



# Stationary states of opinion diffusion

Project for the exam: AMS (DSE)

Paola Serra and Marzio De Corato

# Theoretical Framework

# Statistical Mechanics

*“Ludwig Boltzmann, who spent much of his life studying statistical mechanics, died in 1906, by his own hand. Paul Ehrenfest, carrying on the work, died similarly in 1933. Now it is our turn to study statistical mechanics.” States of Matter (1975), by David L. Goodstein*

# Concepts of statistical mechanics: entropy [1]

**Central problem of thermodynamics:** characterize the actual state of equilibrium among all virtual states

**Entropy postulate:** there exist a function  $S$  of the extensive variables  $(X_0, X_1 \dots X_r)$  called entropy, that assumes the maximum value for a state of equilibrium among all virtual states and that possesses the following properties:

- Extensivity  $S^{(1 \cup 2)} = S^1 + S^2$
- Convexity  $S((1 - \alpha)X^1 + \alpha X^2) \geq (1 - \alpha)S(x^1) + \alpha S(X^2)$
- Monotonicity  $\frac{\partial S}{\partial E}|_{X_1 \dots X_r} = \frac{1}{T} > 0$

The equilibrium state corresponds to the maximum entropy compatible with the constraints

# Concepts of statistical mechanics: entropy [1]

- **Fundamental postulate of statistical mechanics**

$$S = k_b \ln |\Gamma|$$

- Where  $S$  is the thermodynamic entropy,  $k_b$  is Boltzmann constant and  $|\Gamma|$  the volume in the phase space

$$S(X_0, \dots, X_r) = k_b \ln \int_{\Gamma} dx = k_b \int dx \prod_{i=0}^r [\theta(X_i(x) - (X_i - \Delta X_i))\theta(X_i - X_i(x))]$$

(1)

- $(X_0, \dots, X_r)$  are the extensive variables
- The  $\theta$  functions assures that the integrand is not null only in the interval  $X_i - \Delta X_i \leq X_i(x) \leq X_i$

# Concepts of statistical mechanics: micro-canonical ensemble

- Lets focus on a particular observable  $A$  (extensive)

$$S(X; a) = k_b \ln \int_{\Gamma} dx \delta(A(x) - a) \quad (2)$$

$$S(X) = S(X; a^*) \geq S(X; a) \quad (3)$$

$$\begin{aligned} \frac{|\Gamma(a)|}{|\Gamma|} &= \frac{1}{|\Gamma|} \int_{\Gamma} dx \delta(A(x) - a) \\ &= \exp \left\{ \frac{1}{k_b} [S(X; a) - S(X; a^*)] \right\} \end{aligned} \quad (4)$$

$$\simeq \exp \left\{ \frac{1}{k_b} \left[ \frac{\partial^2 S}{\partial A^2} \Big|_{a^*} (a - a^*)^2 \right] \right\}$$

$$a^* = \langle A(x) \rangle = \frac{1}{|\Gamma|} \int_{\Gamma} dx A(x) \quad (5)$$

# Concepts of statistical mechanics: canonical ensemble

$$a^* = \frac{1}{|\Gamma|} \int_{\Gamma} dx_S dx_R A(x_S) \quad (6)$$

$$\langle A(x) \rangle = \int dx_S dx_R A(x_S) \delta(H^{(s)} \quad (7)$$

$$\langle A(x) \rangle = \frac{1}{|\Gamma|} \int dx_S dx_R A(x_S) \delta(H^S(x_S) + H^R(x_R) - H^S(x_S)) \quad (8)$$

$$\langle A(x) \rangle = \frac{1}{|\Gamma|} \int dx_S A(x_S) \times \int dx_R \delta(H^R(x_R) - (E - H^{(S)}(x_S))) \quad (9)$$

$$\int dx_R \delta(H^R(x_R) - (E - H^{(S)}(x_S))) \simeq \exp \left\{ \frac{1}{k_b} S^R(E - H^S) \right\} \quad (10)$$

# Concepts of statistical mechanics: canonical ensemble

$$\exp \left\{ \frac{1}{k_b} S^R(E - H^S) \right\} \simeq \exp \left[ \frac{1}{k_b} S^R(E) \right] \exp \left[ -\frac{1}{k_b} \frac{\partial S^R}{\partial E} \Big|_E H^S(x_S) \right] \quad (11)$$

$$\langle A(x) \rangle = \frac{1}{Z} \int dx_S A(x_S) \exp \left[ -\frac{H^S(x_S)}{k_b T} \right] \quad (12)$$

$$Z = \int dx_S \exp \left[ -\frac{H^S(x_S)}{k_b T} \right] \quad (13)$$

$$\langle A(x) \rangle = \frac{1}{Z} \int dE \int dx \delta(H(x) - E) A(x) \exp\left(-\frac{E}{k_b T}\right) \quad (14)$$

$$\langle A(x) \rangle = \frac{1}{Z} \int dE' a^*(E') \exp \left[ -\frac{E' - TS(E')}{k_b T} \right] \quad (15)$$



# Concepts of statistical mechanics: canonical ensemble[1]

$$Z \simeq \exp \left[ -\frac{E^* - TS(E^*)}{k_b T} \right] = \exp \left( -\frac{F}{k_b T} \right) \quad (16)$$

$$\frac{\partial \ln Z(\beta)}{\partial \beta} = -\frac{1}{Z} \int dx H(x) \exp \left[ -\frac{H}{k_b T} \right] = -\langle H(x) \rangle = -E \quad (17)$$

$$\frac{\partial^2 \ln Z(\beta)}{\partial \beta^2} = \langle H(x)^2 \rangle - \langle H(x) \rangle^2 \quad (18)$$

$$\langle H(x)^2 \rangle - \langle H(x) \rangle^2 = -\frac{\partial E}{\partial (1/k_b T)} = k_b T^2 \frac{\partial E}{\partial T} = k_b T^2 C \quad (19)$$

In this way a statistical quantity the variance has been connected to a thermodynamic quantity: the temperature.

# Numerical simulations

*“Never make a calculation until you know the answer. Make an estimate before every calculation, try a simple physical argument (symmetry! invariance! conservation!) before every derivation, guess the answer to every paradox and puzzle. Courage: No one else needs to know what the guess is. Therefore make it quickly, by instinct. A right guess reinforces this instinct. A wrong guess brings the refreshment of surprise. In either case life as a spacetime expert, however long, is more fun!” John Archibald Wheeler*

# Numerical simulation [1]

- **Simulation** *the evolution equations of a system are defined to such a detail that a computer can make its behaviour explicit, and one looks to see what takes place*
- Numerical experiment
- **Molecular dynamics:** the equation of motion are solved numerically PROS: information of both the dynamical and static properties of the system are explored
- **Monte Carlo:** a fictitious evolution process of the system is solved in order to get the equilibrium distribution PROS 1) also the systems whose dynamics is not defined can be explored 2) a fictitious dynamics can be considered in order to reach the equilibrium faster
- Molecular dynamics may provide a proof of statistical mechanics, Monte Carlo methods presuppose its validity

# Monte Carlo method [1]

We would calculate an integral of type  $\langle A \rangle = \int dx A(x) \rho(x)$  where  $\rho$  is the probability distribution.

Idea: evaluate the integrand in  $N$  point

Idea: the true dynamics is replaced with a fictitious stochastic dynamics. The state at  $t + 1$  depends only from the state at  $t$ .  
→ *MarkovChain*

## Bibliography I



Luca Peliti. *Statistical mechanics in a nutshell*. Princeton University Press, 2011.

# ROC and $\phi$ factor