

## • Equilibrio

1)

a) Eq stabile  $\rightarrow \frac{d^2U}{dx^2} > 0$  (assumo  $\sigma$ )

Eq instabile  $\rightarrow " < 0$  e  $\varepsilon > 0$ )

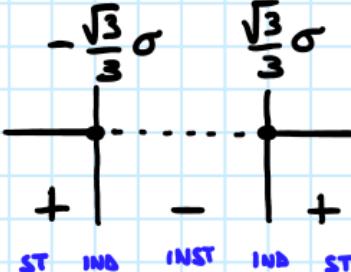
Eq indiffer.  $\rightarrow " = 0$

$$\rightarrow U(x) = \varepsilon \left(1 - \left(\frac{x}{\sigma}\right)^2\right)^2 = \varepsilon \left(1 + \left(\frac{x}{\sigma}\right)^4 - 2\left(\frac{x}{\sigma}\right)^2\right)$$

$$\frac{dU}{dx} = \varepsilon \left(\frac{4x^3}{\sigma^4} - \frac{4}{\sigma^2}x\right) = \frac{4\varepsilon}{\sigma^2}x \left(\frac{x}{\sigma^2} - 1\right) = 0 \Rightarrow x_1 = 0, x_{2,3} = \pm \sigma$$

$$\frac{d^2U}{dx^2} = \varepsilon \left(\frac{12}{\sigma^4}x^2 - \frac{4}{\sigma^2}\right)$$

$$\frac{\varepsilon}{\sigma^2} \left(\frac{12}{\sigma^4}x^2 - 4\right) > 0 \rightarrow \left(\frac{12}{\sigma^4}x^2 - 4\right) > 0$$

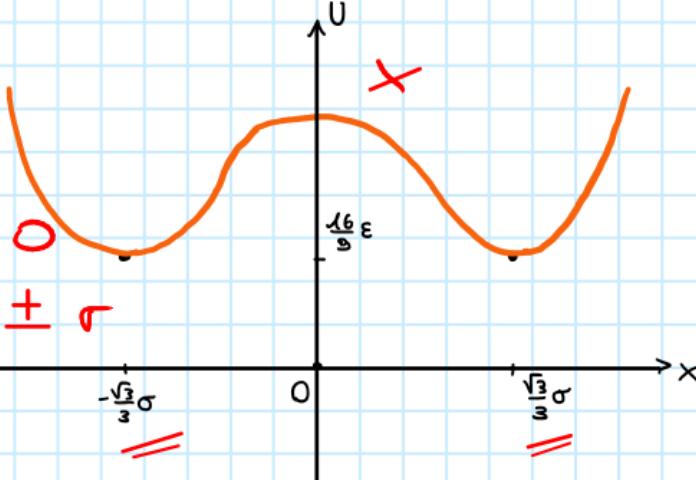


$$\rightarrow x_{1,2} = \frac{0 \pm \sqrt{\frac{192}{\sigma^4}}}{\frac{24}{\sigma^2}} / \begin{cases} +\frac{8\sqrt{3}}{24}\sigma = \frac{\sqrt{3}}{3}\sigma \\ -\frac{8\sqrt{3}}{24}\sigma = -\frac{\sqrt{3}}{3}\sigma \end{cases}$$

$$U(x_1) = \frac{16}{9}\varepsilon$$

$$U(x_2) = \frac{16}{9}\varepsilon$$

$\triangle$  bisogna cercare gli  
annullamenti di  $U''$ !



$$\frac{dE_p}{dx} = -F_x = 0$$

$$\frac{d^2E_p}{dx^2}$$

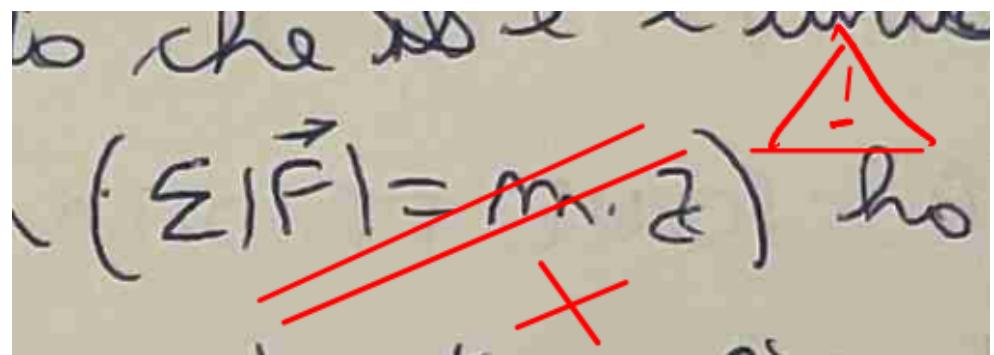
• II Newton

ERRORE

$$|\sum \vec{F}| = m |\vec{a}|$$

$$\sum |\vec{F}| = m \cdot a \quad \text{X}$$

$$\sum |F| = ma$$



• UNITÀ DI MISURA :

$$M = \frac{|\vec{g}| |\vec{r}|^2}{G} = \frac{(9.81 \frac{m}{s^2})(6 \times 10^6)^2 m}{6.674 \times 10^{-11} N m^2 / kg^2} = 5.29 \times 10^{24} \approx 10^{25} \times \text{UNITÀ DI MISURA}$$

$$M \approx 10^{25}$$

• Vettori - scalari :

$$\vec{v}_t'' = \frac{\rho_b \cdot v_b \cdot g}{\xi}$$

$$\vec{v} = \frac{s_b \cdot v_b \cdot g}{\xi}$$

$$-kx = m \cdot \vec{a} \rightarrow \frac{d^2x}{dt^2} = -\frac{k}{m} x$$

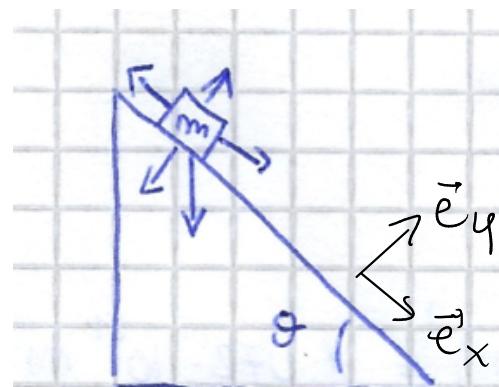
non può uguagliare  
 un vettore e un scalare  
 x diagramma

$$-kx = m\vec{a}$$

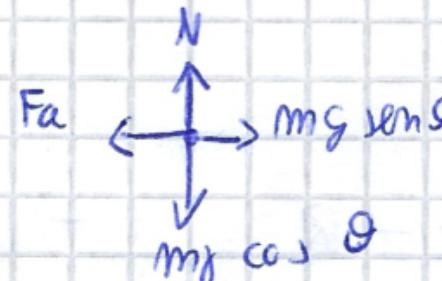
$$\frac{\vec{F}_d}{N} \leq \mu_s \quad \text{che cosa è il rapporto tra 2 vettori ??}$$

$$\mu_s = \frac{\vec{F}_d}{N}$$

- Definire e usare base  $\vec{e}_x, \vec{e}_y$  per esprimere i vettori



diag. corpo libero



II Newton

$$\Sigma_x : mg \sin \theta + F_a = m \cdot a$$

$$\Sigma_y : -mg \cos \theta + N = 0$$

Se no?

Se no?

- Ipotesi  $\Rightarrow$  conclusioni

sapendo che  $\frac{d^2x}{dt^2} = -\frac{k}{m} x$   
da cosa?

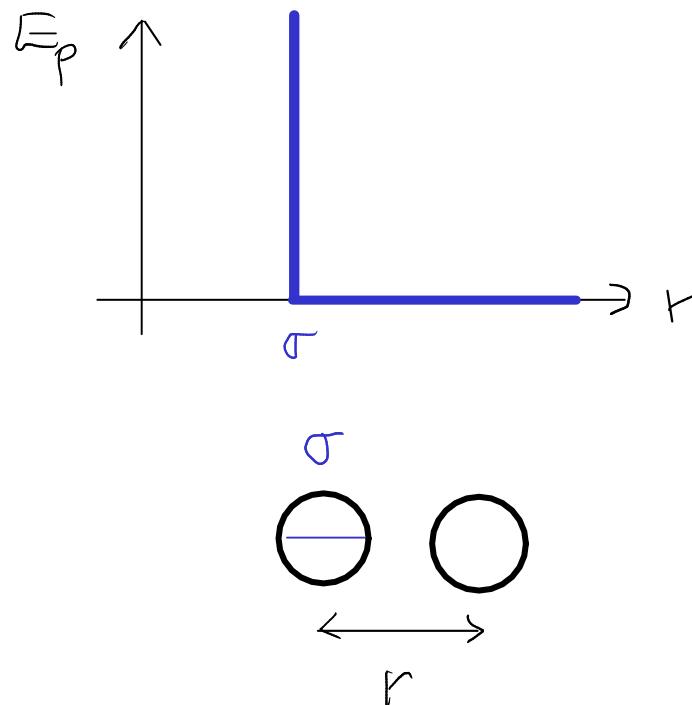
delle x e delle y da che cosa?  
Noto che  $N = mg \cos \theta$ ;  $f_s = mg \sin \theta$   
forza normale  $\otimes$   
So che affinché il blocco sia "fermo"

Deri partire da  
 $\sum \vec{F} = m \vec{a} = \vec{0}$

- Archimede

## INTERPRETAZIONE MICROSCOPICA DELL'ENTROPIA

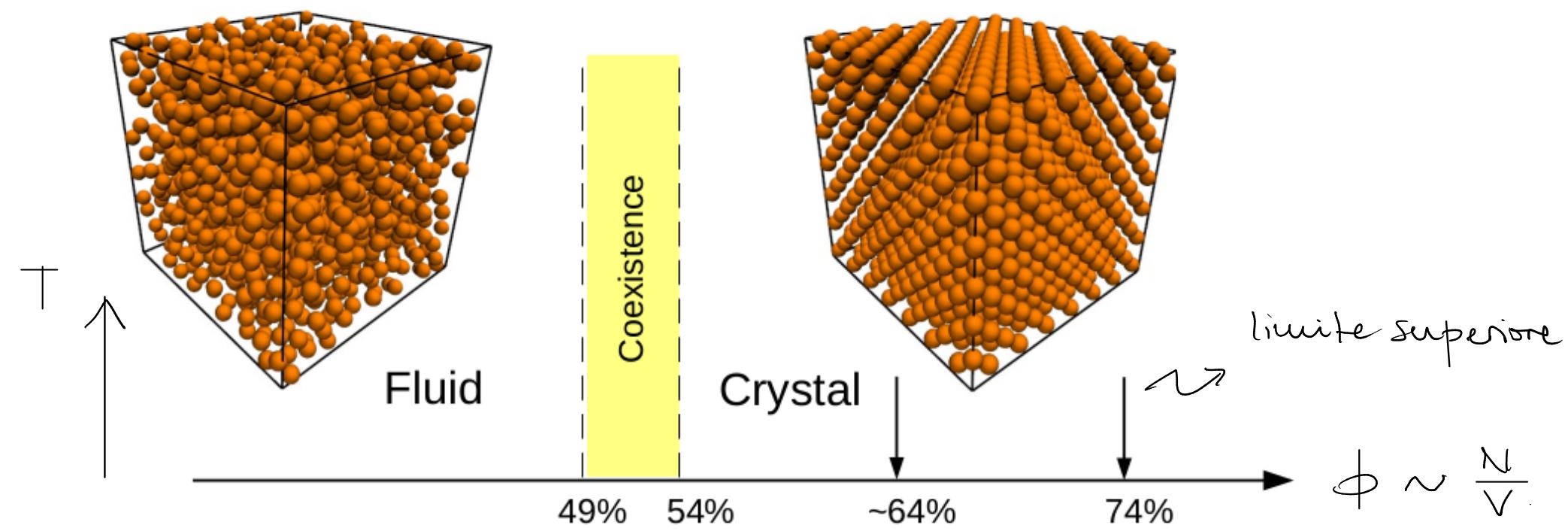
Modelli di sfere dure



$$E_p = \begin{cases} 0 & r > \sigma \\ \infty & r \leq \sigma \end{cases}$$

Sospensioni colloidali

Diagramma di fase



frazione di  
impaccamento

Dinamica molecolare: integrazione numerica delle equazioni del moto

## Phase Transition for a Hard Sphere System

B. J. ALDER AND T. E. WAINWRIGHT

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(Received August 12, 1957)

A CALCULATION of molecular dynamic motion has been designed principally to study the relaxations accompanying various nonequilibrium phenomena. The method consists of solving exactly (to the number of significant figures carried) the simultaneous classical equations of motion of several hundred particles by means of fast electronic computers. Some of the

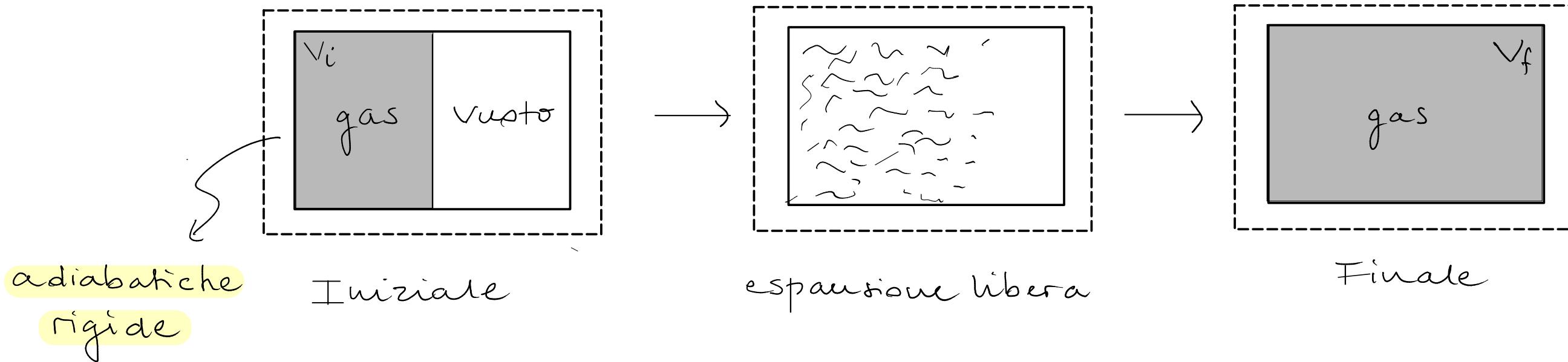


Berni Alder '57

Se  $\phi > 54\%$ , Scristallo > Sfluido

entropia  $\rightleftharpoons$  disordine

Espansione libera di un gas perfetto



adiabatiche  
rigide

Iniziale

espansione libera

Finale

Trasf. adiabatica è reversibile?

$$dS = \frac{\delta Q}{T} \quad QS$$

Variazione di S tra i e f

$$\Delta S = \int_i^f dS = \int_i^f \frac{\delta Q}{T} = \int_i^f \frac{dT}{T} + \int_i^f \frac{P}{T} dV = C_V \int_{U_i}^{U_f} \frac{dU}{U} + nR \int_{V_i}^{V_f} \frac{dV}{V}$$

trasf. immaginaria  
QS tra i e f

$$\delta Q = dU - \delta W = dU + PdV$$

$$= C_V \ln \frac{U_f}{U_i} + nR \ln \frac{V_f}{V_i} = nR \ln \frac{V_f}{V_i} = Nk_B \ln \frac{V_f}{V_i}$$

I pr:  $\Delta U = U_f - U_i = W + Q = 0 \Rightarrow U_f = U_i$

rigide  
+ espansione nel vuoto

Ese:  $V_f = 2V_i \Rightarrow \Delta S = Nk_B \ln 2 > 0$  ok per il II pr.

Macro

Termodinamica

$$\{P, T, V, N, U, S\}$$

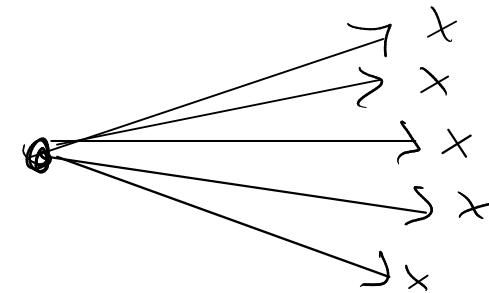
macro - stato

Micro

Dinamica Newtoniana

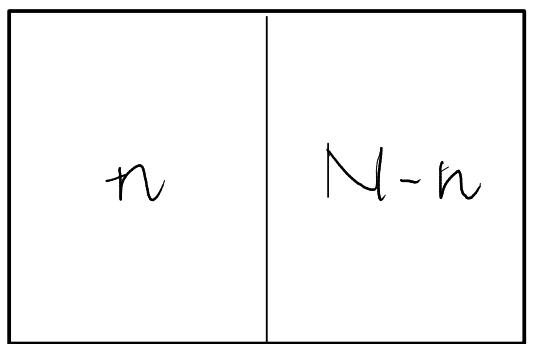
$$\{\vec{r}_1, \dots, \vec{r}_N, \vec{v}_1, \dots, \vec{v}_N\}$$

micro - stato



$S \rightarrow$  numero di micro - stati compatibili  
con un macro - stato

# Modellizzazione Schematica



Numeri di realizzazioni totali

$$\Omega = 2^N$$

macro - stato :  $n$

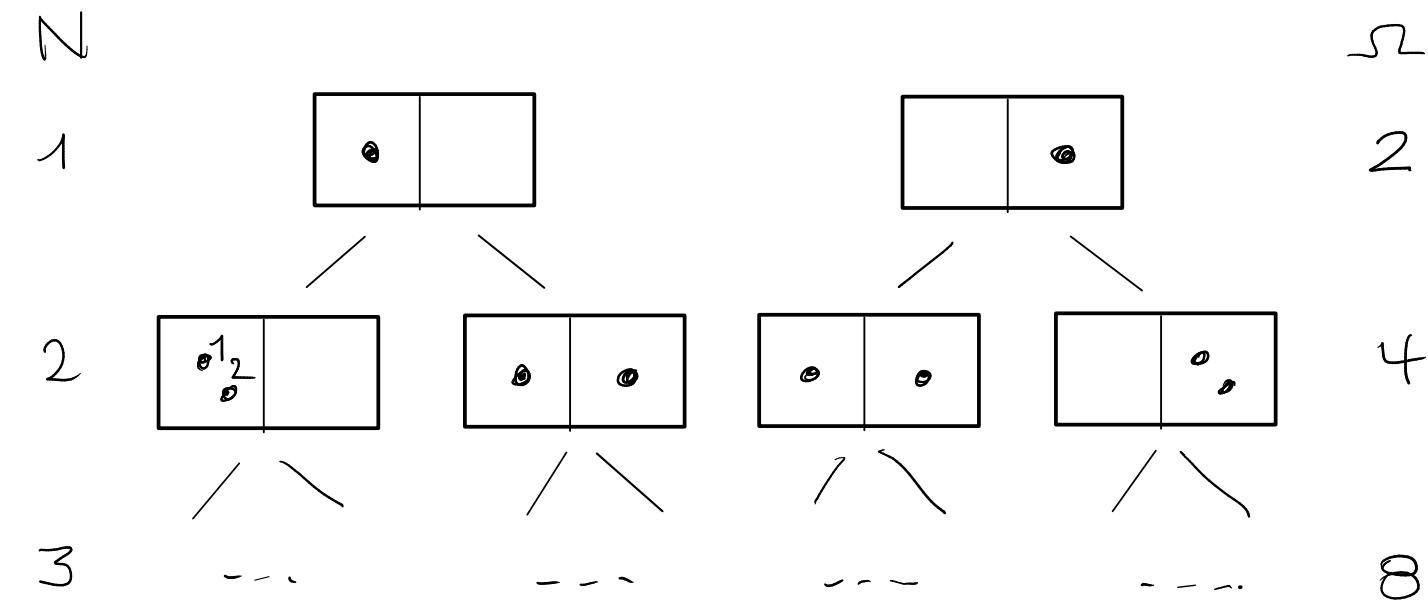
micro - stato : combinazione di  $n$  tra  $N$

Combinazioni compatibili con macro - stato  $n$

$$w_n = C_n^N = \binom{N}{n} = \frac{N!}{n! (N-n)!}$$

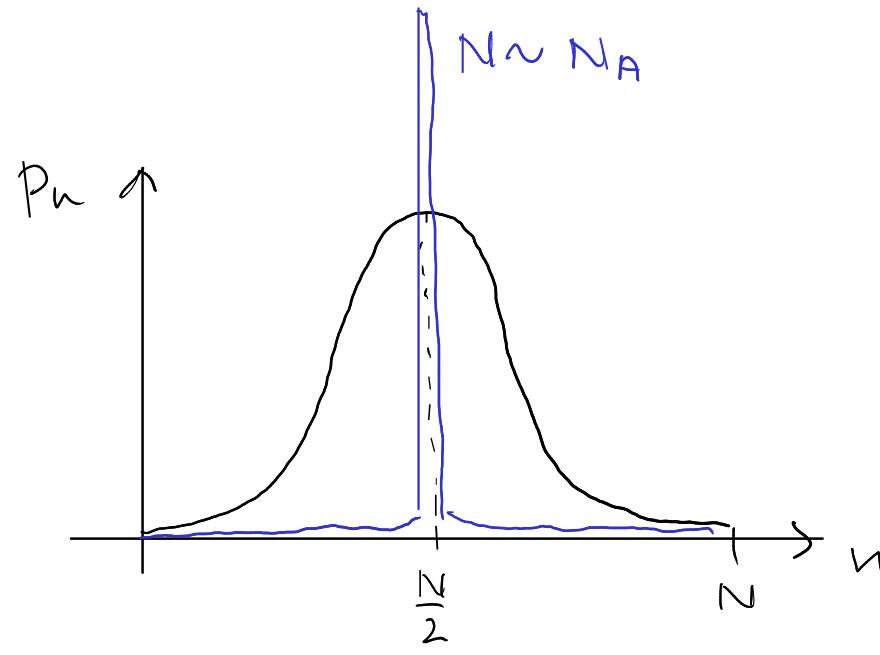
coefficiente binomiale

$$\left[ \sum_{n=0}^N C_n^N = 2^N \right]$$



Probabilità del macro  $n$  stato

$$p_n = \frac{C_n^N}{\sum_{n=0}^N C_n^N} = \frac{w_n}{2^N}$$



$N = N_A$   
 Initiale :  $n = N$   
 Finale :  $n = \frac{N}{2}$

$$P_N = \frac{1}{2^{10^{23}}} = 2^{-10^{23}} \approx 10^{-10^{22}}$$

Entropia di Boltzmann  $\rightarrow$  sistema isolato

Microstati hanno tutti uguali probabilità

$$S \sim \log w$$

↑  
numero di micro-stati  
compatibili con il  
macro-stato



$S$  è additiva

$$\boxed{1} \quad \boxed{2}$$

$$S_{\{1,2\}} = S_1 + S_2$$

$$S_1 \quad S_2$$

$$S \equiv k_B \log w$$



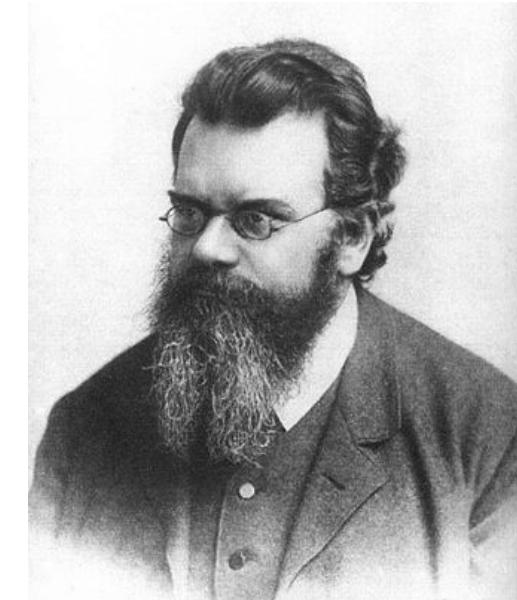
costante di Boltzmann

Nota:  $\log = \ln$   
in base e

$$w_1 \cdot w_2 = w \quad \log(w_1 \cdot w_2) = \log w_1 + \log w_2$$

Equilibrio  $\rightarrow$  stato più probabile (n. massimo di realizzazioni micro)

$S$ : misura della nostra ignoranza / incertezza riguardo allo stato microscopico del sistema



Ludwig Boltzmann  
1844 - 1906

Ese. espansione libera

$$S_n = K_B \ln w_n$$

$$\Delta S = S_{\frac{N}{2}} - S_N = K_B \ln \left[ \frac{\frac{N!}{(\frac{N}{2})! (\frac{N}{2})!}}{1} \right] - K_B \ln \left[ \frac{N!}{N! 1} \right]$$

$$= K_B \ln(N!) - 2 K_B \ln \left[ \left( \frac{N}{2} \right)! \right] = K_B \ln(N!) - 2 K_B \ln \left[ \left( \frac{N}{2} \right)! \right]$$

$$\approx \underbrace{K_B N \ln N}_{\text{term 1}} - \underbrace{K_B N}_{\text{term 2}} - \cancel{2} \underbrace{\frac{N}{2} K_B \ln \left( \frac{N}{2} \right)}_{\text{term 3}} + \cancel{2} \underbrace{K_B \frac{N}{2}}_{\text{term 4}}$$

$$= K_B N \cancel{\ln N} - K_B N \cancel{\ln N} + N K_B \ln 2$$

$$= K_B N \ln 2 \quad \square$$

Approssimazione di Stirling . N > 1

$$\ln(N!) \approx N \ln N - N$$