\ S_{tot} \leq MS(1, M^{-1} U_{tot}, M^{-1} \mathcal{L}_{tot}) = S(M, U_{tot}, \mathcal{L}_{tot}) \end{split}$$

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 $x \in [0,1]$ . The velocity of the material point x is

$$\pi(x,t) = \partial_t \mathcal{L}(x,t)$$

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xample: adiabatic evolution by Euler Equations v c [0,1]. The velocity of the material point v is

-Example: adiabatic evolution by Euler Equations

 $x \in [0,1]$ . The velocity of the material point x is

 $\pi(x,t) = \partial_t \mathcal{L}(x,t)$ 

the force acting on the material element x is

 $\partial_x \tau(U(x,t),\mathcal{L}(x,t))$ 

From dynamics to thermodynamics Thermodynamic crash course Example: adiabatic evolution by Euler Equations

Example: adiabatic evolution by Euler Equations

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$$\mathcal{E}(x,t) = U(x,t) + \frac{\pi(x,t)^2}{2}$$
$$\partial_t r = \partial_x \pi$$
$$\partial_t \pi = \partial_x \tau$$
$$\partial_t \mathcal{E} = \partial_x (\tau \pi)$$
$$\pi(0,t) = 0, \quad \tau(1,t) = \overline{\tau}(t)$$

Example: adiabatic evolution by Euler Equations From dynamics to thermodynamics v c [0,1]. The velocity of the material point v is 2012-03-18 Thermodynamic crash course the force acting on the material element x is the total energy of x is  $\mathcal{E}(x, t) = U(x, t) + \frac{\pi(x, t)^2}{2}$ -Example: adiabatic evolution by Euler Equations  $\pi(0,t) = 0, \quad \tau(1,t) = \overline{\tau}(t)$ 

 $\partial_{\tau} \tau (U(x,t), \mathcal{L}(x,t))$ 

 $\partial_r r = \partial_r \pi$  $\partial_t \pi = \partial_x \tau$  $\partial_{\tau} \mathcal{E} = \partial_{\tau} (\tau \pi)$ 

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# $\partial_t r = \partial_x \pi$ $\partial_t \pi = \partial_x \tau$ $\partial_t \mathcal{E} = \partial_x (\tau \pi)$

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This is an hyperbolic non-linear system of PDE, for smooth initial conditions will stay smooth up to a certain time then it will develop shocks and the solution should be indended in the *weak sense*. In the smooth regime the evolution is isoentropic in the sense... When shocks comes out, we have to consider weak solutions and uniqueness can be lost. Until the solution is smooth, entropy is constant (per material point) and the equation is completely reversible in time.

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 $\partial_t r = \partial_x \pi$  $\partial_t \pi = \partial_x \tau$  $\partial_t U = \tau \partial_x \pi$ 

$$\frac{d}{dt}S(U(x,t),r(x,t)) = \frac{1}{T}\partial_t U - \frac{\tau}{T}\partial_t r = 0$$

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 $\begin{array}{c} \partial_t r = \partial_x \pi \\ \partial_t \pi = \partial_x \tau \\ \partial_t U = \tau \partial_x \pi \\ \frac{d}{dx} S(U(x,t),r(x,t)) = \frac{1}{4} \partial_t U - \frac{\tau}{\pi} \partial_t r = 0 \end{array}$ 

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After shock appears, Entropy should increase:

$$\frac{d}{dt}S(U(x,t),r(x,t))\geq 0$$

Uniqueness of the weak *entropy solution* is an open problem.

 $\begin{array}{c} \partial_t r = \partial_t \pi \\ \partial_t d = -\partial_t \pi \\ \partial_t d = -\partial_t \pi \\ \frac{\partial}{\partial t} = -\partial_t \pi \\ \frac{\partial}{\partial t} \leq U(x,t), r(x,t)) = \frac{1}{T} \partial_t U - \frac{\pi}{T} \partial_t r = 0 \\ After shock appears. Entropy should increase: \\ \frac{\partial}{\partial t} \leq U(x,t), r(x,t) \geq 0 \\ Uniqueness. of the sub-strengy subcline is an open probability of the strength of the results in an open probability of the strength of the s$ 

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#### Example: isothermal transformations by diffusion equations

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

$$\partial_t r(x,t) = \partial_x^2 \overline{\tau}(x,t)$$
  
$$\partial_x r(0,t) = 0, \quad \overline{\tau}(1,t) = \tau_1$$

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Example: isothermal transformations by diffusion equations

 $\tilde{\tau}(x, t) = \tau(r(x, t), T)$   $\partial_t r(x, t) = \partial_x^2 \tilde{\tau}(x, t)$  $\partial_x r(0, t) = 0, \quad \tilde{\tau}(1, t) = \tau$ 

Example: isothermal transformations by diffusion equations

The rubber is immersed in a very viscous liquid at temperature T. Velocity are dunped down by the viscosity. We will see later how to obtain this diffusion equation from a microscopic model.

The convenient coordinates are  $\mathcal{L}, \mathcal{T}$ .

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free energy of the nonequilibrium profile  $\{r(x, t), x \in [0, 1]\}$ :

$$\mathcal{F}(t) = \int_0^1 F(r(x,t),T) \, dx, \qquad (F = U - TS) \tag{6}$$

$$\frac{d}{dt}\mathcal{F}(t) = -\int_0^1 \left(\partial_x \bar{\tau}(x,t)\right)^2 dx + \tau_1 \partial_x \tau(1,t)$$

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$$\begin{split} \tilde{\tau}(x, t) &= \tau(r(x, t), T) \\ & \partial_{x}r(x, t) - \partial_{x}^{2}\tilde{\tau}(x, t) \\ & \partial_{x}r(x, t) - \partial_{x} - \tilde{\tau}(1, t) - \tau_{1} \\ & for energy of the nonsequilibrium profile <math>\{r(x, t), x \in [0, 1]\}: \\ & \mathcal{F}(t) - \int_{0}^{1} F(r(x, t), T) \, dx, \quad (F - U - TS) \qquad (6) \\ & \frac{d}{T}_{x}\mathcal{F}(t) - \int_{0}^{-1} (\partial_{x}\tilde{\tau}(x, t))^{2} \, dx + \tau_{1}\partial_{x}\tau(1, t) \end{split}$$

The rubber is immersed in a very viscous liquid at temperature T. Velocity are dunped down by the viscosity. We will see later how to obtain this diffusion equation from a microscopic model.

The convenient coordinates are  $\mathcal{L}, \mathcal{T}$ .

$$\frac{d}{dt}\mathcal{L}(t) = \int_0^1 \partial_{xx} \bar{\tau}(x,t) \, dx = \partial_x \tau(1,t)$$

i.e.

$$\mathcal{F}(t) - \mathcal{F}(0) = \tau_1 \left( \mathcal{L}(t) - \mathcal{L}(0) \right) - \int_0^t ds \int_0^1 \left( \partial_x \bar{\tau}(x, s) \right)^2 dx$$
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initial global equilibrium  $r(x,0) = r_0$ ,  $\tau_0 = \tau(r_0, T)$ .  $t \to \infty$  we have  $r(x,t) \to r_1$ ,  $\tau_1 = \tau(r_1, T)$ .

$$F(r_1, T) - F(r_0, T) = \tau_1(r_1 - r_0) - \int_0^\infty ds \int_0^1 (\partial_x \bar{\tau}(x, t))^2 dx$$

 $\Delta F < W$ 

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$$\begin{split} & \text{kothermal by diffusion} \\ & & \frac{d}{dt} \mathcal{L}(t) = \int_0^1 d_{0,1} (t,x) \, dx + \partial_{1,1} (1,x) \\ & \text{is} \\ & \mathcal{L}(t) = f(t) = r_1 (\mathcal{L}(t) - \mathcal{L}(t)) - \int_0^1 d_{0,1} \int_0^1 (\partial_{1,1} f(x,x))^2 \, dx \\ & - W - \int_0^1 d_{0,1} \int_0^1 (\partial_{1,1} f(x,t))^2 \, dx \\ & - W - \int_0^1 d_{0,1} \int_0^1 (\partial_{1,1} f(x,t))^2 \, dx \\ & \text{for any base } (x,t) = r_0 \\ & - q = r_1 (t,t) \\ & f(r_1, T) - f(r_0, T) - q(r_1, r_2) - f_0^{-1} d_{0,1} \int_0^1 (\partial_{1,1} f(x,t))^2 \, dx \\ & \Delta T + W \end{aligned}$$

Notice that  $\tau_1(\mathcal{L}(t) - \mathcal{L}(0))$  is the work done up to time t by the force  $\tau_1$ , i.e. equal to W.

Suppose that the initial condition is give by the *global* equilibrium  $r(x,0) = r_0$  corresponding to the tension  $\tau_0$  and the temperature T. The sending  $t \rightarrow infty$ , the solution  $r(x,t) \rightarrow r_1$  where  $\tau(r_1,T) = \tau_1$ . So we have obtained for the difference of the free energy

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From dynamics to thermodynamics Thermodynamic crash course 
$$\begin{split} & \text{Instrumal by diffusion} \\ & & \frac{d}{dt} \mathcal{L}(0) = \int_0^1 \delta_{0,t} \tilde{v}(x,t) \, dx + \delta_{t,t}(1,t) \\ & \text{i.s} \\ & \mathcal{T}(t) = \mathcal{T}(0) = r_1(\mathcal{L}(t)) - \mathcal{L}(0) = \int_0^t ds \int_0^1 \left(\partial_t \tilde{v}(x,s)\right)^2 \, ds \\ & - W - \int_0^t ds \int_0^1 \left(\partial_t \tilde{v}(x,s)\right)^2 \, ds \\ & \frac{\partial H}{\partial t} \frac{\partial H}{\partial t} \frac{\partial H}{\partial t} \frac{\partial H}{\partial t} (t,t) = r_1(t,t) \\ & 1 = m \text{ where} \left( r_1(t) = r_1, \dots, r_n(t,t) \right) \\ & 1 = m \text{ where} \left( r_n(t) = r_n(t,t) - r_n(t,t) \right) \\ & 1 = m \text{ where} \left( r_n(t,t) = r_n(t,t) \right) \\ & 1 =$$

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From dynamics to thermodynamics Thermodynamic crash course 
$$\label{eq:states} \begin{split} & \text{bothermal by diffusion} \\ & \quad \frac{d}{dt}\mathcal{L}(t) - \int_{0}^{1} \partial_{tr} \mathcal{I}(x,t) \, dx + \partial_{tr} (1,t) \\ \text{i.e.} \\ & \mathcal{I}(t) - \mathcal{I}(0) - \tau_{1} \left( \mathcal{L}(t) - \mathcal{L}(0) \right) - \int_{0}^{1} dx \int_{0}^{1} \left( \partial_{tr} \mathcal{I}(x,t) \right)^{2} dx \\ & - W - \int_{0}^{1} dx \int_{0}^{1} \left( \partial_{tr} \mathcal{I}(x,t) \right)^{2} dx \\ \text{into glass parameters} \left( \mathcal{I}(t) - \sigma_{tr} - \sigma_{tr} - \sigma_{tr} \right) \\ & \mathcal{I} + \infty \text{ so have } \mathcal{I}(x, t) + \sigma_{tr} \\ & \pi - (\tau, \tau) \\ & \mathcal{I}(\tau, \tau) - \mathcal{I}(u, \tau) - (\tau, u, \tau) - \int_{0}^{1} dx \int_{0}^{1} \left( \partial_{tr} \mathcal{I}(x,t) \right)^{2} dx \\ & \Delta \mathcal{I} + \mathcal{W} \end{split}$$

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## Irreversible Isothermal Cycle

initial global equilibrium  $r(x,0) = r_0$ ,  $\tau_0 = \tau(r_0, T)$ .

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└── Irreversible Isothermal Cycle

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└─ Irreversible Isothermal Cycle

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Inverse transformation: initial global equilibrium

 $\begin{aligned} r(x,0) &= r_1, \qquad \tau_1 = \tau(r_1, T), \\ \text{and we apply the tension } \tau_0 &= \tau(r_0, T). \\ t &\to \infty \text{ we have } \tilde{r}(x,t) \to r_0, \qquad \tau_0 = \tau(r_0, T). \end{aligned}$ 

$$F(r_0, T) - F(r_1, T) = \tau_0(r_0 - r_1) - \int_0^\infty ds \int_0^1 (\partial_x \tau(\tilde{r}(x, t), T))^2 dx$$

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$$\begin{split} & \text{Inverse transformation: initial global equilibrium} \\ & r(x,0) = r_1, \qquad r_2 = \tau(r_2,T), \\ & \text{and we apply the tension } r_0 = \tau(r_0,T). \\ & t \to \infty \text{ we have } \tilde{r}(x,t) \to r_0, \qquad r_0 = \tau(r_0,T). \end{split}$$

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Summing up we have a cycle and

$$\begin{split} & W = (\tau_1 - \tau_0)(\tau_1 - \tau_0) \\ & \quad - \int_0^{\infty} ds \int_0^{1} \left[ (\partial_x \tau (r(x, t), T))^2 + (\partial_x \tau (\tilde{r}(x, t), T))^2 \right] dx \\ & \text{this work is gone to the thermostat as heat.} \end{split}$$

Summing up we have a cycle and

$$W = (\tau_1 - \tau_0)(r_1 - r_0)$$
  
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### Reversible quasi static isothermal transformation

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

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

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Reversible quasi static isothermal transformation

Pull slowly:  $\bar{\tau}(t)$  smooth and  $\bar{\tau}(0) = \tau_0$ ,  $\bar{\tau}(1) = \tau_1$   $\partial_t r'(x, t) = \partial_x^2 \tau(r'(x, t))$  $\partial_r r'(0, t) = 0$ ,  $\tau(r'(1, t)) = \bar{\tau}(t/\epsilon)$ 

Reversible quasi static isothermal transformation

In order to obtain the reversible (quasi static) transformation, we need to push or pool very slowly, with a tension  $\overline{\tau}(t/\epsilon)$  with  $\overline{\tau}$  that goes smoothly from  $\tau_0$  to  $\tau_1$ .

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!

### Reversible quasi static isothermal transformation

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after the limit as  $t \to \infty$ 

$$F(r_1, T) - F(r_0, T) = \int_0^\infty \tau(r^\epsilon(1, \epsilon t) \partial L^\epsilon(\epsilon t) dt + \epsilon \int_0^\infty ds \int_0^1 (\partial_x \tau(r(x, \epsilon t), T))^2 dx = W + \epsilon \int_0^\infty ds \int_0^1 (\partial_x \tau(r(x, \epsilon t), T))^2 dx$$

and take  $\epsilon \rightarrow 0$ :  $\Delta F = W$ .

From dynamics to thermodynamics Thermodynamic crash course Reversible quasi static isothermal transformation Reversible  $\frac{1}{\sqrt{n}} \int_{0}^{n} \frac{1}{\sqrt{n}} \int_{0}^{n} \frac{1}{\sqrt{n}}$ 

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### Theorem

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

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

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

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

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

$$\begin{split} & \frac{\mathsf{Theorem}}{\mathsf{v}(dx) \ \text{cantered probability on } \mathbb{R}^d, \, e^2 < \infty \\ & \mathsf{v}(dx) \ \text{cantered probability on } \mathbb{R}^d, \, e^2 < \infty \\ & \mathsf{v}(dx) \ \text{cantered probability } \mathsf{v}(dx) \\ & \mathsf{Theorem} \\ & \underbrace{\lim_{x \to \infty} \mathcal{E}_{x}(x) \ \mathrm{cantered probability } \mathcal{E}_{x}(dx) \\ & \mathsf{cantered probability } \mathsf{v}(dx) \\ & \mathsf{cantered probability } \mathsf{R}_{x}(dx) \\ & \mathsf{cantered probability } \mathsf{cantered probability } \mathsf{cantered probability } \mathsf{v}(dx) \\ & \mathsf{red}_{x}(x) \ \mathrm{cantered probability } \mathsf{red}_{x}(x)$$

# 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

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

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

From dynamics to thermodynamics Statistical Mechanics preliminaries: the art of tilting Local Large Deviations Theorem

### Local Large Deviations Theorem

$$\begin{split} \widetilde{S}_n &= \frac{1}{2} \sum_{j=1}^n X_j \text{ on } \mathbb{R}^r \text{ has density } f_n(\mathbf{x}). \end{split}$$
Theorem  $\lim_{n \to \infty} \frac{1}{n} \log f_n(\mathbf{y}) = -I(\mathbf{y}) \text{ .}$   $I(\mathbf{y}) = \sup \left\{ \lambda \cdot \mathbf{y} - \log \int \mathbf{e}^{\lambda \mathbf{y}} d\mathbf{e}(\mathbf{x}) \right\}$ 

(7)

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

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

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$$\begin{split} \Omega \text{ measurable topological space } & (\mathbb{R}^d, \mathbb{S}^d, \dots) \\ \alpha \text{ positive measure (Lebesgue, ...)} \\ & \mathbf{g} : \mathbf{\Omega} \to \mathbb{R}^{\mathsf{r}}, \\ & \mathcal{Z}(\boldsymbol{\lambda}) = \log \int_{\Omega} e^{\boldsymbol{\lambda} \cdot \mathbf{g}(\omega)} d\alpha(\omega) \end{split}$$

From dynamics to thermodynamics Statistical Mechanics Clicity - Preliminaries: the art of tilting Clicity - Tilting lting

 $Ω \text{ measurable topological space } (\mathbb{R}^d, \mathbb{S}^d, ...)$  α positive measure (Lebesgue, ...)  $g: Ω \rightarrow \mathbb{R}^s,$   $Z(λ) = \log \int_Ω e^{λg(ω)} dα(ω)$ 

 $\mathcal{Z}(\lambda)$  is convex and lower semicontinuous (it maybe not continuous). Again strict convexity follows by assuming that every component of **g** is not constant. Furthermore  $\mathcal{D}_{\mathcal{Z}}$  is convex. The Fenchel-Legendre transform is now defined by With respect to  $\alpha_{\lambda}$ , **g** can be seen as a vector valued random variable with average  $\nabla \mathcal{Z}(\lambda)$  and covariance matrix Hess $\mathcal{Z}(\lambda) = \nabla^2 \mathcal{Z}(\lambda)$ . Also

now  $\text{Hess}\mathcal{Z}(\boldsymbol{\lambda}) > 0$  just because **g** is not constant.

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$$\begin{split} \Omega \text{ measurable topological space } & (\mathbb{R}^d, \mathbb{S}^d, \dots) \\ \alpha \text{ positive measure (Lebesgue, ...)} \\ & \mathbf{g} : \mathbf{\Omega} \to \mathbb{R}^r, \\ & \mathcal{Z}(\boldsymbol{\lambda}) = \log \int_{\Omega} e^{\boldsymbol{\lambda} \cdot \mathbf{g}(\omega)} d\alpha(\omega) \\ & \mathcal{Z}^*(\mathbf{x}) = \sup_{\boldsymbol{\lambda}} \{ \boldsymbol{\lambda} \cdot \mathbf{x} - \mathcal{Z}(\boldsymbol{\lambda}) \}. \\ & \bar{\mathbf{x}} = \nabla \mathcal{Z}(\bar{\boldsymbol{\lambda}}) \\ & \bar{\boldsymbol{\lambda}} = \nabla \mathcal{Z}^*(\bar{\mathbf{x}}) \end{split}$$

From dynamics to thermodynamics

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Ω measurable topological space (ℝ<sup>d</sup>, S<sup>d</sup>,...)α positive measure (Lebesgue, ...)g: Ω → ℝ<sup>i</sup>,Z(λ) = log f<sub>Ω</sub> e<sup>λ</sup>E<sup>(ω)</sup>dα(ω)Z<sup>\*</sup>(x) = sop<sub>λ</sub> (λ : x - Z(λ)): $<math>\bar{x} = \nabla Z(\bar{x})$  $\bar{\lambda} = \nabla Z^*(g)$ 

 $\mathcal{Z}(\boldsymbol{\lambda})$  is convex and lower semicontinuous (it maybe not continuous). Again strict convexity follows by assuming that every component of **g** is not constant. Furthermore  $\mathcal{D}_{\mathcal{Z}}$  is convex. The Fenchel-Legendre transform is now defined by With respect to  $\alpha_{\boldsymbol{\lambda}}$ , **g** can be seen as a vector valued random variable

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$$\begin{split} \Omega \text{ measurable topological space } & (\mathbb{R}^d, \mathbb{S}^d, \dots) \\ \alpha \text{ positive measure (Lebesgue, ...)} \\ & \mathbf{g} : \mathbf{\Omega} \to \mathbb{R}^\mathbf{r}, \\ & \mathcal{Z}(\boldsymbol{\lambda}) = \log \int_{\Omega} e^{\boldsymbol{\lambda} \cdot \mathbf{g}(\omega)} d\alpha(\omega) \\ & \mathcal{Z}^*(\mathbf{x}) = \sup_{\boldsymbol{\lambda}} \{ \boldsymbol{\lambda} \cdot \mathbf{x} - \mathcal{Z}(\boldsymbol{\lambda}) \}. \\ & \bar{\mathbf{x}} = \nabla \mathcal{Z}(\bar{\boldsymbol{\lambda}}) \\ & \bar{\boldsymbol{\lambda}} = \nabla \mathcal{Z}^*(\bar{\mathbf{x}}) \end{split}$$

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

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From dynamics to thermodynamics

Statistical Mechanics

Compreliminaries: the art of tilting

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$$\begin{split} \Omega & \mbox{maxuable topological space } (\mathbb{R}^d, \mathbb{S}^d, \dots) \\ & \alpha & \mbox{positive masure } ( \mbox{laborations} (\mathbb{R}^d, \mathbb{S}^d, \dots) \\ & \mbox{g} : \Omega + \pi^d, \\ & \mathcal{Z}(\lambda) = \log f_0 \, e^{h \, \Pi(\omega)} d\alpha(\omega) \\ & \mathcal{Z}^*(\mathbf{x}) = \sup_{\lambda} (\lambda \cdot \mathbf{x} - Z(\lambda)), \\ & \quad \hat{\mathbf{x}} = \nabla Z(\hat{\mathbf{x}}) \\ & \quad \hat{\mathbf{\lambda}} = \nabla Z^*(\hat{\mathbf{x}}) \end{split}$$

 $d\alpha_{\lambda}(\omega) = e^{\lambda g - Z(\lambda)} d\alpha(\omega)$  tilted probability measure on  $\Omega$ 

 $\mathcal{Z}(\boldsymbol{\lambda})$  is convex and lower semicontinuous (it maybe not continuous). Again strict convexity follows by assuming that every component of **g** is not constant. Furthermore  $\mathcal{D}_{\mathcal{Z}}$  is convex. The Fenchel-Legendre transform is now defined by With respect to  $\alpha_{\boldsymbol{\lambda}}$ , **g** can be seen as a vector valued random variable with average  $\nabla \mathcal{Z}(\boldsymbol{\lambda})$  and covariance matrix  $\text{Hess}\mathcal{Z}(\boldsymbol{\lambda}) = \nabla^2 \mathcal{Z}(\boldsymbol{\lambda})$ . Also now  $\text{Hess}\mathcal{Z}(\boldsymbol{\lambda}) > 0$  just because **g** is not constant.

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

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

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

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From dynamics to thermodynamics Statistical Mechanics preliminaries: the art of tilting

 $Z(\lambda + \delta) - Z(\lambda) - \log \int_{\Omega} s^{\delta \cdot \theta} d\sigma_{\lambda}$   $l_{\lambda}(\mathbf{x}) - Z^{+}(\mathbf{x}) - \lambda \cdot \mathbf{x} + Z(\lambda)$ Large deviation rate function, under  $\sigma_{\lambda}^{+}$  on  $\Omega^{+}$ , for  $\mathbf{g}^{(\alpha)} - \frac{1}{2}\sum_{\lambda}^{\infty} \mathbf{g}^{(\alpha)}$  (8)

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

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

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

Large deviation rate function, under  $\alpha^n_{\lambda}$  on  $\Omega^n$ , for

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

# Conditioning

 $\alpha$  positive measure on  $\Omega$ ,  $g: \Omega \to \mathbb{R}^r$ .

From dynamics to thermodynamics Statistical Mechanics preliminaries: the art of tilting Conditioning Conditioning

 $\alpha$  positive measure on  $\Omega$ ,  $g : \Omega \rightarrow \mathbb{R}^{r}$ .

# Conditioning

 $\alpha$  positive measure on  $\Omega$ ,  $g: \Omega \to \mathbb{R}^r$ .

On  $\Omega^n$ , with the product measure  $d\alpha^n = \bigotimes_j d\alpha(\omega_j)$ , define

$$\mathbf{g}^{(n)} = \frac{1}{n} \sum_{j=1}^{n} \mathbf{g}(\omega_j)$$

From dynamics to thermodynamics Statistical Mechanics Preliminaries: the art of tilting Conditioning

#### Conditioning

 $\label{eq:gamma} \begin{array}{l} \alpha \mbox{ positive measure } \alpha \ \Omega, \ g : \Omega \to \mathbb{R}^r. \\ \mbox{ On } \Omega^\alpha, \mbox{ with the product measure } d\alpha^a = \oplus_j d\alpha(\omega_j), \\ \mbox{ define } \\ \mathbf{g}^{(a)} = \frac{1}{a} \sum_{j=1}^n \mathbf{g}(\omega_j) \end{array}$ 

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# Conditioning

 $\alpha$  positive measure on  $\Omega$ ,  $g: \Omega \to \mathbb{R}^r$ .

On  $\Omega^n$ , with the product measure  $d\alpha^n = \bigotimes_j d\alpha(\omega_j)$ , define

$$\mathbf{g}^{(n)} = \frac{1}{n} \sum_{j=1}^{n} \mathbf{g}(\omega_j)$$

On the surface (microcanonical)

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

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

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

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From dynamics to thermodynamics Statistical Mechanics preliminaries: the art of tilting Conditioning Constraints (a) particle measure of  $\Omega_{ij}$  ( $\Omega - \mathbb{R}^{ij}$ ,  $\Omega_{ij}$   $\Omega_{ij}^{(i)}$ , with the product measure of  $u^{i} = \eta_{ij} d_{ij}(\omega_{ij})$ , after  $\theta_{ij}^{(i)} = \frac{1}{2} \sum_{j=1}^{N} \theta_{ij}^{(j)}$ . On the surface (microsconstrai)  $\Gamma_{ij}(v) = \{(\alpha_{ij}, \dots, \alpha_{ij}) \in V_{ij}^{(i)}, v_{ij}^{(i)} > \eta_{ij}\}$ , differe 5 fields (set normalized) measure  $\gamma_{ij}(v_{ij}) \neq \eta_{ij}$  $\int_{ij} F_{ij}^{(i)} \Omega_{ij}^{(i)}(\omega_{ij}, \dots, \omega_{ij}) d_{ij}^{(i)}(\omega_{ij}, \dots, \omega_{ij})$ 

# Tilting and conditioning

Define the (*microcanonical*) volume

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

in the scalar case equal to

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

From dynamics to thermodynamics Statistical Mechanics preliminaries: the art of tilting Tilting and conditioning Tilting and conditioning Define the (microcanonical) volume  $W_n(y) = \int_{\Sigma^-(y)} d^n_{2n}(\omega_1, \dots, \omega_n; y)$ in the scalar case equal to  $W_n(y) = \frac{d}{dy} \int_{\Sigma^{(n)}(y)} dn^n(\omega_1, \dots, \omega_n).$ 

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# Tilting and conditioning

Define the (*microcanonical*) volume

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

in the scalar case equal to

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

Under  $\alpha_{\lambda}^{n}$ ,  $\mathbf{g}^{(n)} = \sum_{j} g(\omega_{j})/n$  has probability density

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

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

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

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From dynamics to thermodynamics Statistical Mechanics preliminaries: the art of tilting Tilting and conditioning 
$$\begin{split} \overline{\text{Thing and conditioning}} \\ \text{Define the (minimum leaf) where } \\ & \mathcal{H}(t) = \int_{K_{m,0}}^{t} d^{k}_{11}(w_1, \dots, w_{m}) \\ \text{ in the static case equal to } \\ & \mathcal{H}_{1}(t) = \frac{d}{dt} \int_{K_{m,0}}^{t} d^{k-1}(w_1, \dots, w_{m}) \\ \text{Under } w_{m}^{k} \ d^{k-1}(x_{1}(t)) + \text{the patholing family} \\ & u_{m}(t) = \int_{K_{m}}^{t} d^{k-1}(w_{m}(t)) \mathcal{H}(t) \\ \text{and the conditional patholing of } d^{k-1}(w_{m}(t)) \mathcal{H}_{2}(t) \\ & d^{k-1}(w_{m}^{k-1}(t)) = d^{k-1}(w_{m}^{k-1}(t)) \\ & d^{k-1}(w_{m}^{k-1}(t)) \\ & d^{k-1}(w_{m}^{k-1}(t)) = d^{k-1}(w_{m}^{k-1}(t)) \\ & d^{k-1}(w_{m}^{k-1}(t))$$

## Boltzmann formula

From dynamics to thermodynamics Statistical Mechanics preliminaries: the art of tilting Boltzmann formula Boltzmann formula

$$\begin{split} W_n(\mathbf{y}) &= e^{-e\left[\lambda \cdot \mathbf{y}-\mathcal{Z}(\lambda)\right]} f_{h,\lambda}(\mathbf{y}) \end{split}$$
 that imply  $\lim_{k\to\infty} \frac{1}{n} \log W_k(\mathbf{y}) = -\mathcal{Z}^*(\mathbf{y}) \end{split}$ 

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

that imply

$$\lim_{n\to\infty}\frac{1}{n}\log W_n(\mathbf{y})=-\mathcal{Z}^*(\mathbf{y})$$

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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  $\epsilon > 0$ 

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

#### Equivalence of Ensembles $y = \nabla Z(\lambda).$

Theorem Theorem exists a constant C > 0 such that for any  $\epsilon > 0$  $\lim_{m \to \infty} \frac{1}{m} \log \int_{\Sigma_{\alpha}(\mathbf{y})} \mathbf{1}_{[|F|\alpha|-f, Edv_{\alpha}] > ]} d\alpha^{(\alpha)}(\omega_{1}, ..., \omega_{n}|\mathbf{y}) \leq -C\epsilon^{2}$ . (9)

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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# Equivalence of Ensembles

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

### Theorem

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

$$\lim_{n\to\infty}\frac{1}{n}\log\int_{\Sigma_{n}(\mathbf{y})}\mathbf{1}_{\left[|F^{(n)}-\int Fd\alpha_{\lambda}|\geq\epsilon\right]}d\alpha^{(n)}(\omega_{1},\ldots,\omega_{n}|\mathbf{y})\leq-C\epsilon^{2}.$$
 (9)

### Theorem

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

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

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Transform Lat  $F(\omega_1, ..., \omega_k)$  a bounded continuous function on  $\Omega^k$  and  $y \in D_{d^{-1}}^{2}$ , then  $\lim_{n\to\infty} \int_{\Sigma_n(y)} F(\omega_1, ..., \omega_k) d\alpha^{(\alpha)}(\omega_1, ..., d\omega_n | y)$   $= \int_{\Omega^k} F(\omega_1, ..., \omega_k) \alpha_k(d\omega_1) ... \alpha_k(d\omega_k)$ 

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  $e^{-x_i^2/2}/\sqrt{2\pi}$ .



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

$$Z(\lambda,\beta) \coloneqq \int e^{-\beta V(r) + \lambda r} dr < +\infty \qquad \forall \beta > 0, \lambda \in \mathbb{R}.$$

From dynamics to thermodynamics

Statistical Mechanics

The microscopic model: chain of anharmonic oscillators

Chain of Oscillators

$$\begin{split} & \underset{m}{\underbrace{(m)}} \hat{f}_{1} \frac{1}{2} \underbrace{(m)}_{1} \hat{f}_{2} \underbrace{(m)}_{1} \underbrace{(m)}_{1}$$

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  $q_i, j = 1, \dots, m$  their positions, and with  $p_i$  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  $V(r) \rightarrow +\infty$  as  $|r| \rightarrow \infty$ and such that It is convenient to work with interparticle distance as coordinates, rather than absolute particle position, so we define  $\{r_i = q_i - q_{i-1} - a, i = 1, \dots, m\}.$ 



*m* = [*nM*], *M* = macroscopic mass.
 (*q<sub>j</sub>*, *p<sub>j</sub>*) ∈ ℝ<sup>2</sup>, *j* = 1, ..., *m*.
 *V*(*q<sub>i+1</sub>* - *q<sub>i</sub>*), *V*(*r*) → +∞.

$$Z(\lambda,\beta) \coloneqq \int e^{-\beta V(r) + \lambda r} dr < +\infty \qquad \forall \beta > 0, \lambda \in \mathbb{R}.$$
$$\{r_j = q_j - q_{j-1} - a, \ j = 1, \dots, m\}, \text{ and}$$

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

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Chain of Oscillators

$$\begin{split} & \underset{(p) \in \{1, 2, 3\}}{\underset{(p) \in \{1, 2\}}{\overset{(p)}{\longrightarrow}}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 2\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow} i\end{array}} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow} i\atop} \underbrace{ \begin{array}{c} \underset{(p) \in \{1, 3\}}{\overset{(p) \in \{1, 3\}}{\longrightarrow} i\atop} i\atop}$$

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  $q_i, j = 1, \dots, m$  their positions, and with  $p_i$  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  $\{r_i = q_i - q_{i-1} - a, j = 1, \dots, m\}.$ 

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$$\underbrace{\begin{array}{c} & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ &$$

$$\dot{r}_j(t) = p_j(t) - p_{j-1}(t), \qquad j = 1, \dots, m, \\ \dot{p}_j(t) = V'(r_{j+1}(t)) - V'(r_j(t)), \qquad j = 1, \dots, m-1, \\ \dot{p}_m(t) = \tau - V'(r_m(t)),$$

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 $\begin{array}{l} \dot{r}_j(t) = \rho_j(t) - \rho_{j-1}(t), \qquad j=1,\ldots,m, \\ \dot{\rho}_j(t) = V'(r_{j+1}(t)) - V'(r_j(t)), \qquad j=1,\ldots,m-1, \\ \dot{\rho}_m(t) = \tau - V'(r_m(t)), \end{array}$ 

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:

$$\underbrace{\begin{array}{c} & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ &$$

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Equilibrium measures:

$$d\alpha_{\tau,\beta}^{n,gc} = \prod_{j=1}^{m} \frac{e^{-\beta(\mathcal{E}_{j}-\tau r_{j})}}{\sqrt{2\pi\beta^{-1}}Z(\beta\tau,\beta)} dr_{j} dp_{j} \qquad \forall \beta > 0.$$

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Chain of Oscillators Chain of Oscillators  $d_{0} = \int_{0}^{1} \int_{0}^{1}$ 

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$$d\alpha_{\tau,\beta}^{n} = \prod_{j=1}^{m} \frac{e^{-\beta(\mathcal{E}_{j}-\tau r_{j})}}{\sqrt{2\pi\beta^{-1}}Z(\beta\tau,\beta)} dr_{j}dp_{j} = \prod_{j=1}^{m} e^{\lambda \cdot \mathbf{g}(r_{i},p_{i})-\mathcal{Z}(\boldsymbol{\lambda})} dr_{j}dp_{j}.$$

$$\Omega = \mathbb{R}^{2}, \qquad d\alpha = drdp,$$

$$\mathbf{g}(r,p) = \mathcal{E}(p,r), \qquad \boldsymbol{\lambda} = (-\beta, -\tau/\beta),$$

$$\mathcal{Z}(\boldsymbol{\lambda}) = \log \left[ Z(\beta\tau,\beta) \sqrt{\frac{2\pi}{\beta}} \right].$$

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

$$\begin{split} \tilde{\Sigma}_m(M, MU, M\mathcal{L}) &\coloneqq \left\{ (r_1, p_1, \dots, r_m, p_m) : \frac{1}{n} \sum_{j=1}^m \mathcal{E}_j = MU, \frac{1}{n} \sum_{j=1}^m r_j = M\mathcal{L} \right\} \\ &= \Sigma_m(U, \mathcal{L}) = \left\{ (r_1, p_1, \dots, r_m, p_m) : \mathcal{E}^{(m)} = U, r^{(m)} = \mathcal{L} \right\}. \end{split}$$

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators  $\begin{aligned}
u_{n,n} = \int_{\mathbb{R}^{2}} \frac{u_{n,n}}{(2\pi)^{2}} \frac{u_{n,n}}}{(2\pi)^{2}} \frac{u_{n,n}}{(2\pi)^{2}} \frac{u_{n,n}}} \frac{u_{n,n}}{(2\pi)^{2}} \frac{u_$ 

$$\Sigma_m(U, \mathcal{L}) = \{(r_1, p_1, \dots, r_m, p_m) : \mathcal{E}^{(m)} = U, r^{(m)} = \mathcal{L}\}.$$

$$W_m(U,\mathcal{L}) = \int_{\Sigma_m(U,\mathcal{L})} \gamma_n(dr_1, dp_1, \ldots, dp_m; U, \mathcal{L})$$

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Entropy!

Entropy!

 $\Sigma_m(U, \mathcal{L}) = \{(r_1, \rho_1, ..., r_m, \rho_m) : \mathcal{E}^{(m)} = U, r^{(m)} = \mathcal{L}\}.$  $W_m(U, \mathcal{L}) = \int_{\Sigma_m(U, \mathcal{L})} \gamma_m(dr_1, d\rho_1, ..., d\rho_m; U, \mathcal{L})$ 

This is the fundamental relation that connects the microscopic system to its thermodynamic macroscopic description.

$$\Sigma_m(U,\mathcal{L}) = \left\{ (r_1, p_1, \ldots, r_m, p_m) : \mathcal{E}^{(m)} = U, r^{(m)} = \mathcal{L} \right\}.$$

$$W_m(U,\mathcal{L}) = \int_{\Sigma_m(U,\mathcal{L})} \gamma_n(dr_1, dp_1, \ldots, dp_m; U, \mathcal{L})$$

The limit

$$S(M, MU, M\mathcal{L}) \coloneqq \lim_{n \to \infty} \frac{1}{n} \log W_m(U, \mathcal{L}) = MS(1, U, \mathcal{L})$$

exists and is concave and homogeneous of degree 1, and

$$S(U,\mathcal{L}) \coloneqq S(1,U,\mathcal{L}) = \inf_{\lambda,\beta>0} \left\{ -\lambda \mathcal{L} + \beta U - \log \left( Z(\lambda,\beta) \sqrt{2\pi\beta^{-1}} \right) \right\}.$$

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Statistical Mechanics

The microscopic model: chain of anharmonic oscillators

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Entropy!

$$\begin{split} & \Sigma_{\rm H}(U,L) = \Big\{ (\tau_1, \mu_1, \ldots, \tau_{\rm dr}, \mu_0) : \mathcal{L}^{(\alpha)} = U, \ell^{(\alpha)} = L \Big\}, \\ & W_{\rm dr}(U,L) = \int_{\Sigma_{\rm dr}(U,L)} \gamma_{\rm dr}(\Phi_1, \Phi_2, \ldots, \Phi_{\rm dr}; U,L) \\ & \text{The limit} \\ & S(M, MU, ML) = \lim_{d \to \infty} \frac{1}{d} \log W_{\rm dr}(U,L) = MS(1, U,L) \\ & \text{obtain an is concerned and homogeneous of diagone 1, and} \\ & S(U,L) = S(1, U,L) = \log (\frac{1}{d}, \left\lfloor -\Delta L + \beta U - \log \left( Z(\Lambda, \beta) \sqrt{2 \pi \beta^{-1}} \right) \right\rfloor \end{split}$$

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

#### Thermodynamic relations

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# Thermodynamic relations

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

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

They can be inverted:

$$\begin{aligned} \mathcal{L}(\lambda,\beta) &= \frac{\partial \log Z(\lambda,\beta)}{\partial \lambda} = \int r \, \frac{e^{\lambda r - \beta V(r)}}{Z(\lambda,\beta)} \, dr = \int r_j \, d\mu_{\tau,\beta}^{gc} \\ \mathcal{U}(\lambda,\beta) &= -\frac{\partial \log \left( Z(\lambda,\beta) \sqrt{2\pi/\beta} \right)}{\partial \beta} = \int V(r) \frac{e^{\lambda r - \beta V(r)}}{Z(\lambda,\beta)} \, dr + \frac{1}{2\beta} \\ &= \int \mathcal{E}_j \, d\mu_{\tau,\beta}^{gc} \end{aligned}$$

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$$\begin{split} U, \mathcal{L} \text{ so where the coordinates:} \\ & \tau (\beta + \lambda - \epsilon - \frac{\partial S}{\partial \mathcal{L}}) = \mathcal{J} = \frac{\partial S}{\partial \mathcal{U}} \\ & \text{They can be inverted.} \\ \mathcal{L}(\lambda, \beta) = \frac{\partial \log Z(\lambda, \beta)}{\partial \lambda} = \int \frac{e^{-\lambda (\lambda, \beta)}}{Z(\lambda, \beta)} dr = \int \tau_1 dr_{\beta, \beta}^{\mu} \\ & U(\lambda, \beta) = -\frac{\partial \log Z(\lambda, \beta) \sqrt{S/\beta}}{\partial \beta} = \int V(\eta) \frac{e^{\lambda - 2V(\eta)}}{Z(\lambda, \beta)} dr + \frac{1}{2} \\ & = \int F_1 dr_{\beta, \beta}^{\mu} \end{split}$$

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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  $\gamma_m$  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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$$S(M, MU, M\mathcal{L}) = M(1 + \log \pi + \log [U - \mathcal{L}^2/2]) = MS(U, \mathcal{L})$$

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Example: harmonic chain

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$$\beta = T^{-1} = \frac{\partial S}{\partial U} = \left[ U - \mathcal{L}^2 / 2 \right]^{-1}, \qquad \tau = -T \frac{\partial S}{\partial \mathcal{L}} = \mathcal{L}$$

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Example: harmonic chain  $\frac{\text{Europe humonic data}}{(1 - 2)^{2} - 2} \frac{(1 - 2)^{2}}{(1 - 1)^{2}} \frac{(1 - 2)^{2}}{$ 

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 $S = 1 + \log(\pi T),$   $F(\mathcal{L}, T) = U - T^{-1}S,$   $\partial_{\mathcal{L}}F = \partial_{\mathcal{L}}U = \mathcal{L}$ 

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Example: harmonic chain  $w_{1}(U_{c}) = \frac{(U_{c})^{-1}}{2} \cdot \frac{$ 

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From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Isocore dynamics: microcanonical measure.  $\frac{1}{100} + \frac{1}{100} + \frac{1}{$ 

$$\begin{split} \dot{r}_{j}(t) &= p_{j}(t) - p_{j-1}(t), \qquad j = 1, \dots, m-1, \\ \dot{p}_{j}(t) &= V'(r_{j+1}(t)) - V'(r_{j}(t)), \qquad j = 1, \dots, m-1, \\ r_{m}(t) &= m\mathcal{L} - \sum_{j=1}^{m-1} r_{j}(t) \,. \end{split}$$

 $\mathcal{H} = \sum_{j} \mathcal{E}_{j} = mU$  and  $\sum_{j=1}^{m} r_{j} = m\mathcal{L}$  are conserved.

Instead of applying a tension  $\tau$ , we fis the ends of the chain between two walls of distance  $m\mathcal{L}$ 

From dynamics to thermodynamics From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Isocore dynamics: microcanonical measure.  $\frac{t(0) - p(1) - p_1(1) - p_1($ 

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 $\mathcal{H} = \sum_{j} \mathcal{E}_{j} = mU$  and  $\sum_{j=1}^{m} r_{j} = m\mathcal{L}$  are conserved. Corresponding conditioned measure (microcanonical) are stationary. Instead of applying a tension  $\tau$ , we fis the ends of the chain between two walls of distance  $m\mathcal{L}$
From dynamics to thermodynamics From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Isocore dynamics: microcanonical measure. How the microscopic dynamics of the microcanonical measure.

$$\begin{split} \dot{r}_j(t) &= \rho_j(t) - \rho_{j-1}(t), \quad j = 1, \dots, m-1, \\ \dot{\rho}_j(t) &= V'(r_{j+1}(t)) - V'(r_j(t)), \quad j = 1, \dots, m-1, \\ r_m(t) &= m\mathcal{L} - \sum_{j=1}^{m-1} r_j(t) \;. \end{split}$$

 $H = \sum_j E_j = mU$  and  $\sum_{j=1}^{m} r_j = mL$  are conserved. Corresponding conditioned measure (microcanonical) are stationary.

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 $\mathcal{H} = \sum_{j} \mathcal{E}_{j} = mU$  and  $\sum_{j=1}^{m} r_{j} = m\mathcal{L}$  are conserved. Corresponding conditioned measure (microcanonical) are stationary.

Usually not the only one! Other conservation laws can be present.

Instead of applying a tension  $\tau$ , we fis the ends of the chain between two walls of distance  $m\mathcal{L}$ 

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#### Definition

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

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

From dynamics to thermodynamics 2012-03-18 Statistical Mechanics The microscopic model: chain of anharmonic oscillators -Local Equilibrium measures

#### ocal Equilibrium measures

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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.

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## Example: Local Gibbs

$$\prod_{j=1}^{n} \frac{e^{-\beta(j/n)(\mathcal{E}_{j}-\tau(j/n)r_{j})}}{\sqrt{2\pi\beta(j/n)^{-1}}Z(\beta(j/n)\tau(j/n),\beta(j/n))}}dr_{j}dp_{j} = g_{\tau(\cdot),\beta(\cdot)}^{n}\prod_{j=1}^{n}dr_{j}dp_{j}$$

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Example: Local Gibbs Example: Local Gibbs

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

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?

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## Example: Local Gibbs

$$\prod_{j=1}^{n} \frac{e^{-\beta(j/n)(\mathcal{E}_{j}-\tau(j/n)r_{j})}}{\sqrt{2\pi\beta(j/n)^{-1}}Z(\beta(j/n)\tau(j/n),\beta(j/n))} dr_{j}dp_{j} = g_{\tau(\cdot),\beta(\cdot)}^{n} \prod_{j=1}^{n} dr_{j}dp_{j}$$

or 1st order perturbations:

$$e^{\frac{1}{n}\sum_{j}F_{j}(r_{j-h},p_{j-h},...,r_{j+h},p_{j+h})}g_{\tau(\cdot),\beta(\cdot)}^{n}\prod_{j=1}^{n}dr_{j}dp_{j}$$
 (10)

with  $F_j$  local functions.

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Example: Local Gibbs Statistical Mechanics Local Gibbs Statistical Mechanics Statistical

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# Example: Local Gibbs

$$\prod_{j=1}^{n} \frac{e^{-\beta(j/n)(\mathcal{E}_{j}-\tau(j/n)r_{j})}}{\sqrt{2\pi\beta(j/n)^{-1}}Z(\beta(j/n)\tau(j/n),\beta(j/n))} dr_{j}dp_{j} = g_{\tau(\cdot),\beta(\cdot)}^{n} \prod_{j=1}^{n} dr_{j}dp_{j}$$

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(10)

with  $F_i$  local functions.

As in extended thermodynamics, define entropy of the local equilibrium

$$S(r(\cdot), u(\cdot)) = \int_0^1 S(r(y), u(y)) \, dy$$

where r(y), u(y) are computed from  $\tau(y), \beta(y)$ 

From dynamics to thermodynamics Statistical Mechanics The microscopic model: chain of anharmonic oscillators Example: Local Gibbs  $f(t) = \frac{1}{2} \int_{0}^{t} \frac{e^{-i(t)t}}{2} \int_{0}^{t} \frac{1}{2} \frac{e^{-i(t)t}}{2} \int_{0}^{t} \frac{e^{-i(t)t}}{2} \int_{0}^{t} \frac{1}{2} \frac{e$ 

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

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Langevin thermostats in each site:

 $w_j(t)$  i.i.d. standard Wiener processes.

From dynamics to thermodynamics Statistical Mechanics Statistical Mechanics Isothermal dynamics Isothermal dynamics

#### Isothermal dynamics

Langevin thermostats in each site:

 $\dot{r}_{i}(t) - p_{i}(t) - p_{j-1}(t), \quad j = 1, ..., n,$   $dp_{i}(t) - (V'(r_{i}, \iota(t)) - V'(r_{i}(t))) dt - p_{i}(t)dt + \sqrt{\beta}dw_{i}(t),$  j = 1, ..., n - 1,  $dp_{0}(t) - (r_{1} - V'(r_{i}(t))) dt - p_{0}(t)dt + \sqrt{\beta}dw_{i}(t)$  $w_{i}(t)$  i.i.d. standard Wiener processes.

Langevin thermostats are attached to each particle. They *maintain* the temperature of each site close to  $\beta^{-1} = T$ , in the sence that if there where not other interactions they would converge exponentially fast to a distribution of the velocities given by the corresponding maxwellian

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Langevin thermostats in each site:

$$\dot{r}_{j}(t) = p_{j}(t) - p_{j-1}(t), \qquad j = 1, \dots, n,$$
  

$$dp_{j}(t) = \left(V'(r_{j+1}(t)) - V'(r_{j}(t))\right) dt - p_{j}(t) dt + \sqrt{\beta} dw_{j}(t),$$
  

$$j = 1, \dots, n-1,$$
  

$$dp_{n}(t) = \left(\tau_{1} - V'(r_{n}(t))\right) dt - p_{n}(t) dt + \sqrt{\beta} dw_{n}(t)$$

 $w_j(t)$  i.i.d. standard Wiener processes.  $d\alpha^n_{\beta,\tau_1}$  is the only stationary probability. From dynamics to thermodynamics Statistical Mechanics Statistical Mechanics Isothermal dynamics Isothermal dynamics Isothermal dynamic

Langevin thermostats in each site:

 $\dot{r}_{j}(t) = \rho_{j}(t) - \rho_{j-1}(t), \quad j = 1,...,n,$   $dp_{j}(t) = (V'(\tau_{j-1}(t)) - V'(\tau_{j}(t))) dt - \rho_{j}(t) dt + \sqrt{j} dw_{j}(t),$  j = 1,...,n - 1,  $dp_{0}(t) - (\tau_{1} - V'(\tau_{n}(t))) dt - \rho_{0}(t) dt + \sqrt{j} dw_{n}(t),$  $w_{j}(t)$  i.i.d. standard Wiener processes.

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From dynamics to thermodynamics Statistical Mechanics Isothermal dynamics Non-equilibrium isothermal dynamics Non-equilibrium isothermal dynamics

We start instead with  $d\alpha^{0}_{\beta,\eta_{1}}$ , for  $\tau_{0} \neq \tau_{1}$ .

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From dynamics to thermodynamics Statistical Mechanics Isothermal dynamics Non-equilibrium isothermal dynamics

We start instead with  $d\alpha^{a}_{\beta,\eta_{1}}$ , for  $\eta_{2} + \eta_{2}$ . Eventually we converge to  $d\alpha^{a}_{\beta,\eta_{1}}$ . At which time scale? How?

We start instead with  $d\alpha_{\beta,\tau_0}^n$ , for  $\tau_0 \neq \tau_1$ . Eventually we converge to  $d\alpha_{\beta,\tau_1}^n$ . At which time scale? How?

From dynamics to thermodynamics

From dynamics

Statistical Mechanics

Isothermal dynamics

Non-equilibrium isothermal dynamics

Non-equilibrium isothermal dynamics

We start instead with  $d\alpha^{a}_{\beta_{1}\gamma_{2}}$ , for  $\tau_{0} + \tau_{1}$ . Eventually we converge to  $d\alpha^{a}_{\beta_{1}\gamma_{2}}$ . At which time scale? How?

Empirical Distribution: diffusive scaling

 $\mu_0(t)(G) = \frac{1}{n} \sum_{i=1}^n G\left(\frac{i}{n}\right) r_i(n^2 t)$ 

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From dynamics to thermodynamics Statistical Mechanics Isothermal dynamics Non-equilibrium isothermal dynamics Non-equilibrium isothermal dynamics

We start instead with  $d\alpha^{a}_{\beta,\eta}$ , for  $\tau_{0} + \tau_{1}$ . Eventually we converge to  $d\alpha^{a}_{\beta,\eta}$ . At which time scale? How?

Empirical Distribution: diffusive scaling  $\mu_{\theta}(t)(G) = \frac{1}{n} \sum_{i=1}^{n} G\left(\frac{i}{n}\right) r_{i}(n^{2}t)$ 

 $\mu_0(0) \rightarrow r_0 dy$ , with  $\tau(r_0, \beta^{-1}) = \tau_0$ .

We start instead with  $d\alpha^n_{\beta,\tau_0}$ , for  $\tau_0 \neq \tau_1$ . Eventually we converge to  $d\alpha^n_{\beta,\tau_1}$ . At which time scale? How?

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 $\mu_n(0) \rightarrow r_0 dy$ , with  $\tau(r_0, \beta^{-1}) = \tau_0$ .

## Isothermal diffusion limit

#### Theorem

$$\frac{1}{n}\sum_{i=1}^{n}G\left(\frac{i}{n}\right)r_{i}(n^{2}t) \underset{n \to \infty}{\longrightarrow} \int_{0}^{1}G(y)r(y,t)dy$$

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

$$\partial_t r(y,t) = \partial_y^2 \tau(r(y,t),T)$$
  
$$\partial_y r(0,t) = 0, \qquad \tau(r(1,t),T) = \tau_1$$

with  $T = \beta^{-1}$ .

From dynamics to thermodynamics Statistical Mechanics Isothermal dynamics Isothermal diffusion limit

Theorem 
$$\begin{split} &\frac{1}{n}\sum_{i=1}^n G\left(\frac{i}{n}\right)r_i(a^2t) \underset{m \to \infty}{\longrightarrow} \int_0^1 G(y)r(y,t)\,dy \end{split}$$
 is probability, with (y,t) solution of  $&\partial_t r(y,t) - \partial_y^2 r((y,t),T) \\ &\partial_t r(y,t) - \partial_y^2 r((t,y,t),T) \\ &\partial_t r(0,t) = 0, \qquad r(r(1,t),T) = r_1 \end{split}$  with  $T = J^{-1}. \end{split}$ 

sothermal diffusion limit

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

### Isothermal Diffusion: local equilibrium

Local Gibbs:

 $g_{\tau(\cdot,t)}^{n} = \prod_{i} e^{-\beta \left( \mathcal{E}_{i} - \tau(i/n,t)r_{i} + \frac{1}{n} (\partial_{y} \tau)(i/n)p_{i} \right) - \mathcal{Z}(\tau(i/n,t))}$ 

From dynamics to thermodynamics Statistical Mechanics Isothermal dynamics Isothermal Diffusion: local equilibrium Isothermal Diffusion: local equilibrium Local Gibbs:  $g_{r(s)}^{n} = \prod_{i} e^{-\beta [\xi_{i} - r(i(a_{i})_{i} - \frac{1}{2} (0, r(i)(a)_{i}) - 2(r(i(a_{i}))_{i}) -$ 

a first order correction to the local Gibbs is needed here: the average of the velocities are a bit tilted because of the gradient in the tension, the intuition is that velocities are small because damped, but of the order 1/n and pushed by the gradient of the tension.

the real distribution of the particles at time  $n^2 t$  is given by the solution of the forward equation

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### Isothermal Diffusion: local equilibrium

Local Gibbs:

 $g_{\tau(\cdot,t)}^{n} = \prod_{i} e^{-\beta \left( \mathcal{E}_{i} - \tau(i/n,t) r_{i} + \frac{1}{n} (\partial_{y} \tau)(i/n) p_{i} \right) - \mathcal{Z}(\tau(i/n,t))}$ 

$$\partial_t f_n(t, r_1, p_1, \dots) = n^2 L f_n(t, r_1, p_1, \dots)$$

$$L = A + S$$
  

$$A = \sum_{i} (p_{i} - p_{i-1})\partial_{r_{i}} + (V'(r_{i+1}) - V'(r_{i}))\partial_{p_{i}} + \tau_{1}\partial_{p_{n}}$$
  

$$S = \sum_{i} \beta^{-1}\partial_{p_{i}}^{2} - p_{i}\partial_{p_{i}}$$

 $f_n(t) \sim g_{\tau(\cdot,t)}^n$  in some sense.



a first order correction to the local Gibbs is needed here: the average of the velocities are a bit tilted because of the gradient in the tension, the intuition is that velocities are small because damped, but of the order 1/n and pushed by the gradient of the tension.

the real distribution of the particles at time  $n^2t$  is given by the solution of the forward equation

## Relative Entropy

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

From dynamics to thermodynamics Constraints of the statistical Mechanics Statistical Mechanics Isothermal dynamics Relative Entropy

#### Relative Entropy

 $H_{0}(t) = \int_{\mathbb{R}^{2n}} f_{0}(t) \log \left( \frac{f_{0}(t)}{g_{\tau(t)}^{0}} \right) \prod_{i} dp_{i} dr_{i}$ 

Add remark of relative entropy in probability, connected to LD, and thermodynamic entropy.

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.

this can be proven by Large deviation via the entropy inequality

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## Relative Entropy

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

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

$$\frac{1}{n}\sum_{j}G(i/n)F(r_{i+1},p_{i+1},\ldots,r_{i+k},p_{i+k}) \underset{n\to\infty}{\longrightarrow} \int_{0}^{1}G(y)\langle F \rangle_{\tau(y,t)} dy$$

in  $f_n(t)$ -probability.

 $\forall \delta > \mathsf{0}$ 

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

From dynamics to thermodynamics Statistical Mechanics Isothermal dynamics Relative Entropy

Relative Entropy  

$$H_0(r) = \int_{\mathbb{R}^n} f_0(r) \log\left(\frac{f_0(r)}{K_{1/2}^n}\right) \prod_{i=1}^n d_i dr_i$$
  
If  $H_0(r) = c(r)$  then  $f_0(r)$  has the factor equilibrium property:  
 $\frac{1}{n} \sum_{i=1}^n C(r) F(r_{i+1}, p_{i+1}, \dots, r_{i-n}, p_{i-1}) = \prod_{i=1}^n \int_0^r C(r)(F)_{r(2,I)} dr$   
 $\frac{1}{n} \int_0^r F_0(r) probability$   
 $\forall d = 0$   
 $\int F F_0(r) dpdr = \frac{1}{2} \int d^{-d^2} \frac{dr_{i-1}}{dr_{i-1}} dpdr + \frac{H_0(r)}{dr_{i-1}}$ 

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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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## Relative Entropy method

#### Compute

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

From dynamics to thermodynamics Statistical Mechanics Isothermal dynamics Relative Entropy method

remember that  $\tau(r, T) = \langle V' \rangle_{r,T}$ . par



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

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

## Relative Entropy method

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

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

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

in anharmonic case we need

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

From dynamics to thermodynamics Statistical Mechanics Isothermal dynamics Relative Entropy method

remember that  $\tau(r, T) = \langle V' \rangle_{r,T}$ . par

$$\label{eq:relative fixing method} \\ \hline \\ Compute \\ \frac{d^2_{11}(1)}{dt} \simeq \int \frac{d^2 L'_{11} d^2_{11} - \partial_{1} d^2_{11}}{dt} \, L_{11}(1) d_{11} d_{11} \\ - \int \sum_{i} (\partial_{i} r_{i})(r_{i}) \, I_{11}^{i}(r_{i}) - r_{i}(r_{i})(r_{i}) - \frac{d^2_{i}}{dt}(r_{i} - r(l), r_{i}) \right) L_{11}(1) d_{11} \\ \hline \\ the thermosic case  $\mathcal{P}(r_{i}) - r_{i}(r) + r_{i}$  and  $\frac{d^2_{21}(r_{i})}{dt} \leq \sigma(r) \\ the abstronged case or small \\ = \frac{1}{2} \sum_{i} \mathcal{V}(r_{i}) - r_{i}^{i} \frac{1}{2} \sum_{i} \frac{1}{2} \sum_{i} \mathcal{V}(r_{i}) - r_{i}^{i} \frac{1}{2} \sum_{i} \mathcal{V}(r_{i}) - r_{i}^{i} \frac{1}{2} \sum_{i} \frac{1}{2} \sum_{i} \mathcal{V}(r_{i}) - r_{i}^{i} \frac{1}{2} \sum_{i} \frac{1}{2} \sum_{$$$

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if we can justify

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

then we are left with

$$\int \sum_{i} (\partial_t \tau) (i/n, t) [\tau(\bar{r}_{i,k}) - \tau(r(i/n, t)) - \frac{d\tau}{dr}(\bar{r}_{i,k} - r(i/n, t))] f_n(t) d\alpha_{0,\beta}^n + o(k, n)$$

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

From dynamics to thermodynamics if we can justify  $\frac{1}{k}\sum_{i=1}^{k} V'(r_{i+j}) \sim \tau \left(\frac{1}{k}\sum_{i=1}^{k} r_{i+j}, T\right)$ 2012-03-18 -Statistical Mechanics then we are left with -Isothermal dynamics  $\int \sum_{i} (\partial_t \tau)(i/n, t) [\tau(\tilde{\tau}_{i,k}) - \tau(r(i/n, t)) - \frac{d\tau}{dr}(\tilde{\tau}_{i,k} - r(i/n, t))] f_0(t) d\alpha_{0,i}^0$  $r_{i,k} = \frac{1}{k} \sum_{j=1}^{k} r_{i+j} \qquad \frac{o(k,n)}{n} \xrightarrow[n \to \infty, k \to \infty]{} 0$ 

+o(k,n)

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$$\begin{split} \int \sum_{i} (\partial_t \tau) (i/n, t) [\tau(\bar{r}_{i,k}) - \tau(r(i/n, t)) - \frac{d\tau}{dr} (\bar{r}_{i,k} - r(i/n, t))] f_n(t) d\alpha_{0,\beta}^n \\ \leq C \int \sum_{i} (\bar{r}_{i,k} - r(i/n, t))^2 f_n(t) d\alpha_{0,\beta}^n + o(k, n) \\ r_{i,k} = \frac{1}{k} \sum_{j=1}^k r_{i+j} \qquad \frac{o(k, n)}{n} \underset{n \to \infty, k \to \infty}{\longrightarrow} 0. \end{split}$$



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From dynamics to thermodynamics Statistical Mechanics Statistical Mechanics Isothermal dynamics relative entropy (end) relative entropy (end)

Use again the relative entropy inequality:

 $\leq \frac{C}{x} \log \int e^{\delta \sum_{i} (\tilde{c}_{i,k} - r(i/n,t))^2} g_{\delta}(t) d\alpha_{0,\beta}^n + C \frac{H_{\delta}(t)}{x} + o(n,k)$  $\leq C \frac{H_{\alpha}(t)}{s} + o_1(n, k)$ 

and conclude by Gronwall that  $H_{\delta}(t) \sim o(n)$ .

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From dynamics to thermodynamics Statistical Mechanics Statistical Mechanics Isothermal dynamics relative entropy (end) relative entropy (end)

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From dynamics to thermodynamics EC-Statistical Mechanics Isothermal dynamics L-I-block estimate

#### 1-block estimate

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

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

We have here already some information about the local equilibrium: the velocities are automatically distributed by a maxwellian at temperature  $T = \beta^{-1}$ .

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From dynamics to thermodynamics EC-Statistical Mechanics Isothermal dynamics L-I-block estimate 
$$\begin{split} \frac{1 \operatorname{block}\operatorname{estimate}}{\frac{\lim_{n \to \infty} \lim_{k \to \infty} \int_{0}^{1} \int_{\mathbb{R}^{n}} \frac{1}{k} \sum_{j=1}^{n} \frac{|z_{j}|^{2}}{k} \sum_{j=1}^{n} \frac{|z_{j}|^{2}}{k} \sum_{j=1}^{n} \frac{|z_{j}|^{2}}{k} \sum_{j=1}^{n} \frac{|z_{j}|^{2}}{k} e_{ij}, \tau \Big| \int_{0}^{1} d_{i}(1) dw_{0,i}^{2} = 0}{\frac{1}{\tau} \int_{0}^{1} \frac{d(1)}{k} \sum_{j=1}^{n} \frac{d(1)}{k} du_{0,j}^{2} \leq \frac{1}{\kappa}} \end{split}$$

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

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$$\frac{1}{t} \int_0^t f_n(t) = \overline{f}_n$$
$$\sum_i \int \frac{(\partial_{p_i} \overline{f}_n)^2}{\overline{f}_n} d\alpha_{0,\beta}^n \leq \frac{C}{n}$$

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

$$\begin{split} \frac{1}{2} \frac{\log |\log_{1} f_{0}|}{\int_{0}^{1} \int_{0}^{1} \frac{1}{q_{0}^{2}} \left[\frac{1}{q_{0}^{2}} \sum_{j=1}^{N} \left[\frac{1}{q_{0}^{2}} \sum_{j=1}^{N}$$

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

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$$\frac{1}{t} \int_{0}^{t} f_{n}(t) = \bar{f}_{n}$$
$$\sum_{i} \int \frac{(\partial_{p_{i}}\bar{f}_{n})^{2}}{\bar{f}_{n}} d\alpha_{0,\beta}^{n} \leq \frac{C}{n}$$
$$\Longrightarrow \bar{f}_{n}\Big|_{[i,i+k]} \xrightarrow{n \to \infty} \tilde{f}^{(i,k)}(r_{1},\ldots,r_{k})$$

independent of the *p*'s!

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

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

$$\int AF \, d\nu_i = \int (A+S)F \, d\nu_i = \lim_{n \to \infty} \int LF_i \, \bar{f}_n d\alpha_{\beta,0}^n$$
$$= \lim_{n \to \infty} \frac{1}{n^2 t} \int_0^t ds \int n^2 LF_i \, f_n(s) d\alpha_{\beta,0}^n$$
$$= \lim_{n \to \infty} \frac{1}{n^2 t} \int F_i \, [f_n(t) - f_n(0)] d\alpha_{\beta,0}^n = 0.$$
$$\implies d\nu_i = \int d\alpha_{\beta,\tau}^\infty \, d\tilde{\nu}_i(\tau)$$

From dynamics to thermodynamics 5 Statistical Mechanics 5 Isothermal dynamics 5 I-1-block estimate

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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  $\tau$ . 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

$$\underbrace{\begin{array}{c} & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

$$\begin{split} \dot{r}_{j}(t) &= p_{j}(t) - p_{j-1}(t), \qquad j = 1, \dots, n, \\ dp_{j}(t) &= \left( V'(r_{j+1}(t)) - V'(r_{j}(t)) \right) dt, \qquad j = 1, \dots, n-1, \\ dp_{n}(t) &= \left( \tau_{1} - V'(r_{n}(t)) \right) dt \end{split}$$

From dynamics to thermodynamics Prom dynamics to thermodynamics Constraints Cons



$$\begin{split} \dot{r}_j(t) &= \rho_j(t) - \rho_{j-1}(t), \qquad j = 1, \dots, n, \\ d\rho_j(t) &= \left(V'(r_{j+1}(t)) - V'(r_j(t))\right) dt, \qquad j = 1, \dots, n-1, \\ d\rho_n(t) &= \left(\tau_1 - V'(r_n(t))\right) dt \end{split}$$

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Deterministic dynamics: difficult!

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

From dynamics to thermodynamics



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# Hyperbolic Adiabatic Dynamics

3 conserved quantities:

stretch  $\mathcal{R}_n(t)[G] = \frac{1}{n} \sum_i G(i/n) r_i(nt)$ momentum  $\pi_n(t)[G] = \frac{1}{n} \sum_i G(i/n) p_i(nt)$ energy  $\mathfrak{e}_n(t)[G] = \frac{1}{n} \sum_i G(i/n) \mathcal{E}_i(nt)$  From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Hyperbolic Adiabatic Dynamics Hyperbolic Adiabatic Dynamics

B conserved quantities: stretch  $\mathcal{R}_{n}(t)[G] = \frac{1}{n} \sum_{i} G(i/n)r_{i}(nt)$ momentum  $\pi_{n}(t)[G] = \frac{1}{n} \sum_{i} G(i/n)p_{i}(nt)$ energy  $e_{n}(t)[G] = \frac{1}{n} \sum_{i} G(i/n)E_{i}(nt)$ 

we expect the convergence to the hyperbolic system of PDE this is an open problem also in the smooth regime of the equations, and it is not true for the harmonic case.

Its validity depends from the ergodic properties of the corresponding infinite dynamics.

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 $(\mathcal{R}_n(t), \pi_n(t), \mathfrak{e}_n(t)) \longrightarrow (r(x, t)dx, \pi(x, t)dx, \mathfrak{e}(x, t)dx)$  $\partial_t r = \partial_x \pi$  $\partial_t \pi = \partial_x \tau$  $\partial_t \mathfrak{e} = \partial_x (\tau \pi)$  $\partial r(0, t) = 0, \qquad \tau(r(1, t), U(1, t)) = \tau_1$ 

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Hyperbolic Adiabatic Dynamics Hyperbolic Adiabatic Dynamics

$$\begin{split} & 1 \operatorname{semical} g_{n}(G(G) = 1 + \sum_{i} G(i) g_{i}(x_{i}) \\ & \operatorname{semical} g_{n}(i) (G) = 1 + \sum_{i} G(i) g_{i}(x_{i}) \\ & \operatorname{semical} g_{n}(x_{i}) (G(G) - \frac{1}{2} \sum_{i} G(i) g_{i}(x_{i}) \\ & \operatorname{semical} g_{n}(x_{i}) = e_{n}(i) (G(G) - \frac{1}{2} \sum_{i} G(i) g_{i}(x_{i}) \\ & \operatorname{semical} g_{n}(x_{i}) = e_{n}(i) \\ & \operatorname{semical} g_{n}(x_{i}) \\ & \operatorname{$$

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# Ergodicity of the infinite dynamics

Consider the dynamics of the infinite system:

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

From dynamics to thermodynamics Provide Statistical Mechanics Adiabatic dynamics Ergodicity of the infinite dynamics Ergodicity of the infinite dynamics

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Under this ergodic property, the 1-block estimate that we described before it is possible to prove, and relative entropy method works fine at least in the smooth regime of the macroscopic equations.

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We say that it is *ergodic* if all stationary translational invariant probability measures locally absolutely continuous are convex combinations of the Gibbs measures:

$$d\alpha_{\beta,\pi,\tau} = \prod_{j \in \mathbb{Z}} e^{-\beta \mathcal{E}_j + \pi p_j + \tau r_j - \mathcal{Z}(\beta,\pi,\tau)} dr_j dp_j$$

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Not true for harmonic chain or any other completely integrable system.

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Ergodicity of the infinite dynamics Ergodicity of the infinite dynamics

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## Velocity echeangeability

### 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

 $d\nu(\mathbf{p}|\mathbf{r})$ 

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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

is excheangeable, then it is a convex combination of Gibbs measures.

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.

From dynamics to thermodynamics Constraints Stochastic dynamic perturbations

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

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

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

momentum exchange For each couple of nearest neighbor particle, we randomly exchange momentum,  $(p_i, p_{i+1}) \rightarrow (p_{i+1}, p_i)$ , with intensity 1. The resulting infinite dynamics has the ergodic property. From dynamics to thermodynamics
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Stochastic dynamic perturbations

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With this stochastic perturbation, we can prove the convergence to the Euler system of PDE, at least in the smooth regime.

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

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### Harmonic case

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

$$\partial_t r = \partial_x \pi$$
$$\partial_t \pi = \partial_x r$$
$$\partial_t \mathfrak{e} = \partial_x (r\pi)$$
$$\partial r(0, t) = 0, \qquad r(1, t) = \tau_1$$

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

From dynamics to thermodynamics 5 Statistical Mechanics C Adiabatic dynamics C Harmonic case narmonic case

If  $V(r) = \frac{d^2}{2}$ , we have  $\tau(\mathcal{L}, U) = \mathcal{L}$ , and the system bacame  $\partial_t r = \partial_t \pi$   $\partial_t = -\partial_t r$   $\partial_t = -\partial_t (r\pi)$   $\partial_t = \partial_t (r\pi)$   $\partial_t (0, t) = 0$ ,  $r(1, t) = r_1$ Linear wave exactly t = solicit (ct, r) as function of the solution

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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Linear wave equation + explicit  $\mathfrak{e}(x, t)$  as function of the solution of it. No dissipation on the hyperbolic space-time scale. From dynamics to thermodynamics 5 Statistical Mechanics C Adiabatic dynamics C Harmonic case

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From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Adiabatic diffusion of Energy 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.

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# Chain of Anharmonic oscillators

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

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

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

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$$dq_i = p_i dt$$
  
 $dp_i = -\partial_{q_i} \mathcal{H} dt$ 

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Chain of Anharmonic oscillators Chain of Anharmonic oscillators 
$$\begin{split} \rho_i, q_i \in \mathbb{R}, \ i \in \mathbb{N}, \ |\alpha - N \ or \ h - \mathbb{Z}, \\ \mathcal{H} &= \sum_i \left[ \frac{d^2}{2} + V(q_i - q_{i-1}) + U(q_i) \right] \\ &\quad - \sum_i q_i \\ &\quad dq_i - p_i \ dt \\ &\quad dq_i - dt, \ dt \end{split}$$

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$$dQ_{\beta} = \frac{e^{-\beta \mathcal{H}}}{Z_{\beta}} dp dq \qquad \beta = T^{-1} > 0$$

 From dynamics to thermodynamics
 Chain of Anharmonic oscillators

 End dynamics
  $\mu_{e,e,E}, i, k, k = k = k = k$  

 Adiabatic dynamics
  $\mu_{e,e,E}, i, k, k = k = k = k$  

 Chain of Anharmonic oscillators
  $\frac{d_{e,e,e,R}}{d_{e,e,e,R}}$ 
 $d_{e,e,e,R}, i, k = k = k = k$   $d_{e,e,e,R}, i, k = k = k = k$ 
 $d_{e,e,e,R}, i, k = k = k$   $d_{e,e,e,R}, i, k = k = k$ 
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 $e_i = \frac{p_i^2}{2} + V(q_i - q_{i-1}) + U(q_i)$  Energy of atom *i*.

$$e_i = \frac{p_i^2}{2} + V(q_i - q_{i-1}) + U(q_i) \qquad \text{Energy of atom } i.$$

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From dynamics to thermodynamics EC Statistical Mechanics Adiabatic dynamics

$$\begin{split} e_i &= \frac{p_i^2}{2} + V(q_i - q_{i-1}) + U(q_i) \qquad \text{Energy of atom } i. \\ \dot{e}_i &= \left(j_{i-1,i} - j_{i,i+1}\right) \quad \text{local conservation of energy}. \end{split}$$

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 $\dot{e}_i = (J_{i-1,i} - J_{i,i+1})$  local conservation of energy.

From dynamics to thermodynamics E-Statistical Mechanics Adiabatic dynamics

$$\begin{split} e_i &= \frac{p_i^2}{2} + V(q_i - q_{i-1}) + U(q_i) \qquad \text{Energy of atom } i. \\ \dot{e}_i &= \begin{pmatrix} y_{i-1,i} & -y_{i,i+1} \end{pmatrix} \quad \text{local conservation of energy.} \\ y_{i,i+1} &= -\rho_i V^i(q_{i+1} - q_i) \qquad \text{hamiltonian energy currents} \end{split}$$

$$e_i = \frac{p_i^2}{2} + V(q_i - q_{i-1}) + U(q_i) \qquad \text{Energy of atom } i.$$

 $\dot{e}_i = (J_{i-1,i} - J_{i,i+1})$  local conservation of energy.

 $J_{i,i+1} = -p_i V'(q_{i+1} - q_i)$  hamiltonian energy currents

## Non-stationary behavior

We would like to prove that

$$\frac{1}{N}\sum_{i}G(i/N)e_{i}(N^{2}t) \underset{N \to \infty}{\longrightarrow} \int G(y)u(t,y)dy$$

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:

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

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

#### Non-stationary behavior

We would like to prove that  $\frac{1}{N}\sum_{\gamma}G(x)(N)v_{1}(X^{2}x)\sum_{M=m}\int G(x)v_{2}(x,y)dy$ with w(x,y) aluston of the nonlinear bast quantum:  $\partial_{M}a = \partial_{\mu}D(w)\partial_{\mu}a$  with the thermal conductivity diffind by the Greene-Kube formula  $D(w) = \chi_{0}^{-1}\sum_{m}\int_{0}^{m}\left((\mu_{1}x)(\chi_{0}x)(\eta_{m})dy\right)dy dx, \qquad \beta = \beta(w)$ 

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Not clear under which initial conditions such limit would be true

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

#### Non-stationary behavior

We would like its prove that  $\frac{1}{N}\sum_{i}G(i)(N_i(k^*)) \max_{m=i} \int G(i)u(x_i)dy \\ \text{with } u(x_i) \text{ isothism } dh \text{ monotone has the quarkine:} \\ \partial_i u = \partial_i D(u)\partial_i u \\ \text{with the thermal conductively defined by the Green-Kode formula <math display="block">D(u) = \sum_{i} \sum_{m} \int_{-\infty}^{\infty} (j_{i+1}(x_i))u(y_i) w \\ (i, j_{i+1}) = \partial_i u(y_i) \\ N(u) = (u, u) = \sum_{i} \sum_{m} \int_{-\infty}^{\infty} (j_{i+1}(x_i))u(y_i) w \\ (i, j_{i+1}) = \sum_{i} \partial_i u(y_i) \\ N(u) = (u, u) = \sum_{i} \sum_{m} \int_{-\infty}^{\infty} (j_{i+1}(x_i))u(y_i) w \\ (i, j_{i+1}) = \sum_{i} \sum_{m} \int_{-\infty}^{\infty} (j_{i+1}(x_i))u(y_i) w \\ (i, j_{i+1}) = \sum_{i} \sum_{m} \int_{-\infty}^{\infty} (j_{i+1}(x_i))u(y_i) w \\ (i, j_{i+1}) = \sum_{i} \sum_{m} \int_{-\infty}^{\infty} (j_{i+1}(x_i))u(y_i) w \\ (i, j_{i+1}) = \sum_{i} \sum_{m} \sum_{j=1}^{\infty} (j_{i+1}(x_i))u(y_i) w \\ (i, j_{i+1}) = \sum_{i} \sum_{j=1}^{\infty} (j_{i+1}(x_i))u(y_i) w \\ (i, j_{i+1}) = \sum_{j=1}^{\infty} (j_{i+1}(x_j))u(y_i) w \\ (i, j_{i+1})u(y_i) = \sum_{j=1}^{\infty} (j_{i+1}(x_j))u(y_i) w \\ (i, j_{i+1})u(y_i) = \sum_{j=1}^{\infty} (j_{i+1}(x_j))u(y_i)u(y_i) w \\ (i, j_{i+1})u(y_i)u($ 

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# Equilibrium Fluctuations: Linear response

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

From dynamics to thermodynamics From dynamics I dechanics Adiabatic dynamics Equilibrium Fluctuations: Linear response Equilibrium Fluctuations: Linear response

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Consider the system in equilibrium at temperature  $T = \beta^{-1}$ , and perturbe it at time 0 in atom 0 by adding some energy there:

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Equilibrium Fluctuations: Linear response Equilibrium Fluctuations: Linear response

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$$dQ'_{\beta} = \frac{e_0}{\langle e_0 \rangle_{\beta}} dQ_{\beta}$$

We want to study the time evolution of

$$< e_i(t) >_{Q'_{\beta}} = \int e_i dQ'_{\beta,t} = rac{< e_i(t)e_0(0) >}{< e_0 >}$$

 Equilibrium Fluctuations: Linear response

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## Linear response

Assuming that the corresponding limits exist, we have that

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

with 
$$\chi(\beta) = \sum_i (\langle e_i e_0 \rangle_\beta - \langle e_i \rangle_\beta \langle e_0 \rangle_\beta).$$



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with  $\chi(\beta) = \sum_i (\langle e_i e_0 \rangle_{\beta} - \langle e_i \rangle_{\beta} \langle e_0 \rangle_{\beta})$ . In fact, using stationarity and translation invariance

$$< e_{0} >_{\beta} \sum_{i \in \mathbb{Z}} i^{2} < e_{i}(t) >_{Q_{\beta}'} = \sum_{i \in \mathbb{Z}} i^{2} < (e_{i}(t) - e_{i}(0))e_{i}(0) >_{\beta}$$
$$= 2 \int_{0}^{t} ds \int_{0}^{s} d\tau \sum_{i} \langle J_{i,i+1}(s - \tau)J_{0,1}(0) \rangle$$
$$\xrightarrow{t \to \infty} 2 \int_{0}^{\infty} \sum_{i} \langle J_{i,i+1}(s)J_{0,1}(0) \rangle ds$$

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Linear response



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Define

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#### Linearized heat equation

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

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 $C(i,j,t) = \langle e_i(t)e_j(0) \rangle_{\beta} - \bar{e}^2$ 

From dynamics to thermodynamics EC Statistical Mechanics Adiabatic dynamics Linearized heat equation

#### Linearized heat equation

Define  $C(i,j,t) = < v_i(t)v_0(0) >_\beta - \vec{v}^2$ Conjecture:  $\boxed{NC([Me];[My], N^2t) \xrightarrow[N \to \infty]{} (2\pi D)^{-1/2} \exp\left(-\frac{(x-y)^2}{2tD}\right)}$ 

### Define

$$C(i,j,t) = \langle e_i(t)e_j(0) \rangle_{\beta} - \bar{e}^2$$

Conjecture:

$$\boxed{\mathsf{NC}([\mathsf{N}x],[\mathsf{N}y],\mathsf{N}^2t) \xrightarrow[\mathsf{N}\to\infty]{} (2\pi\mathcal{D})^{-1/2} \exp\left(-\frac{(x-y)^2}{2t\mathcal{D}}\right)}$$

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Linearized heat equation

#### Linearized heat equation

| Define         | $C(i, j, t) = \langle a_j(t)a_j(0) \rangle_{ij} - \tilde{a}^2$  |
|----------------|---|
| Conjecture:    |   |
| NC([           | $Wx$ ], $[Ny], N^2t$ ) $\xrightarrow[N\to\infty]{} (2\pi D)^{-1/2} \exp\left(-\frac{(x-y)^2}{2tD}\right)$ |
| i.e. the limit | follows the linearized heat equation  |
|                | $\partial_{\alpha}C = D\partial_{\alpha}C$  |

### Define

$$C(i,j,t) = \langle e_i(t)e_j(0) \rangle_\beta - \bar{e}^2$$

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 $\partial_t C = \mathcal{D} \partial_{xx} C$ 

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From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Linearized heat equation

#### Linearized heat equation

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i.e. the limit follows the linearized heat equation

 $\partial_t C = \mathcal{D} \partial_{xx} C$ 

this is more challenging than proving existence for  $\mathcal{D}$ .

# How to prove this?

Define, for a *good* choice of a sequence of smooth local functions  $\mathcal{F}_n$ 

$$\Phi_n = \mathsf{J}_{0,1} - \mathcal{D}(e_1 - e_0) - \mathcal{LF}_n$$

with L the generator of the dynamics,

From dynamics to thermodynamics ECONT CONT CO

#### How to prove this?

Define, for a good choice of a sequence of smooth local functions  $\mathcal{F}_{\alpha}^{-}$  $\Phi_{\alpha} = j_{0,1} - \mathcal{D}(\phi_{1} - a_{0}) - L\mathcal{F}_{\alpha}$ with L the generator of the dynamics,

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# How to prove this?

Define, for a good choice of a sequence of smooth local functions  $\mathcal{F}_n$ 

$$\Phi_n = \mathsf{J}_{0,1} - \mathcal{D}(e_1 - e_0) - \mathcal{LF}_n$$

with *L* the generator of the dynamics, and pick a nice test function G(x):

$$\frac{1}{N}\sum_{i,j}G\left(\frac{i}{N}\right)F\left(\frac{j}{N}\right)\left[C(i,j,N^{2}t)-C(i,j,0)\right]$$
$$=\frac{1}{N}\sum_{i,j}G\left(\frac{i}{N}\right)F\left(\frac{j}{N}\right)\left\langle (e_{i}(N^{2}t)-e_{i}(0))e_{j}(0)\right\rangle$$

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics How to prove this?

#### How to prove this

Define, for a good choice of a sequence of smooth local functions  $\mathcal{F}_{\alpha}^{-} = p_{0,1} - D(e_1 - e_0) - L\mathcal{F}_{\alpha}$ with *L* the generator of the dynamics, and pick a nice test function C(x),  $\frac{1}{N} \sum G\left(\frac{i}{N}\right) F\left(\frac{i}{M}\right) \left[C(i,j,N^2t) - C(i,j,0)\right]$ 

 $\frac{1}{N}\sum_{i,j}^{N} G\left(\frac{1}{N}\right)F\left(\frac{j}{N}\right)\left[C(i,j,N^{*}t) - C(i,j,0)\right]$   $= \frac{1}{N}\sum_{i,j}^{N} G\left(\frac{j}{N}\right)F\left(\frac{j}{N}\right)\left(\left(a_{i}(N^{2}t) - a_{i}(0)\right)a_{j}(0)\right)$ 

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$$=\int_{0}^{t}\sum_{i,j}\nabla G\left(\frac{i}{N}\right)F\left(\frac{j}{N}\right)\left\langle J_{i,i+1}(N^{2}s)e_{j}(0)\right\rangle ds$$

From dynamics to thermodynamics Prove Statistical Mechanics Adiabatic dynamics How to prove this?

#### How to prove this?

Defines, for a generation of a sequence of smooth local functions  $\mathcal{F}_{a}^{-}$   $\Phi_{a} = \chi_{1,2} - \mathcal{P}(a_{1} - u_{0}) - \mathcal{L}\mathcal{F}_{a}$ with *L* the generator of the dynamics, and pick a noise test function  $\mathcal{G}(x)$ :  $\frac{1}{N} \sum_{ij} G\left(\frac{1}{N}\right) F\left(\frac{1}{N}\right) \left[C(i_{i}, h^{2}t) - C(i_{i}, 0)\right]$  $- \frac{1}{N} \sum_{ij} G\left(\frac{1}{N}\right) \left[F\left(\frac{1}{N}\right) \left[(u_{i}(h^{2}t) - u_{i}(0))u_{i}(0)\right)\right]$ 

 $= \int_{0}^{t} \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \langle j_{1,i+1}(N^{2}s) e_{j}(0) \rangle ds$ 

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$$= \int_{0}^{t} \frac{1}{N} \sum_{i,j} \Delta G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \mathcal{D}\left\langle e_{i}(N^{2}s)e_{j}(0)\right\rangle ds$$
$$+ \int_{0}^{t} \frac{1}{N^{2}} \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \left\langle (N^{2}L)\tau_{i}\mathcal{F}_{n}(N^{2}s)e_{j}(0)\right\rangle ds$$
$$+ \int_{0}^{t} \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \left\langle \tau_{i}\Phi_{n}(N^{2}s)e_{j}(0)\right\rangle ds$$

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$$\begin{split} &-\int_{0}^{t}\frac{1}{N}\sum_{i,j}\Delta G\left(\frac{i}{N}\right)F\left(\frac{i}{N}\right)D\left(a_{i}(N^{2}s)a_{i}(0)\right)ds \\ &+\int_{0}^{t}\frac{1}{N^{2}}\sum_{i,j}\nabla G\left(\frac{i}{N}\right)F\left(\frac{i}{N}\right)\left((N^{2}t)\gamma_{c}\mathcal{F}_{a}(N^{2}s)a_{i}(0)\right)ds \\ &+\int_{0}^{t}\sum_{i,j}\nabla G\left(\frac{i}{N}\right)F\left(\frac{i}{N}\right)\left(\gamma_{c}\Phi_{a}(N^{2}s)a_{j}(0)\right)ds \end{split}$$

$$= \int_{0}^{t} \frac{1}{N} \sum_{i,j} \Delta G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \mathcal{D}\left\langle e_{i}(N^{2}s)e_{j}(0)\right\rangle ds$$
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$$+ \int_{0}^{t} \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \left\langle \tau_{i}\Phi_{n}(N^{2}s)e_{j}(0)\right\rangle ds$$

$$\sim \int_{0}^{t} \frac{1}{N} \sum_{i,j} \Delta G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \mathcal{D}NC(i,j,N^{2}t) ds$$
  
+  $\frac{1}{N^{2}} \sum_{i,j} \nabla G\left(\frac{i}{N}\right) F\left(\frac{j}{N}\right) \left\langle \tau_{i}(\mathcal{F}_{n}(N^{2}t) - \mathcal{F}_{n}(0))e_{j}(0) \right\rangle ds$   
+  $\int_{0}^{t} \sum_{i,j} F\left(\frac{j}{N}\right) \nabla G\left(\frac{i}{N}\right) \left\langle \frac{1}{2k} \sum_{|i-l| \leq k} \tau_{l} \Phi_{n}(N^{2}s)e_{j}(0) \right\rangle ds$ 

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$$\begin{split} &-\int_0^{-1} \frac{1}{h^2}\sum_{ij}^{ij} \Delta \alpha \left(\frac{i}{h}\right) F\left(\frac{i}{h^2}\right) T\left(\alpha (\delta^2 \cdot) v(0)\right) dt \\ &+\int_0^{-1} \frac{1}{h^2}\sum_{ij}^{ij} \Delta \alpha \left(\frac{i}{h}\right) F\left(\frac{i}{h}\right) \left((\delta^2 \cdot) v^2 \cdot A(\delta^2 \cdot) v(0)\right) dt \\ &+\int_0^{-1} \frac{1}{h^2}\sum_{ij}^{ij} \Delta \alpha \left(\frac{i}{h}\right) F\left(\frac{i}{h}\right) \left(\delta^2 \cdot A^2 \cdot v(0)\right) dt \\ &-\int_0^{-1} \frac{1}{h^2}\sum_{ij}^{ij} \Delta \alpha \left(\frac{i}{h}\right) F\left(\frac{i}{h}\right) TW(1, I, A^2 \cdot) dt \\ &+\frac{1}{h^2}\sum_{ij}^{ij} \nabla \alpha \left(\frac{i}{h}\right) F\left(\frac{i}{h}\right) \left(v(2, iA^2 \cdot) - x_i(0) v(0)\right) dt \\ &+\int_0^{-1} \sum_{ij}^{ij} F\left(\frac{i}{h}\right) C\left(\frac{i}{h}\right) \left(\frac{1}{h^2}\sum_{ij} v^2 \cdot v^2 \cdot A(\delta^2 \cdot) v(0)\right) dt \end{split}$$

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$$\Phi_n = J_{0,1} - \mathcal{D}(e_1 - e_0) - LF_n$$
$$\hat{\Phi}_{n,k} = \frac{1}{2k} \sum_{|j| \le k} \tau_j \Phi_n$$

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

$$\|F\|^{2}\bar{e}^{2}\left\{\left(\int_{0}^{t}N\sum_{i}G'\left(\frac{i}{N}\right)\tau_{i}\hat{\Phi}_{n,k}(N^{2}s)ds\right)^{2}\right\}$$
$$=C\left\{\left(\int_{0}^{N^{2}t}\frac{1}{N}\sum_{i}G'\left(\frac{i}{N}\right)\tau_{i}\hat{\Phi}_{n,k}(s)ds\right)^{2}\right\}$$

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics  $\begin{array}{c}
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We are left to prove that this is negligeable as  $N \to \infty$ ,  $k \to \infty$  and  $n \to \infty$ .

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For a deterministic hamiltonian infinite dynamics, I do not know how to show that this variance is small.

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For stochastic dynamics there is a technique to prove this (in some cases...):

Varadhan's Non Gradient methods.

S.R.S. Varadhan (1990): Non-gradient Ginzburg-Landau conservative model (reversible).

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Stochastic dynamics perturbations

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

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From dynamics to thermodynamics 5 Statistical Mechanics Adiabatic dynamics Stochastic dynamics perturbations

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From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Stochastic dynamics perturbations

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For stochastic dynamics, roughly the idea is the following:

$$\Phi_n = J_{0,1} - \mathcal{D}_T (e_1 - e_0) - LF_n$$
$$\hat{\Phi}_{n,K} = \frac{1}{2k} \sum_{|j| \le k - r_{\Phi}} \tau_j \Phi_n$$

How can the space-time variance be small?

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

#### Varadhan's non-gradient method

For stochastic dynamics, roughly the idea is the following:  $\Phi_{a}=j_{0,1}-\mathcal{D}_{T}\left(e_{1}-e_{0}\right)-LF_{a}$ 

$$\begin{split} \Phi_n = j_{0,1} - \mathcal{D}_T \left( \phi_1 - \phi_0 \right) - LF_n \\ \hat{\Phi}_{n,K} = \frac{1}{2k} \sum_{|j| \leq k - \phi_0} \tau_j \Phi_n \end{split}$$
 How can the space-time variance be small?

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How can the space-time variance be small? For the <u>finite</u> set  $\Lambda_k = \{-k, \dots, k\}$ , consider the generator  $L_{\Lambda_k}$ , with free B.C. From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Varadhan's non-gradient method

#### Varadhan's non-gradient method

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How can the space-time variance be small? For the <u>finite</u> set  $\Lambda_k = \{-k, \ldots, k\}$ , consider the generator  $L_{\Lambda_k}$ , with free B.C. The corresponding dynamics conserve the energy of the box  $\sum_{i \in \Lambda_K}$ , if the *noise* is sufficiently nice (ellipticity, spectral gap ...), there will be ergodicity in the corresponding microcanonical surface, and it will be possible to solve the equation

$$L_{\Lambda_{\mathcal{K}}}u_{k}=\frac{1}{2k}\sum_{i=-k}^{k-1}\mathsf{J}_{i,i+1}$$

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

#### Varadhan's non-gradient method

For stochastic dynamics, roughly the idea is the following:

$$\Phi_{\alpha} = j_{0,1} - D_T (\theta_1 - \theta_0)$$

$$\hat{\Phi}_{\alpha,K} = \frac{1}{2k} \sum_{\alpha=\alpha+1,\dots,n} \tau_j \Phi_\alpha$$

How can the space-time variance be small? For the finite set  $A_{ii} = (-k, ..., k)$ , consider the generator  $L_{jk_{ii}}$ , with free B.C. the corresponding dynamics conserve the energy of the box  $\sum_{i > k_{ii}}$ , if the noise is sufficiently nice (elipticity, spectral gap ...), there will be ergodicity in the corresponding microcanneid surface, and it will be possible to solve the equation

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

#### Varadhan's non-gradient method

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

$$L_{\Lambda_{\mathcal{K}}}u_{k} = \frac{1}{2k}\sum_{i=-\mathcal{K}}^{k-1} \mathsf{J}_{i,i+1}$$

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

$$\begin{split} L_{n_0} u_k &= \frac{1}{2k} \sum_{k=K}^{k-1} \sum_{j=1}^{k-1} j_{j+1} \\ \text{going back to the full generator of the infinite dynamics:} \\ &= \frac{1}{2K} \sum_{k=1}^{k-1} j_{j+1} - (L-L_{n_0}) u_k + L u_k \\ \text{It is the boundary term } (L-L_{n_0}) u_k \text{ target single to the standard to Tries, -k-1}, in the source finit. \end{split}$$

$$L_{\Lambda_{\mathcal{K}}}u_{k}=\frac{1}{2k}\sum_{i=-\mathcal{K}}^{k-1}\mathsf{J}_{i,i+1}$$

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$$\frac{1}{2\kappa}\sum_{i=-k}^{k-1} \mathsf{J}_{i,i+1} = -(L-L_{\Lambda_k})u_k + Lu_k$$

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

$$L_{h_K} u_k = \frac{1}{2k} \sum_{i=-K}^{k-1} j_{i,i+1}$$
 ing back to the full generator of the infinite dynamics:

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It is the boundary term  $(L-L_{\lambda_k})_{kk}$  that gives origin to the gradient  $\mathfrak{D}_T(a_k-a_{-k})$ , in the proper limit. This requires some work and two ingredients: bounds on the spectral gap and a sector condition.

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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

 $r_i = q_i - q_{i-1}$ 

 $\underbrace{\begin{array}{c} & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & &$  $\gamma_0 = 0$ r.

From dynamics to thermodynamics 2012-03-18 -Statistical Mechanics Adiabatic dynamics -Chain un unpinned anharmonic oscillators with

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# Chain un unpinned anharmonic oscillators with conservative noise

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Equilibrium measure are product:

$$dQ_{\beta} = \prod_{i} \frac{e^{-\beta(p_{i}^{2}/2 + V(r_{i}))}}{Z_{\beta}} dp_{i} dr_{i} \qquad \beta = T^{-1} > 0$$

 $r_i = q_i - q_{i-1}$ 

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

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# Energy Conserving Noise

We use the vector fields tangent to the microcanonical surface:

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

The Hamiltonian vector field is

$$A = \sum_{i} (p_{i} - p_{i-1}) \partial_{r_{i}} - V'(r_{i}) (\partial_{p_{i}} - \partial_{p_{i-1}}) = \sum_{i} (X_{i} - Y_{i-1,i})$$

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

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We add stochastic dynamics with generator defined by

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

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

We use the vector fields tangent to the microcanonical surface: 
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It will be interesting extend this to different type of noise or chaotic mechanism.

S. Olla - CEREMADE From dynamics to thermodynamics

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Energy Conserving Noise Energy Conserving Noise We use the vector fields tangent to the microcanonical surface

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

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From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Currents

Currents

$$\begin{split} g_{i,i+1}^2 = Y_{i,i+1} e_i &= -\rho_i V'(r_{i+1}) \\ g_{i,i+1}^2 = Y_{i,i+1}^2 e_i &= -\rho_i^2 V''(r_{i+1}) + V'(r_{i+1})^2 \\ \end{split}$$
 NON GRADIENT CURRENTS

$$\begin{aligned} \mathsf{J}_{i,i+1}^{a} &= Y_{i,i+1} e_i = -p_i V'(r_{i+1}) \\ \mathsf{J}_{i,i+1}^{s} &= Y_{i,i+1}^2 e_i = -p_i^2 V''(r_{i+1}) + V'(r_{i+1})^2 \end{aligned}$$

#### NON GRADIENT CURRENTS

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Currents

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Currents Currents

 $j_{i,i+1}^{2} = Y_{i,i+1}e_{i} = -p_{i}V'(r_{i+1})$  $j_{i,i+1}^{4} = Y_{i,i+1}^{2}e_{i} = -p_{i}^{2}V''(r_{i+1}) + V'(r_{i+1})^{2}$ 

NON GRADIENT CURRENTS In the harmonic case ( $V(r) = r^2/2$ ) we have the decomposition:

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

for a homogeneous second order polynome F(r, p) and  $\mathcal{D}$  constant.

$$J_{i,i+1}^{a} = Y_{i,i+1}e_{i} = -p_{i}V'(r_{i+1})$$
  
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#### NON GRADIENT CURRENTS

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for a homogeneous second order polynome F(r, p) and  $\mathcal{D}$  constant.

$$\Phi_n = J_{0,1} - \mathcal{D}_T (e_1 - e_0) - LF_n$$
$$\hat{\Phi}_{n,K} = \frac{1}{2K} \sum_{|j| \le K} \tau_j \Phi_n$$

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics  $\begin{pmatrix}
\varphi_{x,y_1} - D_{x}(\varphi_{x,y_1}) - U_{x,y_1} \\
\varphi_{x,y_2} - D_{x,y_2} \\
\psi_{x,y_1} - D_{x,y_2} \\
\psi_{x,y_2} - D_{x,y_2} \\
\psi_{x,y_1} - D_{x,y_1} \\
\psi_{x,y_1} - D_{x,y_2} \\
\psi_{$ 

By a general inequality valid for all Markov processes:

$$\left\| \left( \int_0^t N \sum_j G'(i/N) \tau_i \hat{\Phi}_{n,K}(N^2 s) ds \right)^2 \right)$$
  
 
$$\leq Ct \left\{ \sum_i G'(i/N) \tau_i \hat{\Phi}_{n,K}, (-S)^{-1} \sum_i G'(i/N) \tau_i \hat{\Phi}_{n,K} \right\}$$
  
 
$$\sim \leq Ct \|G'\|_{L^2}^2 K \left\langle \hat{\Phi}_{n,K}, (-S_{\Lambda_K})^{-1} \hat{\Phi}_{n,K} \right\rangle$$

$$\Phi_n = J_{0,1} - \mathcal{D}_T (e_1 - e_0) - LF_n$$
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$$\sim \leq Ct \|G'\|_{L^2}^2 K \left\langle \hat{\Phi}_{n,K}, (-S_{\Lambda_K})^{-1} \hat{\Phi}_{n,K} \right\rangle$$

We are left to prove that this is negligeable as  $N \to \infty$ ,  $K \to \infty$  and  $n \to \infty$ .

### Microcanonical variance

 $\langle \cdot \rangle_{K,E}$ : microcanonical expectation on the energy shell

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

Hypothesis on  $V \implies$  connected surface.

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Microcanonical variance

#### Microcanonical variance

 $<\cdot>_{K,E}: \text{ microcanonical expectation on the energy shell}$   $\Sigma_{K,E} = \left\{ (r_1, p_1, \dots, r_K, p_K) : \sum_{i=1}^K e_i = KE \right\}$ Hypothesis on  $V \longrightarrow \text{ connected surface.}$ 

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#### Microcanonical variance

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Hypothesis on  $V \implies$  connected surface. For two local functions f, g define

$$\langle\!\langle f,g \rangle\!\rangle = \lim_{K \to \infty} \frac{1}{K} \left( \sum_{i=-k+\ell}^{k-\ell} \tau_i f, (-S_K)^{-1} \sum_{i=-k+\ell}^{k-\ell} \tau_i g \right)_{K,E}$$

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 $<\cdot>_{K,E}: microcanonical expectation on the energy shell <math display="block">\Sigma_{K,E} = \left\{(r_1, \rho_1, \ldots, r_K, \rho_K): \sum_{i=1}^K n_i = KE\right\}$  Hypothesis on  $V \longrightarrow \text{connected surface}.$  For two local functions f, g define

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#### Microcanonical variance

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We need to prove that there exists  $F_n$  such that

$$\langle\!\langle \Phi_n, \Phi_n \rangle\!\rangle \longrightarrow 0$$

for  $\Phi_n = J_{0,1} - D(e_1 - e_0) - LF_n$ .

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From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Microcanonical variance

#### Microcanonical variance

$$\begin{split} >_{K,E} : & \text{microcanonical expectation on the energy shell} \\ & \Sigma_{K,E} = \left\{ (r_1, \rho_1, \ldots, r_K, \rho_K) : \sum_{i=1}^{K} e_i = KE \right\} \end{split}$$

Hypothesis on  $V \longrightarrow$  connected surface. For two local functions f, g define

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### variational formulas

Let  $\Phi = X_0F + Y_{0,1}G$ , for some local F, G, then

$$\lim_{K \to \infty} \frac{1}{2k} \left( \sum_{i=-k+\ell}^{k-\ell} \tau_i \Phi, (-S_K)^{-1} \sum_{i=-k+\ell}^{k-\ell} \tau_i \Phi \right)_{k,E} = \langle\!\langle \Phi_n, \Phi_n \rangle\!\rangle$$
  
$$\leq \sup_{(\xi^0, \xi^1) \text{ closed}} \left\{ 2 < F, \xi^0 > +2 < G, \xi^1 > -\gamma \left( < (\xi^0)^2 + (\xi^1)^2 > \right) \right\}$$

From dynamics to thermodynamics EC Statistical Mechanics Adiabatic dynamics Variational formulas

#### variational formulas

Let  $\Phi = X_0F + Y_{0,1}G$ , for some local F, G, then

$$\begin{split} &\lim_{K\to\infty}\frac{1}{2k}\left(\sum_{i=-k+\ell}^{k-\ell}\tau_i\Phi,(-S_K)^{-1}\sum_{i=-k+\ell}^{k-\ell}\tau_i\Phi\right)_{k,E}=(\Phi_n,\Phi_n)\\ &\leq \sup_{\{0,\ell\neq\}}\left(2< F,\xi^0>+2< G,\xi^1>-\gamma\left(<(\xi^0)^2+(\xi^1)^2>\right)\right) \end{split}$$

#### variational formulas

Let  $\Phi = X_0F + Y_{0,1}G$ , for some local F, G, then

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Def:  $(\xi^0, \xi^1) \in L^2 \times L^2$  is a closed form if

$$X_{i}(\tau_{j}\xi^{0}) = X_{j}(\tau_{i}\xi_{0}) \qquad Y_{j,j+1}(\tau_{i}\xi^{1}) = Y_{i,i+1}(\tau_{j}\xi^{1})$$
$$X_{i}(\tau_{j}\xi^{i}) = Y_{j,j+1}(\tau_{i}\xi^{0}) \qquad i \neq j, j+1$$
...

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Variational formulas variational formulas

Let  $\Phi = X_0F + Y_{0,1}G$ , for some local F, G, then

$$\begin{split} &\lim_{R\to\infty}\frac{1}{2R} \sum_{i_1,\ldots,i_{n-1}}^{i_{n-1}} d_{i_1} \Phi_{i_2} - (-S_R)^{-1} \sum_{i_1,\ldots,i_{n-1}}^{i_{n-1}} d_{i_1} \Phi_{i_2} - (\Phi_{i_n} \Phi_{i_n}) \\ &\leq \sup_{i_1\in \mathbb{Z}/2} \sum_{i_1,\ldots,i_{n-1}}^{i_{n-1}} d_{i_1} E_i^{-1} + 2 < E_i^{-1} \leq i_1 < i_1 \leq i_1 < i_$$

 $X_i(\tau_j\xi^i)=Y_{j,j+1}(\tau_i\xi^0)\qquad i\neq j,j+1$ 

#### exact forms

We need to show that closed form are approximated (in  $L^2(Q_\beta)$ ) by exact forms:

Def:  $(\xi^0, \xi^1) \in L^2 \times L^2$  is an exact form if there exists F local and a constant  $a \in \mathbb{R}$  such that

$$\xi^{0} = X_{0}\left(\sum_{i \in \mathbb{Z}} \tau_{i}F\right)$$
  
$$\xi^{1} = Y_{0,1}\left(\sum_{i \in \mathbb{Z}} \tau_{i}F\right) + ap_{0}V'(r_{1})$$

From dynamics to thermodynamics Constraints and the second secon exact forms We need to show that closed form are approximated (in  $L^2(Q_3)$ ) by exact form: Def.  $(\mathcal{C}, \mathcal{C}) \in L^2 \times L^2$  is an exact form if there exists F local and a constant a c is such that

 $\xi^0 = X_0(\sum_{i \in \mathbb{Z}} \tau_i F)$  $\xi^1 = Y_{0,1}(\sum_{i \in \mathbb{Z}} \tau_i F) + ap_0 V'(r_1)$ 

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### exact forms

We need to show that closed form are approximated (in  $L^2(Q_\beta)$ ) by exact forms:

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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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#### exact form

We need to show that closed form are approximated (m  $L^2(Q_1))$  by read form: Def  $(\tilde{Q}^2,\tilde{Q}) \in \mathcal{I} \times d\tilde{\mathcal{I}}$  is an exact form if there exists F local and a constant a  $\in \mathbb{R}$  such that  $\begin{aligned} \tilde{\mathcal{L}}^2 = XQ_{12} \sum_{i=1}^{N} F_i \\ \tilde{\mathcal{L}}_i = \tilde{\mathcal{L}}_i \sum_{i=1}^{N} F_i = xq_i \sum_{i=1}^{N} F_i + xq_i \sum_{i=1}^{N} F_i \\ \end{bmatrix}$ This is proven by a candid construction, integrating the form

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From dynamics to thermodynamics 81 Constraints Constra

Ingredients to prove this: • Spectral gap bound for  $S_K$ :  $SG(S_K) \ge CK^{-2}$ . • Sector condition:  $| < vAu > |^2 \le C < v(-S)v > < u(-S)u >$ .

Ingredients to prove this:

- Spectral gap bound for  $S_K$ :  $SG(S_K) \ge CK^{-2}$ .
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• Spectral gap bound for  $S_K$ :  $SG(S_K) \ge CK^{-2}$ .

i.e. for any smooth local f such that  $\langle f \rangle_{K,E} = 0$ 

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

$$\begin{aligned} Y_{i,i+1} &= p_i \partial_{r_{i+1}} - V'(r_{i+1}) \partial_{p_i}, \\ X_i &= Y_{i,i} = p_i \partial_{r_i} - V'(r_i) \partial_{p_i}, \end{aligned}$$

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

 $< \ell^2 >_{K,E} \le C_1 \sum_{i=1}^{K} ((X_i \ell)^2)_{K,E} + C_2 \kappa^2 \sum_{i=1}^{K-1} ((Y_{i,i+1} \ell)^2)_{K,E}$ 

$$\begin{split} Y_{i,i+1} &= p_i \partial_{\kappa+1} - V'(r_{i+1}) \partial_{\mu}, \\ X_i &= Y_{i,i} = p_i \partial_{\kappa} - V'(r_i) \partial_{\mu}, \end{split}$$

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

 $f_{i,odd}(p) = \frac{1}{2}(f(p^{(i)}) - f(p)), \qquad f_{i,even}(p) = \frac{1}{2}(f(p^{(i)}) + f(p)),$ with  $p_i^{(i)} = -p_i$  and  $p_j^{(i)} = p_j$  if  $j \neq i$ . From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Sector Condition Sector Condition For any i decompose f = f<sub>1,odd</sub> + f<sub>1,onn</sub>

$$\begin{split} f_{i,odd}(\rho) &= \frac{1}{2}(f(\rho^{(i)}) - f(\rho)), \qquad f_{i,outh}(\rho) = \frac{1}{2}(f(\rho^{(i)}) + f(\rho)), \\ \text{with } \rho_i^{(i)} &= -\rho_i \text{ and } \rho_i^{(i)} = \rho_i \text{ if } j + i. \end{split}$$

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

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

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Sector Condition Sector Condition

For any i decompose  $f - f_{i,ded} + f_{j,dent}$  $f_{i,ded}(p) = \frac{1}{2} (f(p^{(i)}) - f(p)), \qquad f_{i,rest}(p) = \frac{1}{2} (f(p^{(i)}) + f(p)),$ with  $p_{i}^{(i)} = -p_{i}$  and  $p_{i}^{(i)} = p_{i}$  if  $j \neq i$ .  $(wAw) = \sum (v(X_{i} - Y_{i-1,i})w)$ 

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

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with  $p_i^{(i)} = -p_i$  and  $p_j^{(i)} = p_j$  if  $j \neq i$ .  
 $\langle vAu \rangle = \sum_i \langle v(X_i - Y_{i-1,i})u \rangle$ 

From dynamics to thermodynamics EC Statistical Mechanics Adiabatic dynamics Sector Condition

#### Sector Condition For any *i* decompose *f* = *f*<sub>1,odd</sub> + *f*<sub>1,mm</sub>

$$\begin{split} & f_{i,\text{netre}}(\rho) = \frac{1}{2} (f(\rho^{(i)}) - f(\rho)), \qquad f_{i,\text{netre}}(\rho) = \frac{1}{2} (f(\rho^{(i)}) + f(\rho)), \\ & \text{with } \rho_i^{(i)} = -\rho_i \text{ and } \rho_i^{(i)} - \rho_i \text{ if } j \neq i. \\ & (\nu A u) = \sum \left( \nu (X_i - Y_{i-1,i}) u \right) \end{split}$$

$$\begin{split} & \langle v X_i u \rangle = \begin{pmatrix} v_{i,odd} X_i v_{i,owen} \end{pmatrix} + \begin{pmatrix} v_{i,owen} X_i w_{i,odd} \end{pmatrix} \\ & = \begin{pmatrix} v_{i,odd} X_i v_{i,owen} \end{pmatrix} - \begin{pmatrix} u_{i,odd} X_i v_{i,owen} \end{pmatrix} \\ & \leq \begin{pmatrix} v_{i,odd}^2 \end{pmatrix}^{1/2} \left( (X_i v_{i,owen})^2 \right)^{1/2} + \begin{pmatrix} u_{i,odd}^2 \end{pmatrix}^{1/2} \left( (X_i v_{i,owen})^2 \right)^{1/2} \\ & \leq C \left( (X_i v)^2 \right)^{1/2} \left( (X_i u)^2 \right)^{1/2} + \begin{pmatrix} (X_i u)^2 \right)^{1/2} \left( (X_i v)^2 \right)^{1/2} \end{split}$$

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

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with  $p_i^{(i)} = -p_i$  and  $p_j^{(i)} = p_j$  if  $j \neq i$ .  
 $\langle vAu \rangle = \sum_i \langle v(X_i - Y_{i-1,i})u \rangle$ 

and similarly for  $\langle vY_{i-1,i}u \rangle$ .  $\implies |\langle vAu \rangle| \leq C \langle v(-S)v \rangle \langle u(-S)u \rangle$ .

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From dynamics to thermodynamics EC-Statistical Mechanics Adiabatic dynamics Sector Condition

#### Sector Condition

For any i decompose  $I = f_{i,ikkl} + f_{i,men}$   $f_{i,mkl}(p) = \frac{1}{2}(I(p^{(i)}) - I(p)), \quad f_{i,mek}(p) = \frac{1}{2}(I(p^{(i)}) + I(p)),$ with  $p_i^{(i)} = -p_i$  and  $p_j^{(i)} = p_j$  if  $j \neq i$ .  $(oku) = \sum (v(X_i - Y_{i-1,j})u)$ 

$$\begin{split} & (vX, u) = \begin{pmatrix} v_{i,kall}, X_{ii}, z_{iik}, u \end{pmatrix} + \begin{pmatrix} v_{i,kall}, X_{iii}, z_{ikl} \end{pmatrix} \\ & = \begin{pmatrix} v_{i,kall}, X_{iik}, z_{ikl} \end{pmatrix} + \begin{pmatrix} v_{i,kall}, X_{ikl}, z_{ikl} \end{pmatrix} \\ & \leq \begin{pmatrix} v_{i,kall} \end{pmatrix}^{1/2} \left( (X_{ikl}, z_{ikl}) \right)^{1/2} + \begin{pmatrix} v_{i,kall} \end{pmatrix}^{1/2} \left( (X_{il}, z_{ikl}) \right)^{1/2} \\ & \leq ((X_{ikl})^2)^{1/2} \left( (X_{ikl})^2 \right)^{1/2} + ((X_{ikl})^2)^{1/2} \\ & \text{and initiality for } < (v_{i-1})^2 \cdot v_{i-1} \\ & = \downarrow \quad |(vkh)| \leq (v_{i-1})^2 \cdot v_{i-1} \\ & = \downarrow \quad |(vkh)| \leq (v_{i-1})^2 \cdot v_{i-1} \\ \end{split}$$

### 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

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

From dynamics to thermodynamics 81 Constraints Constra  $\begin{array}{l} \label{eq:constraints} \\ \mbox{Equilibrium fluctuations} \\ \mbox{Equilibrium fluctuations} \\ \mbox{fail} \\ \mbox{$\kappa^{\mu} - \frac{1}{\sqrt{M}} \sum_{i} N_{ii} \left( \kappa(i) - e \right) $} \\ \mbox{It convergs in lase the $a $ data constant content quasian field $Y$} \\ \mbox{$\mathcal{I}[Y(Y)Y(G)] - x$} \int F(y)G(y) dy $} \end{array}$ 

### equilibrium fluctuations

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#### Theorem

$$Y_t^N = \frac{1}{\sqrt{N}} \sum_i \delta_{i/N} \left\{ \epsilon_i (N^2 t) - e \right\}$$

converges in law to the solution of the linear SPDE

$$\partial_t Y = \mathcal{D} \; \partial_y^2 Y \; dt + \sqrt{2\mathcal{D}\chi} \; \partial_y B(y,t)$$

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From dynamics to thermodynamics Statistical Mechanics Contemport Contemport

Equivalently we can express the result is term of the fluctuation field  $Y^N = \frac{1}{\sqrt{N}} \sum_{i} \delta_{ijN} \left( \phi_i(0) - e \right)$  It converges in law to a data correlated contend gaussian field Y $\mathbb{E}[Y(F)Y(G)] - \chi \int F(y)G(y) dy$ 

#### Theorem

equilibrium fluctuations

 $Y_t^N = \frac{1}{\sqrt{N}} \sum_j \delta_{i/N} \left\{ e_i(N^2 t) - e \right\}$ converges in law to the solution of the linear SPDE  $\partial_t Y = D \ \partial_t^2 Y \ dt + \sqrt{2D\chi} \ \partial_r B(y, t)$ 

start with the martingale decomposition:

$$\mathcal{G}_{k} = \sigma \{ e_{1}, \dots, e_{k}, p_{k+1}, r_{k+1}, \dots, p_{L}, r_{L} \}$$

$$f_{k} \coloneqq E[f|\mathcal{G}_{k}], \qquad f_{L} = f_{L}(e_{1}, \dots, e_{L})$$

$$< f^{2} >_{L,E} = \sum_{k=0}^{L-1} < (f_{k} - f_{k+1})^{2} >_{L,E} + < f_{L}^{2} >_{L,E}$$

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics proof of spectral gap bound

#### proof of spectral gap bound

#### start with the martingale decomposition:

$$\begin{split} \mathcal{G}_k &= \sigma \; \{ e_1, \ldots, e_k, p_{k+1}, r_{k+1}, \ldots, p_1, r_L \} \\ f_k &:= E[f|\mathcal{G}_k], \qquad f_L = f_L(e_1, \ldots, e_L) \\ < f^2 >_{L,E} = \sum_{i=1}^{L-1} < (f_k - f_{k+1})^2 >_{L,E} + < f_L^2 >_{L,E} \end{split}$$

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

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

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics proof of spectral gap bound

#### proof of spectral gap bound

start with the martingale decomposition

$$\begin{split} \mathcal{G}_{k} &= \sigma \left\{ e_{1}, \ldots, e_{k}, p_{k+1}, r_{k-1}, \ldots, p_{k}, r_{k} \right\} \\ f_{k} &= E[f(\mathcal{G}_{k}], \qquad f_{k} - f_{k}(e_{1}, \ldots, e_{k}) \\ &< f^{2} >_{LE} = \sum_{k=0}^{k-2} < (f_{k} - f_{k+1})^{2} >_{LE} + < f_{k}^{2} >_{LE} \\ X_{k}^{2} \text{ has his unform spectral gap in the correspondir scanonical surface } (X_{k}, e_{k} = 0): \end{split}$$

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

 proof of the spectral gap bound

 $Y_{k,k+1} = \rho_k \partial_{r_{k+1}} - V'(r_{k+1}) \partial_{\rho_k}$ 

 $Y_{k,k+1} = p_k \partial_{r_{k+1}} - V'(r_{k+1}) \partial_{p_k}$ 

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics Proof of the spectral gap bound

#### proof of the spectral gap bound

 $Y_{k,k+1} = \rho_k \partial_{r_{k+1}} - V'(r_{k+1}) \partial_{\rho_k}$ 

 $Y_{k,k+1}f_{L} = \rho_{k}V'(r_{k+1})(\partial_{e_{k}} - \partial_{e_{k+1}})f_{L}(e_{1}, \dots, e_{L})$ 

 $Y_{k,k+1} = p_k \partial_{r_{k+1}} - V'(r_{k+1}) \partial_{p_k}$ 

 $Y_{k,k+1}f_L = p_k V'(r_{k+1})(\partial_{e_k} - \partial_{e_{k+1}})f_L(e_1,\ldots,e_L)$ 

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From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics proof of the spectral gap bound

#### proof of the spectral gap bound

 $Y_{k,k+1}=p_k\partial_{r_{k+1}}-V'(r_{k+1})\partial_{p_k}$ 

 $Y_{k,k+1}f_L = \rho_k V'(r_{k+1})(\partial_{e_k} - \partial_{e_{k+1}})f_L(e_1, \ldots, e_L)$ 

 $<(Y_{k,k+1}f_{L})^{2}>_{L,E}\sim \ \left\{e_{k}e_{k+1}\left[\left(\partial_{e_{k}}-\partial_{e_{k+1}}\right)f_{L}\right]^{2}\right\}_{L,E}$  Dirichlet form of the Ginzburg Landau model!

$$Y_{k,k+1} = p_k \partial_{r_{k+1}} - V'(r_{k+1}) \partial_{p_k}$$

$$Y_{k,k+1}f_L = p_k V'(r_{k+1})(\partial_{e_k} - \partial_{e_{k+1}})f_L(e_1,\ldots,e_L)$$

$$<(Y_{k,k+1}f_L)^2>_{L,E} \sim \langle e_k e_{k+1} [(\partial_{e_k} - \partial_{e_{k+1}})f_L]^2 \rangle_{L,E}$$

Dirichlet form of the Ginzburg Landau model!

From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics proof of the spectral gap bound

#### proof of the spectral gap bound

 $Y_{k,k+1} = \rho_k \partial_{r_{k+1}} - V'(r_{k+1}) \partial_{\rho_k}$ 

 $Y_{k,k+1}f_{L} = \rho_{k}V'(r_{k+1})(\partial_{e_{k}} - \partial_{e_{k+1}})f_{L}(e_{1}, \dots, e_{L})$ 

 $<(Y_{k,k+1}f_k)^2>_{L,E}\sim \ \left\{e_ke_{k+1}\left[(\partial_{e_k}-\partial_{e_{k+1}})f_L\right]^2\right\}_{L,E}$  Dirichlet form of the Ginzburg Landau model! We are left to prove G for this GL model:

 $< t_L^2 >_{L,E} \le C_2 L^2 \sum_{k=1}^{L-1} \left( e_k e_{k+1} \left[ (\partial_{e_k} - \partial_{e_{k+1}}) f_L \right]^2 \right]_{L,E}$ 

$$Y_{k,k+1} = p_k \partial_{r_{k+1}} - V'(r_{k+1}) \partial_{p_k}$$

$$Y_{k,k+1}f_L = p_k V'(r_{k+1})(\partial_{e_k} - \partial_{e_{k+1}})f_L(e_1,\ldots,e_L)$$

$$<(Y_{k,k+1}f_L)^2>_{L,E} \sim \left\langle e_k e_{k+1} \left[ (\partial_{e_k} - \partial_{e_{k+1}}) f_L \right]^2 \right\rangle_{L,E}$$

Dirichlet form of the Ginzburg Landau model! We are left to prove G for this GL model:

$$< f_L^2 >_{L,E} \le C_2 L^2 \sum_{k=1}^{L-1} \langle e_k e_{k+1} [(\partial_{e_k} - \partial_{e_{k+1}}) f_L]^2 \rangle_{L,E}$$
From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics L proof of the spectral gap bound proof of the spectral gap bound

The microcanonical marginal density on the energies  $e_1, ..., e_L$  has a linear behavior at large values, and not strictly convex, also the weight  $e_k e_{k+1}$  does not allow easy telescoping arguments.

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From dynamics to thermodynamics Statistical Mechanics Adiabatic dynamics - Proof of the spectral gap bound proof of the spectral gap bound

The microcanonical marginal density on the energies  $e_1, \ldots, e_t$  has a linear behavior at large values, and not strictly convex, also the weight  $e_te_{t-1}$  does not allow easy telescoping arguments. Caputo approach + a smart telescoping + the elementary inequality

 $\int_{-\infty}^{1} g(t)^{2} dt \leq \frac{1}{2} \int_{-\infty}^{1} g'(t)^{2} t(1-t) dt$ 

The microcanonical marginal density on the energies  $e_1, \ldots, e_L$  has a linear behavior at large values, and not strictly convex, also the weight  $e_k e_{k+1}$  does not allow easy telescoping arguments. Caputo approach + a smart telescoping + the elementary inequality

 $\int_0^1 g(t)^2 dt \leq \frac{1}{2} \int_0^1 g'(t)^2 t(1-t) dt$ 

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