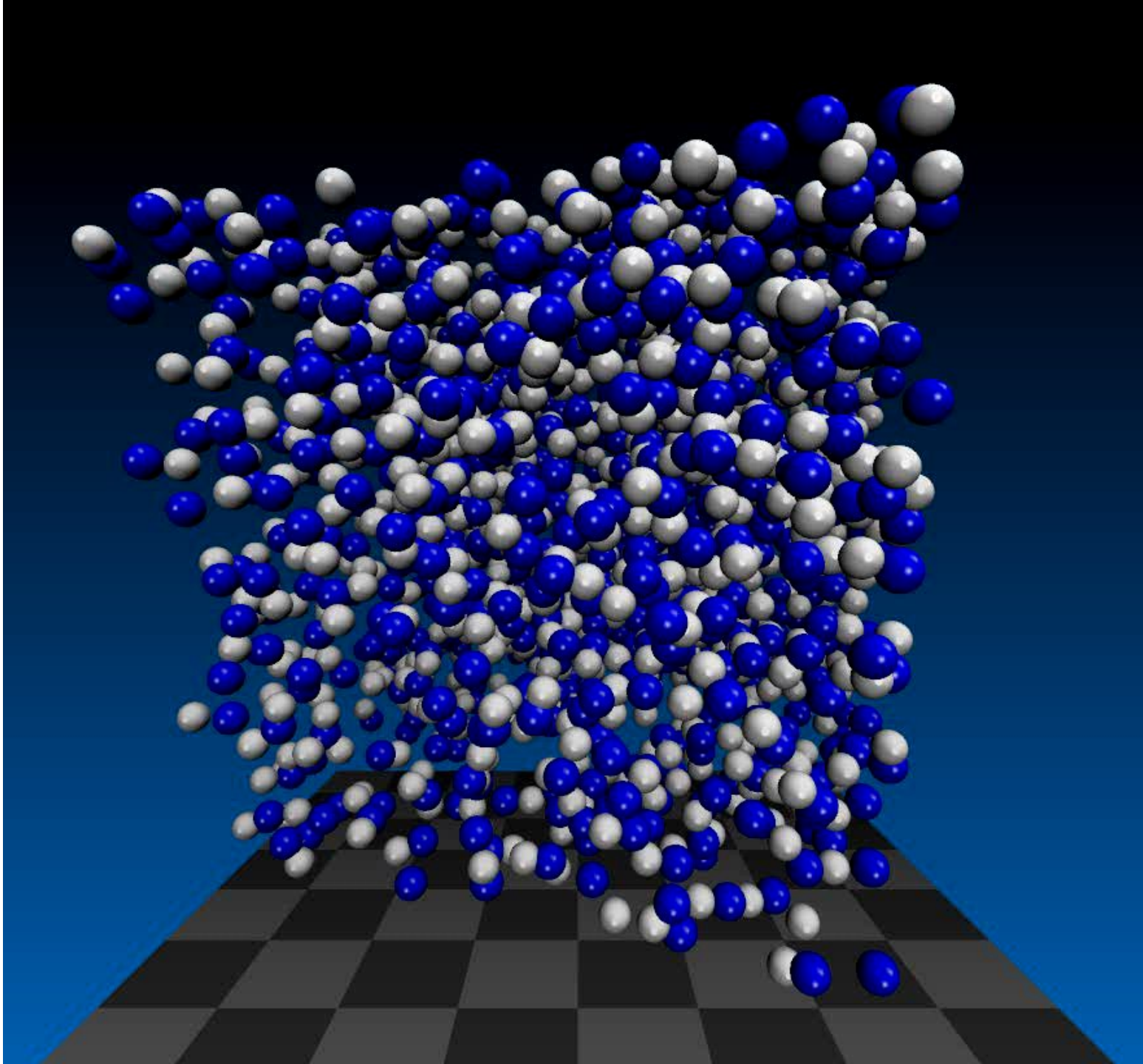
Dinámica Molecular

2MeV

T

0.1 MeV



Dinamica Molecular 1

Cuestiones a ver en esta clase

a) Teorema ergodico

b) camino al equilibrio

c) ecuaciones de movimiento

d) resolucion de las ecuaciones de movimiento

e) que ensemble estamos simulando?

e) trucos

Teorema Ergodico

Espacios

Espacio $\mu \Rightarrow$ 6 dimensiones, $d^3p\ d^3q$

1 punto representa las coordenadas y momentos de 1 particula

La configuracion del sistema completo necesita N puntos

Espacio $\Gamma \Rightarrow$ 6N dimensiones, $(d^3p_1\ d^3q_1; d^3p_2\ d^3q_2; \ldots.)$

1 punto en Γ representa un estado del sistema de N particulas

El ensemble Gibbsiano:

Dada una condicion Macroscopica (i.e. E,V,N), todos los posibles estados compatibles con ella definiran una "nube de puntos" en Γ representada por:

$$\rho(p,q,t)$$

Entonces $\rho(p,q,t)d^{3N}pd^{3N}q$ es el numero de estados en ....

Dado el hamiltoniano $H(p,q)$ tendremos

$$\dot{p_i} = -\frac{\partial H}{\partial q_i}; 1 \leq i \leq N$$

$$\dot{q_i} = \frac{\partial H}{\partial p_i}; 1 \leq i \leq N$$

El Teorema de Liouville

$$\frac{\partial \rho}{\partial t} + \sum \left[\frac{\partial \rho}{\partial p_i} \dot{p}_i + \frac{\partial \rho}{\partial q_i} \dot{q}_i \right] = 0$$

1punto en el ensemble es un estado, el numero de estados se conserva $\Rightarrow$ continuidad, sea ϖ un volumen con superficie S en Γ :

$$-\frac{\partial}{\partial t} \int_{\varpi} d\varpi \rho = \int_{S} dS \vec{n} \cdot \vec{v} \rho$$

con $\vec{n}$ normat exterior y $\vec{v} = (\ldots, \dot{p}_i, \ldots, \ldots, \dot{q}_i, \ldots)$

$$\int_{\varpi} d\varpi \left[\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{v} \rho \right] = 0$$

pero ϖ es un volumen arbitrario ...

$$-\frac{\partial \rho}{\partial t} = \nabla \cdot \vec{v}\rho$$

$$-\frac{\partial \rho}{\partial t} = \sum\left[\frac{\partial \rho}{\partial p_i}\dot{p}_i + \frac{\partial \rho}{\partial q_i}\dot{q}_i\right] +$$

$$+\rho\sum\left[\frac{\partial}{\partial p_i}\dot{p}_i + \frac{\partial}{\partial q_i}\dot{q}_i\right]$$

0 !!!

Pero el ultimo termino es 0 en virtud de las ec. de Hamilton

$$\frac{d\rho}{dt} = 0$$

es la derivada siguiendo las lineas de flujo $\Rightarrow$fluido incompresible !!!!!!!

O sea que se preserva el volumen.

$$\frac{\partial}{\partial p_i}\dot{p}_i = \frac{\partial}{\partial p_i}\left[-\frac{\partial H}{\partial q_i}\right]$$

$$\frac{\partial}{\partial q_i}\dot{q}_i = \frac{\partial}{\partial q_i}\left[\frac{\partial H}{\partial p_i}\right]$$

Sumando

$$\frac{\partial}{\partial p_i}\left[-\frac{\partial H}{\partial q_i}\right] + \frac{\partial}{\partial q_i}\left[\frac{\partial H}{\partial p_i}\right] = 0 = \frac{\partial}{\partial p_i}\dot{p}_i + \frac{\partial}{\partial q_i}\dot{q}_i$$

$$-\frac{\partial \rho}{\partial t} = \nabla \cdot \vec{v}\rho$$

$$-\frac{\partial \rho}{\partial t} = \sum\left[\frac{\partial \rho}{\partial p_i}\dot{p}_i + \frac{\partial \rho}{\partial q_i}\dot{q}_i\right] +$$

$$+\rho\sum\left[\frac{\partial}{\partial p_i}\dot{p}_i + \frac{\partial}{\partial q_i}\dot{q}_i\right]$$

0 !!!

Pero el ultimo termino es 0 en virtud de las ec. de Hamilton

$$\frac{d\rho}{dt} = 0$$

derivada convectiva

es la derivada siguiendo las lineas de flujo $\Rightarrow$fluido incompresible !!!!!!!

O sea que se preserva el volumen. en Γ space

$$\rho \sum_{i=1} \left(\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right) = \rho \sum_{i=1} \left(\frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial q_i \partial p_i} \right) = 0$$

usando corchetes de Poisson

$$\frac{\partial \rho}{\partial t} = -\{\rho, H\}$$

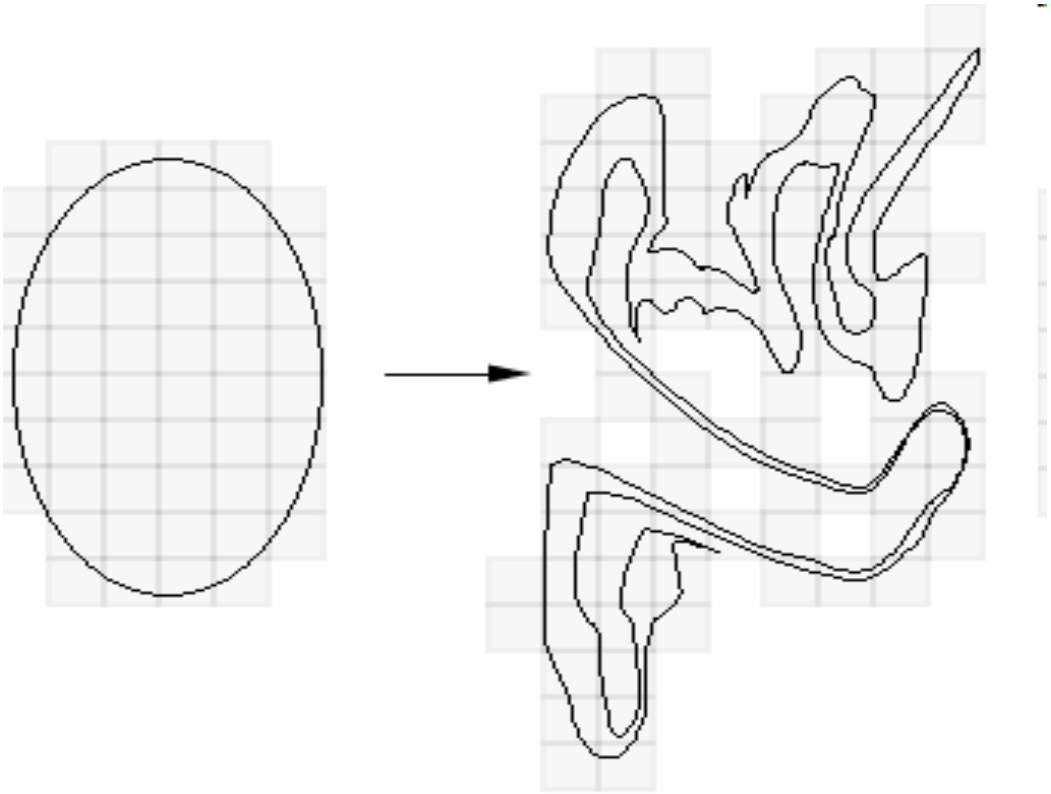
usando el Liovilliano

$$i\hat{\boldsymbol{L}} = \sum_{i=1} \left[\frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} \right] \Rightarrow$$

$$\frac{\partial \rho}{\partial t} + i\hat{\boldsymbol{L}}\rho = 0$$

$$\frac{\partial \langle A \rangle}{\partial t} = \frac{1}{i\hbar} \langle [A, H] \rangle$$

Atención



Hay diversos posibles evoluciones que dan lugar a una preservacion del volumen

Birkoff probo que, dada una funcion dinamica que es integrable sobre todo el espacio de fases

$$\int_{\Gamma} d\mu_0 |b(x)| < \infty$$

Entonces

$$\lim_{T\to\infty} \frac{1}{(T - t_0)} \int_{t_0}^{T} b(x)dt = \overline{b(x)}$$

es el promedio temporal.

Este promedio existe para casi toda condicion inicial

Ademas probo un segundo teorema que bajo ciertas condiciones

a) $\overline{b(x)}$es constante independiente de x (para casi todo el espacio)

b) se satisface con $\langle b \rangle$ el promedio sobre el espacio de fases

$$\overline{b(x)} = \langle b \rangle$$

Camino al equilibrio

Atencion : En realidad no trabajamos sobre todo el espacio de fases sino que tenemos una integral aislante que es la energia luego debemos restringirnos al hyperplano de la energia constante.

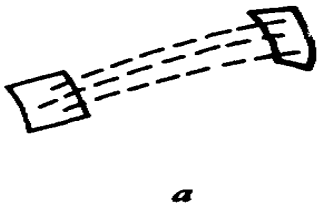
Ademas necesitamos que el espacio sea metricamente transitivo (todo el espacio sea accesible)

Sin embargo necesitamos, ademas, que el flujo "cubra todo el espacio de fases accesible al sistema"

Pero la trayectoria es una linea y no cubre totalmente el espacio!

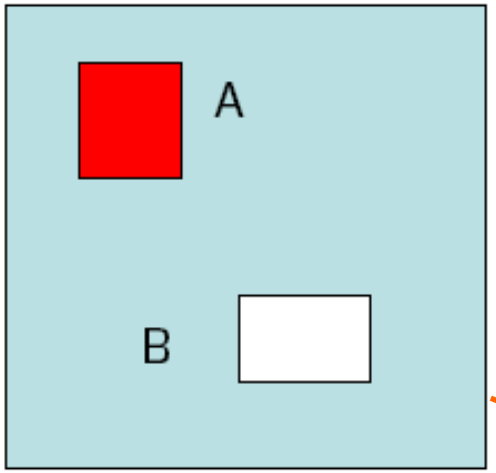
pero....

definiendo la medida $\mu(\Gamma) = \int_\Gamma d\mu = \int_\Gamma dx\, F(x) = 1$



a

b



Pesa las distintas
Regiones del
espacio de fases
De modo que no
Diverja la integral

Sea este el esquema de la condicion inicial y la region de control
Con "volumenes" (medidas)$\mu_0(A)$ y $\mu_0(B)$

Al evolucionar en el tiempo $\mu_0(A) \rightarrow \mu_0(A_t)$

Sea el flujo mixing aquel que:

$$\lim_{t\to\infty} \frac{\mu_0(A_t \cap B)}{\mu_0(B)} = \mu_0(A) \quad = \quad \frac{\mu_0(A)}{\mu_0(\Gamma)}$$

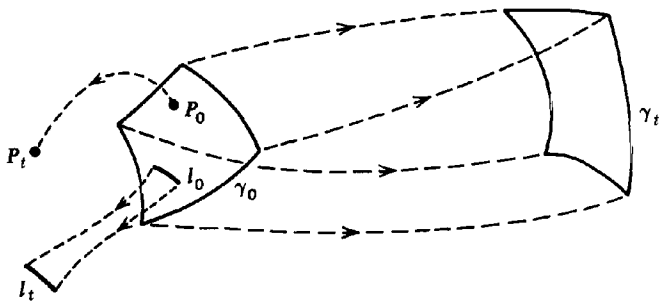
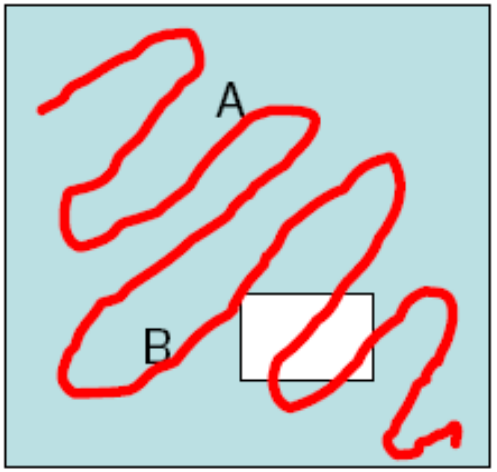


Figure A.5.2. Motion of a phase element.



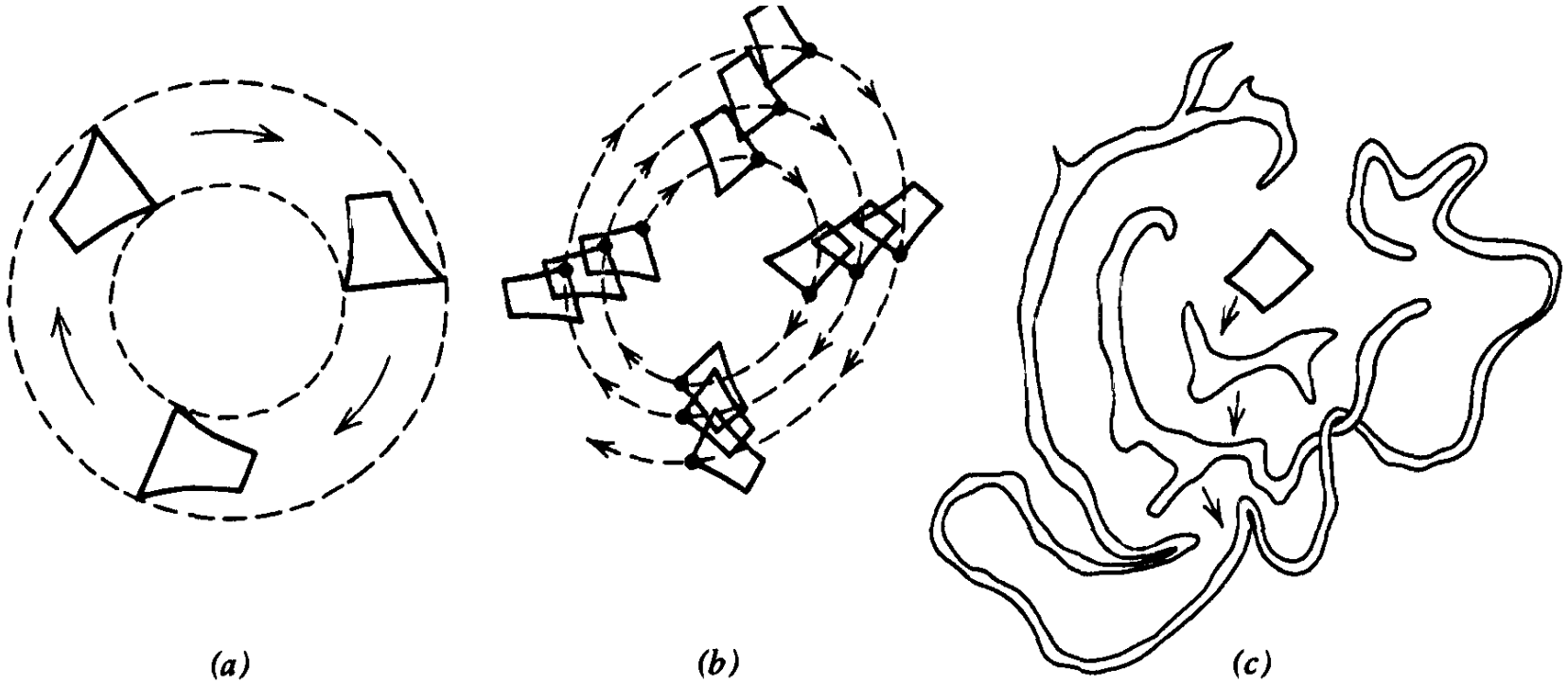


Figure A.6.1. Various types of flow in phase space: (*a*) nonergodic; (*b*) ergodic but not mixing; (*c*) mixing.

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VI. GEOMETRIC ILLUSTRATION OF THE APPROACH TO EQUILIBRIUM AND THE SECOND LAW

As Thermodynamics describes a N-body systems by a few control parameters M only, which are much less than the total number $6N$ of degrees of freedom, it gives only *probabilistic* answers (the *average* of some observable $< O >$ over the whole ensemble of all systems with the same values of the M control-parameters). Therefore, Thermodynamics describes the evolution of the whole ensemble. There is also a geometric interpretation of the evolution of a non-equilibrized ensemble to the microcanonical uniform filling of the energy-shell in the $6N$-dim. phase space.

Even though every trajectory spreads over the available phase space and returns after $t_{Poincarre}$, different points of the manifold have different $t_{Poincarre}$ which are normally incommensurable. I.e. the ensemble spreads irreversibly over the accessible phase-space.

Due to the redundancy of the information given by the few (M) control-parameters one cannot distinguish the distribution in phase-space from its direct neighborhood. Therefore, in the case of a strongly folded (eventually fractal) non-equilibrium phase-space distribution Boltzmann's entropy is the area of the closure of the distribution [34]. The area of the closure can be calculated by box-counting [34, 35] c.f. fig.(5). Mathematically, the area of the closure is obtained in the limit of box-sides $\delta \to 0$. However, by several reasons this limit should not be taken in physical applications (see below). This figure illustrates also how a non-equilibrium ensemble develops in time, and how for a mixing dynamics it becomes more and more dense in the larger available phase-space, so that the area of its closure $e^{S(t)}$ approaches the larger area of the new microcanonical ensemble $\propto (V_a + V_b)^N$. This is the *geometric meaning of the Second Law of Thermodynamics*. Due to the inherent redundant information given by Thermodynamics, represented here by a finite, non-zero, resolution δ of the box-counting, this is achieved in a finite equilibration time [38].

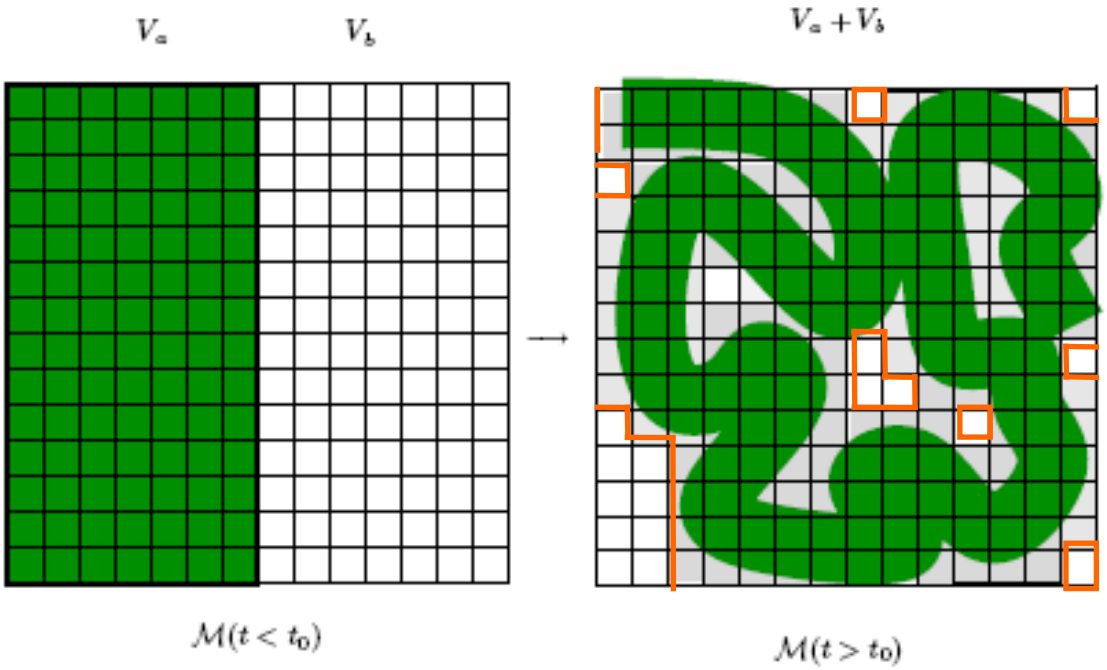


FIG. 5: At time $t \leq t_0$ the system is assumed to be equilibrized and be represented by the compact microcanonical set in phase-space $\mathcal{M}(t_0) = \mathcal{E}(V_a)$, left side. At times t_0 the accessible volume is suddenly enlarged to $V_a + V_b$. The system develops into an increasingly folded but non-crossing "spaghetti"-like distribution $\mathcal{M}(t)$ in phase-space with rising time $t > t_0$ after opening the volume V_b. The right figure shows only the early form of the distribution. At much later times it will become more and more fractal (Gibbs ink-lines) and finally dense in the new larger phase space. The grid illustrates the boxes or size δ^{6N} of the box-counting method. All boxes which overlap with $\mathcal{M}(t)$ contribute to the box-counting volume and are shaded gray. Their number is N_δ. Then the box-counting area is $= N_\delta \delta^d$ where d is the dimension of the microcanonical manifold.

Lyapunov exponents

Marcan el ritmo de divergencia de dos trayectorias inicialmente muy cercanas en el espacio de fases

$$\frac{dx}{dt} = V_i(x) \ , \ i = 1, M$$

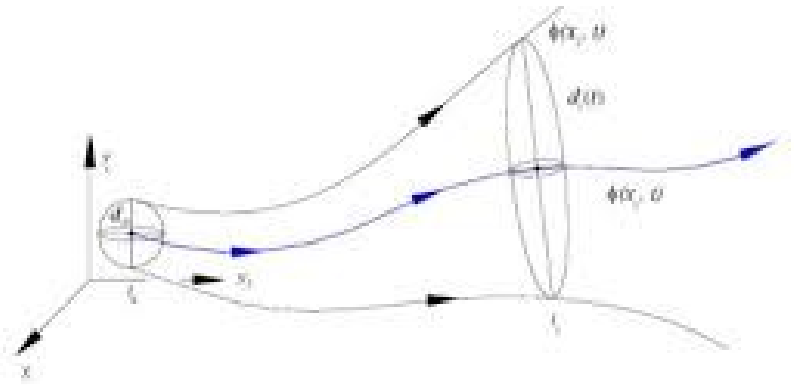
Sean dos trayectorias en el espacio de fases con condiciones iniciales x_0 y $x_0 + \Delta x_0$

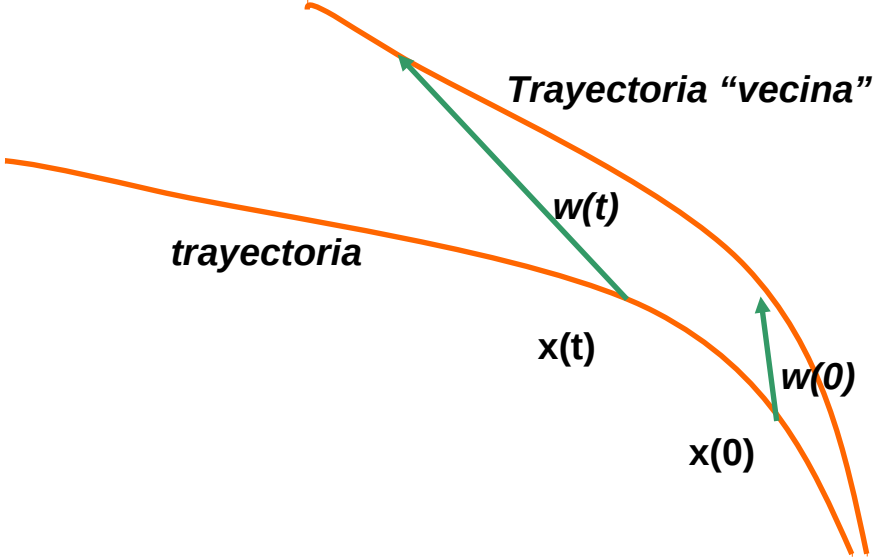
Estas dos trayectorias generan el vector tangente

$$\vec{\Delta}(x_0, t) \ , \text{ de donde } d(x_0, t) = \left\| \overrightarrow{\Delta x}(x_0, t) \right\|$$

si escribimos $\omega = \overrightarrow{\Delta x}$, y tomamos la forma linealizada de V

$$\frac{d\omega}{dt} = M(x(t)) \cdot \omega$$





con $M = \frac{\partial V}{\partial x}$, que es el jacobiano de V

Sea

$$\sigma(x_0, w) = \lim_{t\to\infty, d(0)\to 0} \left(\frac{1}{t}\right) \ln \frac{d(x_0, t)}{d(x_0, 0)}$$

Que es el ritmo exponencial de divergencia de las trayectorias

En un espacio M-dimensional existe una base $\{\hat{e}_i\}$ de ω

$$\sigma_i(x_0) = \sigma(x_0, \hat{e}_i)$$

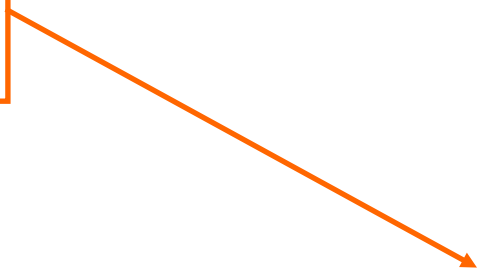
Existen entonces M exponentes

$$\sigma_1 \geq \sigma_2 \geq \ldots \sigma_{M-1} \geq \sigma_M$$

Estos son independientes de la metrica del espacio

Como hay una divergencia exponencial el maximo domina la evolucion

Para el caso Hamiltoniano



$$V = \left(\frac{-\partial H}{\partial q}, \frac{\partial H}{\partial p} \right)$$

Hay una simetria en este caso

$$\sigma_i = \sigma_{2N-i+1}$$

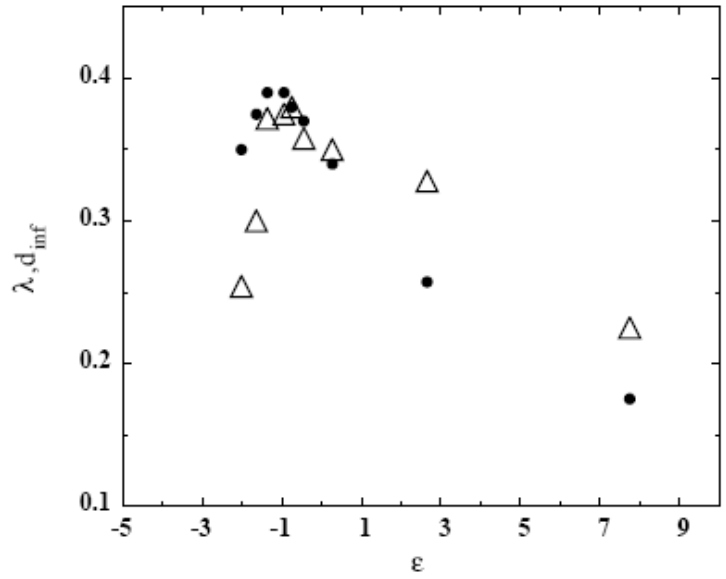


Fig. 2. MLE (triangles) and $d_\infty/4$ (full circles) as a function of energy for two-dimensional Lennard-Jones drops with $N = 100$ particles.

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Local (in time) maximal Lyapunov exponents of fragmenting drops

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$$\lambda = \lim_{t\to\infty} \lim_{d(0)\to 0} \left[\frac{1}{t} \ln \frac{d(t)}{d(0)}\right].$$

$$d(t) = \left(\sum_{i=1}^{N} \{a[\mathbf{r}_m(t) - \mathbf{r}_s(t)]^2 + b[\mathbf{p}_m(t) - \mathbf{p}_s(t)]^2\}_i \right)^{1/2}.$$

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THE EUROPEAN PHYSICAL JOURNAL A

Lyapunov exponent, generalized entropies and fractal dimensions of hot drops

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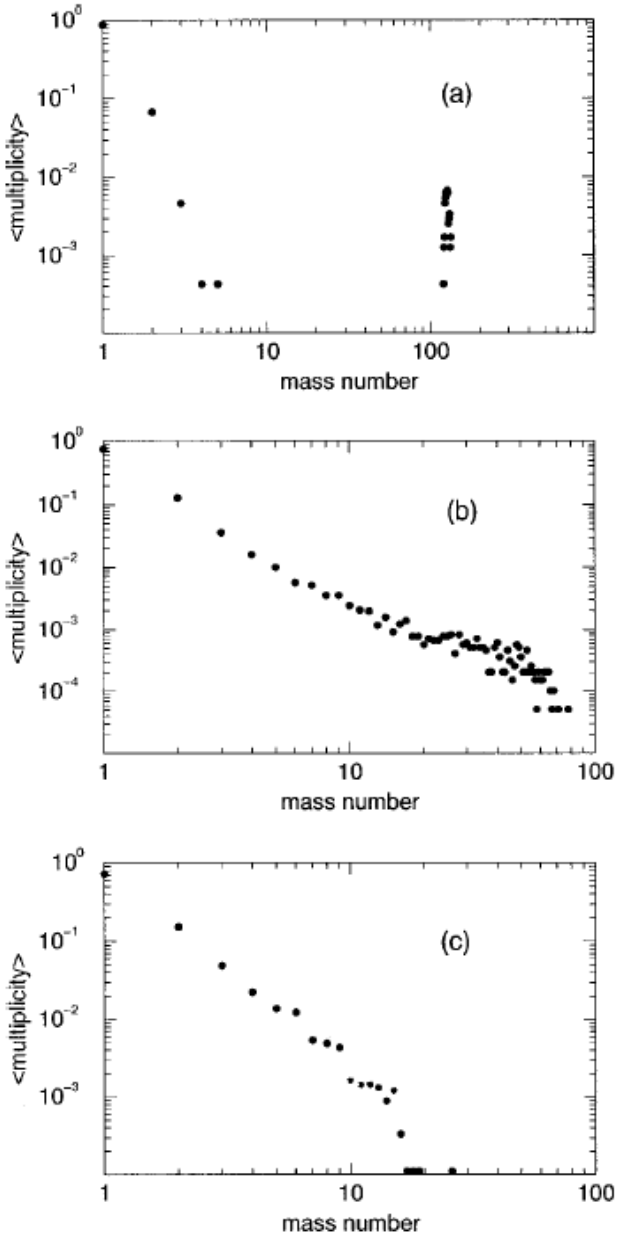

FIG. 1. Asymptotic mass spectra for three different energies in the fragmentation regime: (a) $E=-2.0\epsilon$, (b) $E=+0.5\epsilon$, and (c) $E=+3.0\epsilon$.

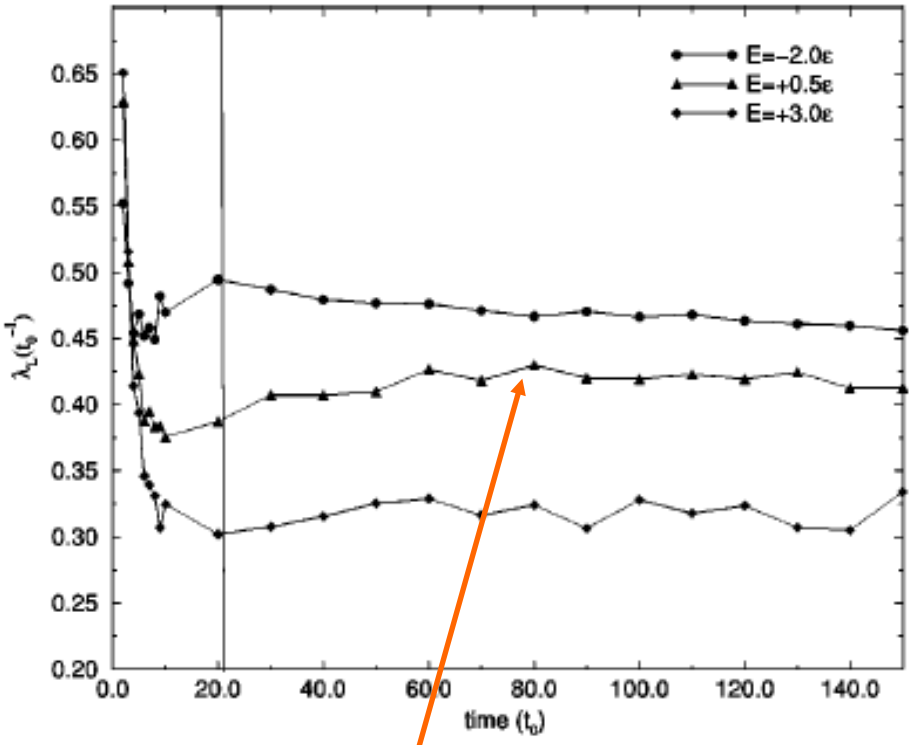

FIG. 3. Maximum local Lyapunov exponent (λ_L) as a function of time for the same three energies of Fig. 1: solid circles for $E=-2.0\epsilon$, solid triangles for $E=+0.5\epsilon$, and solid diamonds for $E=+3.0\epsilon$.

TRF < 0 !!!!!!!

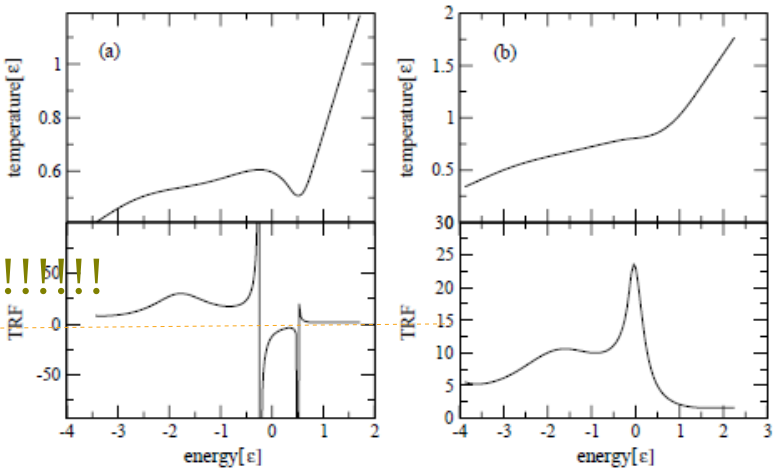

Fig. 4. Here we show the CC (upper panels) and the associated TRF (lower panels) for two values of the volume. The left-hand side corresponds to $R = 15\sigma$ (dilute case) and the right-hand side to $R = 8\sigma$ (transition to dense state). It can be seen that for the dilute case two poles are present which limit the region of negative TRF. On the other hand, at $R = 8\sigma$ the TRF is always positive and displays a maximum.

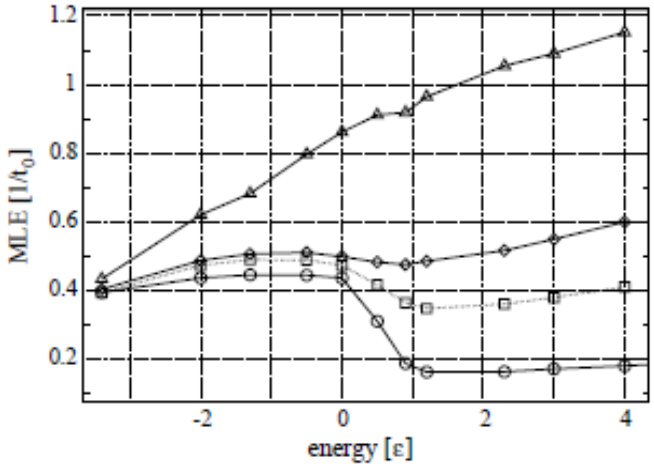

Fig. 5. In this figure we plot the MLE as a function of the energy deposited in the system for the four values of the containing volume considered in this work. Symbols have the same meaning as in fig. 1). It can be seen that the MLE clearly signals the transition from a liquid-like regime to a vapor-like regime (according to the ECRA analysis).

$$d_{\infty}^{n}(t) = \left(\frac{\sum_{i=1}^{N} \left[(p_1(t) - p_2(t))^2 \right]_i}{\frac{1}{2} \sum_{i=1}^{N} \left[p_1(t) \right]_i^2} \right)^{\frac{1}{2}} .$$

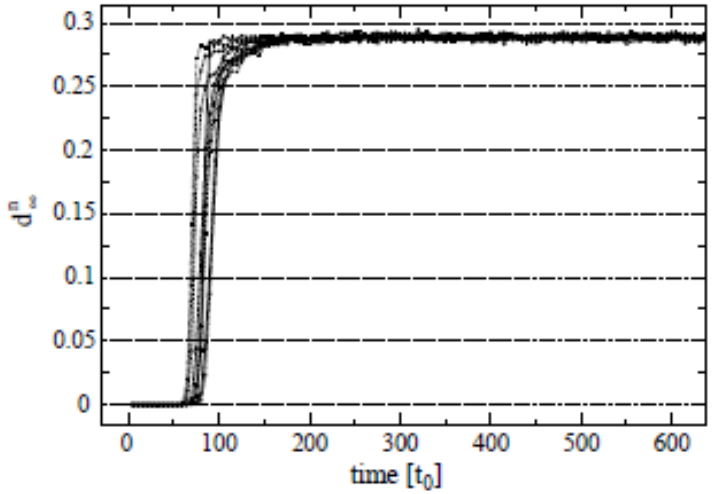

Fig. 7. d_{∞} scaled with the square root of the kinetic energy for a volume of radius $R = 8\sigma$. Different curves correspond to different energies in the range $-3.4 \leq E \leq 4.0$ Notice that after a short time all the curves collapse into a single one.

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THE EUROPEAN PHYSICAL JOURNAL A

Dynamical properties of constrained drops

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La entropia de Kolmogorov

Sea una trayectoria en el espacio de fases.

$$\vec{x}(t) = [x_1(t), x_2(t), \ldots, x_d(t)]$$

El espacio de fases esta dividido en celdas de tamaño l^d

Sea $P_{i_0 \ldots . i_n}$ la Probabilidad conjunta de que

punto		*celda*
$\vec{x}(0)$	$\mapsto$	i_0
$\ldots$		$\ldots$
$\vec{x}(n\tau)$		i_n

Entonces la informacion necesaria para localizar a la trayectoria en unas celdas

$i_0 \ldots . i_n$ con precision l es

Entonces la informacion necesaria para localizar a la trayectoria en unas celdas $i_0 \ldots . i_n$ con precision l es

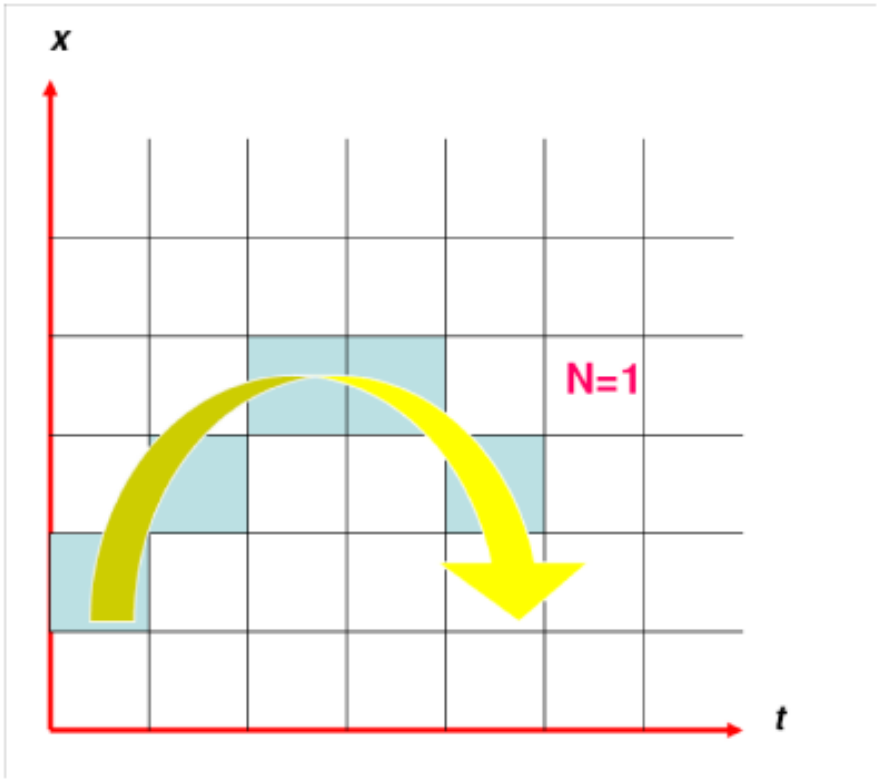
$$K_n = -\sum_{i_0 \ldots . i_n} P_{i_0 \ldots . i_n} \log P_{i_0 \ldots . i_n}$$

La K-entropy es definida como el ritmo promedio de perdida de informacion

$$K = \lim_{\tau \to 0} \lim_{l \to 0} \lim_{N \to \infty} \frac{1}{N\tau} \sum (K_{n+1} - K_n)$$

Aproximamos $P_{i0} P_{i1} \approx P_{i0} \cdot \frac{1}{N}$

numero de posibles nuevos intervalos involucrados en la evolucion a partir de i_0



N=numero de celda visitadas

En este caso la evolucion pasa de celda a celda, de donde "puntos inicialmente adyacentes siguen estando adyacentes"

Entonces

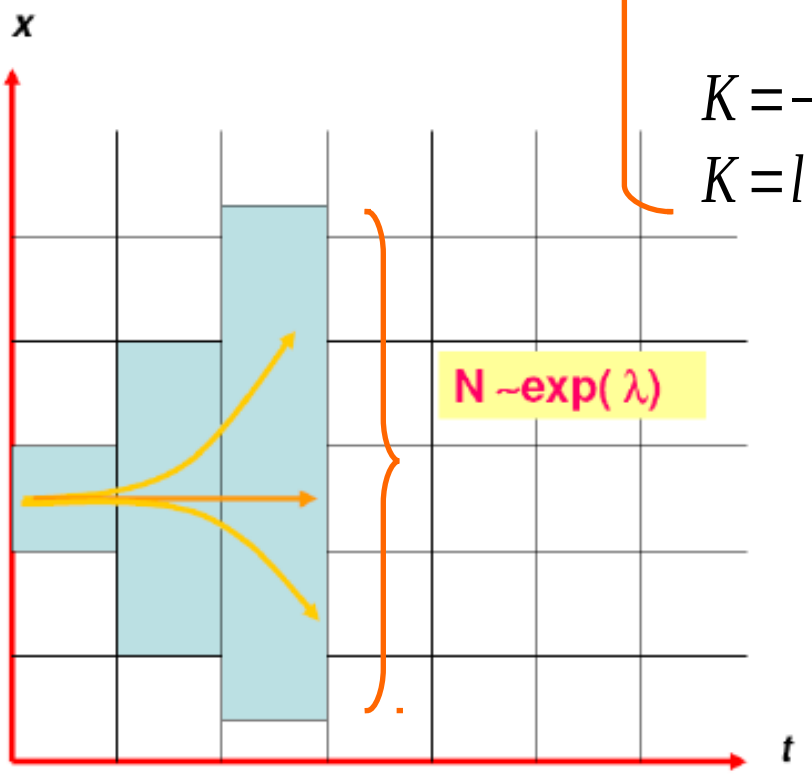
$$P_{i_0} = l \rightarrow P_{i_0 i_1} = l \cdot 1 \Rightarrow K = 0$$

Pero si ocurre (exponencial)

$$K = -\left[\sum l e^{-\lambda} \ln\left(l e^{-\lambda}\right) - l \ln l\right]$$

$$K = -e^{\lambda} l e^{-\lambda} \ln\left(l e^{-\lambda}\right) + l \ln l$$

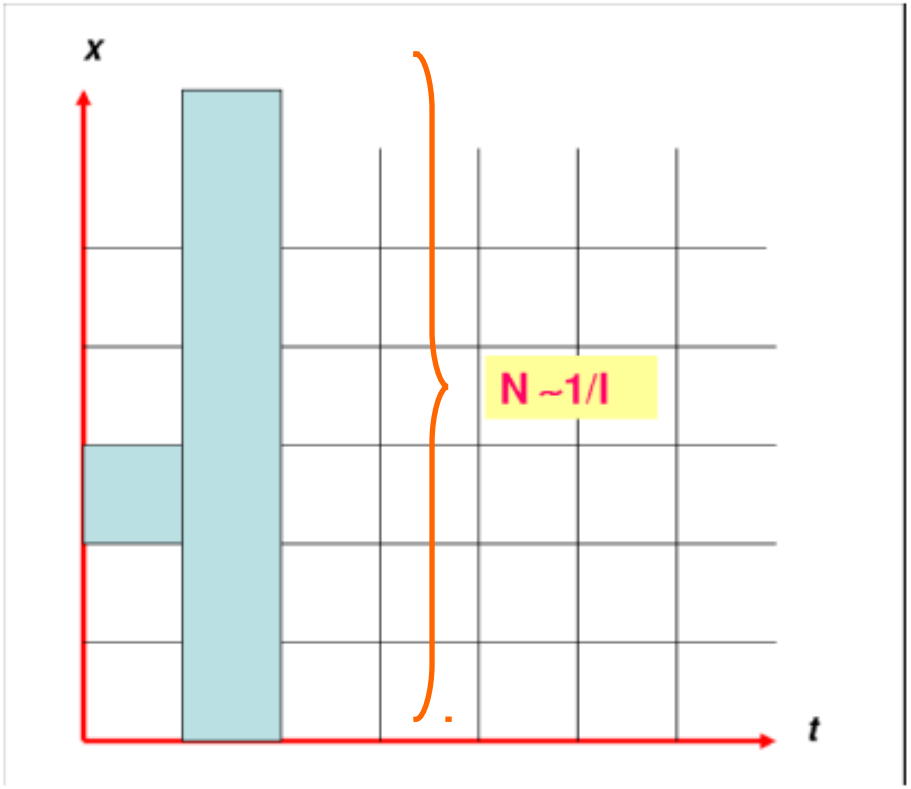
$$K = l \ln l - l \ln l + l\lambda = l\lambda$$



En este caso

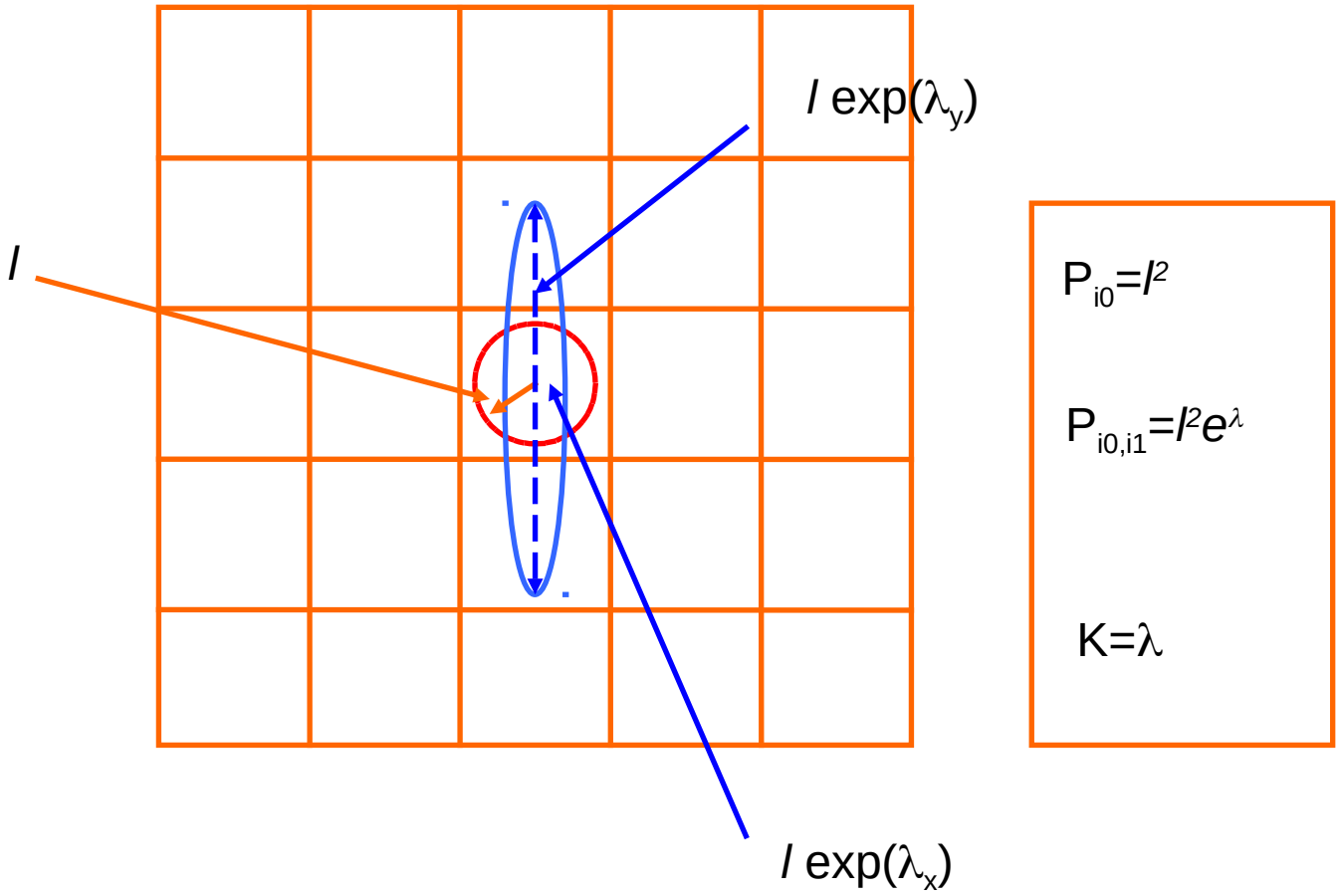
$$P_{i_0} = l \;\rightarrow\; P_{i_0 i_1} = l \cdot e^{-\lambda} \;\Rightarrow\; K = \lambda > 0$$

Finalmente (aleatoria)



$$P_{i_0} = l \;\rightarrow\; P_{i_0 i_1} \propto l^2 \;\Rightarrow\; K \propto -\log l \rightarrow \infty$$

En dos dimensiones



Nuevamente K y λ , ademas al contraerse no baja el numero de celd

Los sistemas se caracterizan por

K-Systems

entropia de Kolmogorov positiva

Mixing-Systems

"shaking" (un lyapunov positivo)

Ergodicos

(satisfacen lo visto al ppo.)

tal que

$$K - \text{Systems} \Rightarrow \textit{Mixing} - \text{Systems} \Rightarrow \text{Ergodicos}$$

Ecuaciones de movimiento

Tomemos en cuenta que para solo en r obtenemos

$$f(t) = f(0) + \Delta r \frac{\partial}{\partial r} f(0) + \frac{1}{2!}(\Delta r)^2 \cdot \frac{\partial^2}{\partial r^2} f(0) + \ldots$$

Como $\Delta r = \dot{r}(0) \cdot t$

Entonces

$$f(t) = f(0) + \dot{r}(0) \cdot t \frac{\partial}{\partial r} f(0) + \frac{1}{2!}\left(\dot{r}(0) \cdot t\right)^2 \frac{\partial^2}{\partial r^2} f(0) + \ldots$$

.

usando

$$iL_r = \dot{r}(0) \frac{\partial}{\partial r}$$

liouvilliano

$$\frac{\partial F(q,p;t)}{\partial t} \equiv \partial_t F(q,p:t) = [H(q,p), F(q,p;t)]_P$$

Ecuación de Liouville

$$\partial_t F(t) = LF(t)$$

$$LF(t) = [H,F]_P = \sum_{n=1}^{N} \{ \frac{\partial H}{\partial q_n} \frac{\partial F}{\partial p_n} - \frac{\partial H}{\partial p_n} \frac{\partial F}{\partial q_n} \}$$

Liouvilliano

Se suele usar $i\partial_t F = L'F$ con $L' = iL$

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots + \frac{x^n}{n!} + \ldots$$

$$e^x = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} x^n$$

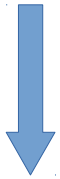
, puede ser reescrito como

$$e^x = \sum_{n=0}^{\infty} \frac{1}{n!} x^n$$

$$f(t) = f(0) + iL_r f(0) + \frac{1}{2!}(iL_r)^2 f(0) + \ldots$$

$$= \exp\left(\dot{r}\ (0) \cdot t \frac{\partial}{\partial r}\right) f(0)$$

$$= f\left[p(0), (r + \dot{r}\ (0) \cdot t)\right]$$



propagacion

.

Sea ahora la expresion completa del propagador

$$iL = \dot{r}\ \frac{\partial}{\partial r} + \dot{p}\ \frac{\partial}{\partial p}$$

$$[iLt] = [iL_x t] + [iL_p t]$$

Atencion :

$$\exp[iLt] \neq \exp[iL_x t]\exp[iL_p t]$$

Para operadores que no conmutan tenemos

$$\exp[A+B] \neq \exp[A]\exp[B]$$

$$iLf = \dot{r}\,\frac{\partial}{\partial r}f + \dot{p}\,\frac{\partial}{\partial p}f = \dot{f} = [iL_r + iL_p]f \qquad \#$$

.

Usando la expresion de Totter, un paso en la evolucion temporal es

$$\exp(iL_p\Delta/2)\exp(iL_x\Delta)\exp(iL_p\Delta/2) \qquad \#$$

.

Tenemos entonces que aplicar esto a f

$$\exp(iL_p\Delta/2)\exp(iL_x\Delta)\exp(iL_p\Delta/2)f = \exp(iL_p\Delta/2)\exp(iL_x\Delta)[\exp(iL_p\Delta/2)f]$$

.

que es lo que ya hicimos pero con p

PHYSICAL REVIEW A VOLUME 28, NUMBER 6 DECEMBER 1983

Applications of the generalized Trotter formula

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(Received 30 December 1982; revised manuscript received 14 June 1983)

Trotter

La identidad de trotter es :

$$e^{(A+B)} = \lim_{P \to \infty} \left(e^{A/2P} e^{B/P} e^{A/2P} \right)^P$$

Para P finito

$$e^{(A+B)} = \left(e^{A/2P} e^{B/P} e^{A/2P} \right)^P e^{O(1/P^2)}$$

Para el liouvilliano

$$\frac{A}{P} \equiv \frac{iL_p t}{P} \equiv \Delta \dot{p}(0) \frac{\partial}{\partial p}$$

$$\frac{B}{P} \equiv \frac{iL_x t}{P} \equiv \Delta \dot{x}(0) \frac{\partial}{\partial x}$$

$$\text{con } \Delta = t/P \text{ un paso} \Rightarrow \left(e^{iL_p \Delta/2} e^{iL_x \Delta} e^{iL_p \Delta/2} \right)$$

Teniendo en cuenta que

$$\exp(iL_p\Delta/2)f[p(0),r(0)] = f\left\{\left[p(0)+\frac{\Delta}{2}\,\dot{p}\,(0)\right],r(0)\right\} \qquad \#$$

.

operando con el otro termino del propagador

$$\exp(iL_x\Delta)f\left\{\left[p(0)+\frac{\Delta}{2}\,\dot{p}\,(0)\right],r(0)\right\} = f\left\{\left[p(0)+\frac{\Delta}{2}\,\dot{p}\,(0)\right],\left[r(0)+\Delta\,\dot{r}\,(\frac{\Delta}{2})\right.\right.$$

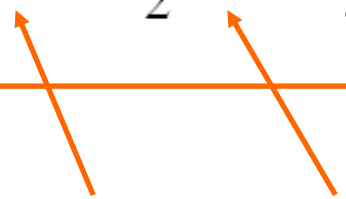
.

finalmente

$$\exp(iL_p\Delta/2)f\left\{\left[p(0)+\frac{\Delta}{2}\,\dot{p}\,(0)\right],\left[r(0)+\Delta\,\dot{r}\,(\frac{\Delta}{2})\right]\right\} \qquad \#$$

$$\# \qquad \#$$

$$= f\left\{\left[p(0)+\frac{\Delta}{2}\,\dot{p}\,(0)+\frac{\Delta}{2}\,\dot{p}\,(\Delta)\right],\left[r(0)+\Delta\,\dot{r}\,(\frac{\Delta}{2})\right]\right\} \qquad \#$$



Lo cual resulta en

$$p(0) \rightarrow p(0) + \frac{\Delta}{2}[F(0) + \boldsymbol{F(\ \Delta)}]$$

$$r(0) \rightarrow r(0) + \Delta\ \dot{r}\ (\frac{\Delta}{2})$$

$$= r(0) + \Delta\ \dot{r}\ (0) + \frac{\Delta^2}{2\mathrm{m}}F(0)$$

Velocity Verlet

Que estamos resolviendo?

Como habiamos visto el microcanonico podia ser escrito como

Definiendo Σ como

$$\Sigma(E,V,N) = \int \Theta(E-H)d^{3N}qd^{3N}p/C_N$$

De donde

$$S(E,V,N) = k\ln\Sigma$$

Sea entonces un hamiltoniano $H = \sum p_i^2/2m$
$+\sum_{i<j} v_{ij} = K + U$, entonces se pueden hacer las integrales en p usando las formulas para la esfera de radio $[2m(E-U)]^{1/2}$ para una esfera de $3N$ dimensiones (ver Huang o Munster)

$$\Sigma(E,V,N) = \int (E-U)^{3N/2}\Theta(E-U)d^{3N}q \Big/ [C_0\Gamma(3N/2+1]$$

.

tambien podemos usar $\omega = \partial\Sigma/\partial E$

$$\omega = \int (E-U)^{3N/2-1}\Theta(E-U)d^{3N}q \Big/ [C_0\Gamma(3N/2]$$

.

con $C_0 = C_N/(2\pi m)^{3N/2}$ y Γ es aqui la funcion gamma

.

Los promedios se calculan del siguiente modo

We first calculate

$$\sum(E) = \frac{1}{h^{3N}} \int_{\mathscr{H} < E} d^3p_1 \cdots d^3p_N \, d^3q_1 \cdots d^3q_N \tag{6.43}$$

where h is a constant of the dimension of momentum $\times$ distance, introduced to make $\sum(E)$ dimensionless. The integration over q_i can be immediately carried out, giving a factor of V^N. Let

$$R = \sqrt{2mE} \tag{6.44}$$

Then

$$\sum(E) = \left(\frac{V}{h^3}\right)^N \Omega_{3N}(R) \tag{6.45}$$

where Ω_n is the volume of an n-sphere of radius R:

$$\Omega_n(R) = \int_{x_1^2 + x_2^2 + \cdots + x_n^2 < R^2} dx_1 \, dx_2 \cdots dx_n \tag{6.46}$$

Clearly,

$$\Omega_n(R) = C_n R^n \tag{6.47}$$

where C_n is a constant. To find C_n, consider the identity

$$\int_{-\infty}^{+\infty} dx_1 \cdots \int_{-\infty}^{+\infty} dx_n \, e^{-(x_1^2 + \cdots + x_n^2)} = \left(\int_{-\infty}^{+\infty} dx \, e^{-x^2}\right)^n = \pi^{n/2} \tag{6.48}$$

The left side of (6.48) can be re-expressed as follows. Let $S_n(R) \equiv d\Omega_n(R)/dR$ be the surface area of an n-sphere of radius R. Then

$$\begin{aligned} \int_{-\infty}^{+\infty} dx_1 \cdots \int_{-\infty}^{+\infty} dx_n \, e^{-(x_1^2 + \cdots + x_n^2)} &= \int_0^\infty dR \, S_n(R) \, e^{-R^2} \\ &= nC_n \int_0^\infty dR \, R^{n-1} e^{-R^2} \\ &= \tfrac{1}{2} nC_n \int_0^\infty dt \, t^{(n/2)-1} e^{-t} = \tfrac{1}{2} nC_n \Gamma(n/2) \end{aligned} \tag{6.49}$$

where $\Gamma(z)$ is the gamma function. Comparison of (6.49) and (6.48) yields

$$C_n = \frac{\pi^{n/2}}{\Gamma(n/2 + 1)} \tag{6.50}$$

$$\log C_n \underset{n \to \infty}{\to} \frac{n}{2} \log \pi - \frac{n}{2} \log \frac{n}{2} + \frac{n}{2} \tag{6.51}$$

Hence

$$\sum(E) = C_{3N} \left[\frac{V}{h^3} (2mE)^{3/2}\right]^N \tag{6.52}$$

$$< A >= \int A(E-U)^{3N/2-1}\Theta(E-U)d^{3N}q / [\omega C_0 \Gamma(3N/2)]$$

O tambien

$$< A >= \int A(E-U)^{3N/2}\Theta(E-U)d^{3N}q / [C_0 \Gamma(3N/2+1]/\Sigma$$

Pero queremos ver molecular dynamics

El sistema descripto por el $H = \sum p^2/(2m) + U$

El termino de energia potencial depende de las coordenadas y quizas del volumen del sistema

El sistema es tal que se conserva

$$E = H \qquad \vec{M} = \sum \vec{p}$$

O sea que tenemos 4 integrales de movimiento.

Luego es un caso especial del EVN que llamamos $EVNM$

$$\Phi(E,N,V,M) = \int \Theta(E-H)\delta\left(\vec{M} - \sum \vec{p}\right) d^{3N}q \; d^{3N}p / C_N$$

Con C_N una constante

La entropia de Boltzmann es

$$S(E,N,V,M) = k \ln \Phi$$

Usando tecnicas usuales de integracion

$$\Phi(E,N,V,M) = \int\left[E - \frac{M^2}{2Nm} - U\right]^{3(N-1)/2} \times \Theta(E - \frac{M^2}{2Nm} - U)d^{3N}q \times \{C_0\Gamma[3(N-1)/2+1]\}^{-1}$$

con $C_0 = C_N N^{3/2}/(2\pi m)^{3(N-1)/2}$, entonces calculan $\omega = \partial\Phi/\partial E$

$$\Phi(E,N,V,M) = \int\left[E - \frac{M^2}{2Nm} - U\right]^{3(N-1)/2-1} \times \Theta(E - \frac{M^2}{2Nm} - U)d^{3N}q \times \{C_0\Gamma[3(N-1)/2]\}^{-1}$$

Para el valor medio de una variable dinamica obtienen

$$\langle A\rangle = \int A\left[E - \frac{M^2}{2Nm} - U\right]^{3(N-1)/2-1} \times \Theta(E - \frac{M^2}{2Nm} - U)d^{3N}q \times \{\omega C_0\Gamma[3(N-1)/2]\}^{-1}$$

Ahora calculan la energia cinetica media y obtienen

$$\langle K \rangle = 3(N-1)kT/2 + M^2/(2Nm)$$

Para el *EVN* teniamos

$$\langle K \rangle = 3(N)kT/2$$

y vemos que son diferentes aun cuando $\vec{M} = 0$

Para la ecuacion de estado obtienen

$$P = NkT/V - \left\langle \frac{\partial U}{\partial V} \right\rangle$$

Igual que en el *ENV*

PHYSICAL REVIEW A VOLUME 37, NUMBER 1 JANUARY 1, 1988

Fundamental treatment of molecular-dynamics ensembles

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(Received 22 April 1987)

Aplicacion a Lennard Jones

Problema a resolver :

Sistema confinado en un volumen V

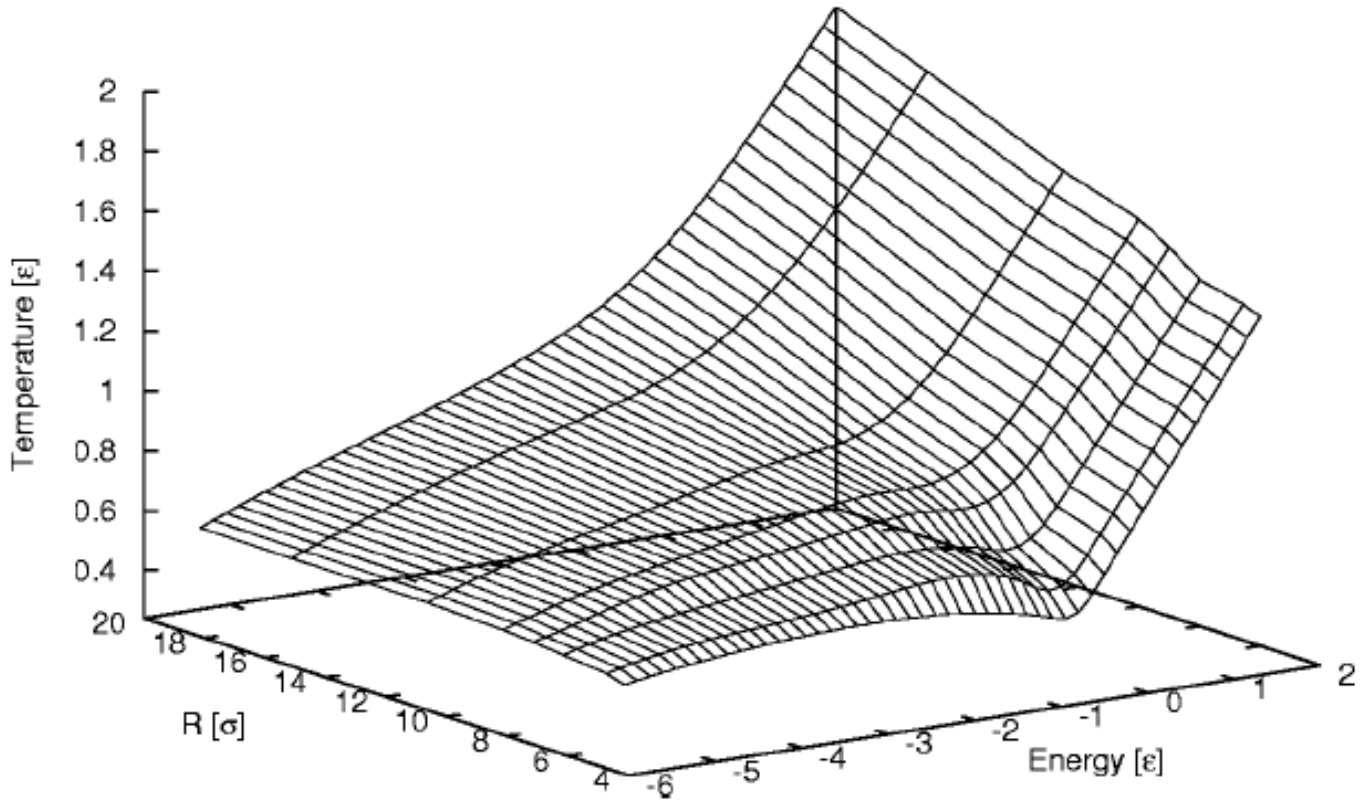


FIG. 3. Temperature of the constrained system as a function of its energy and radius.

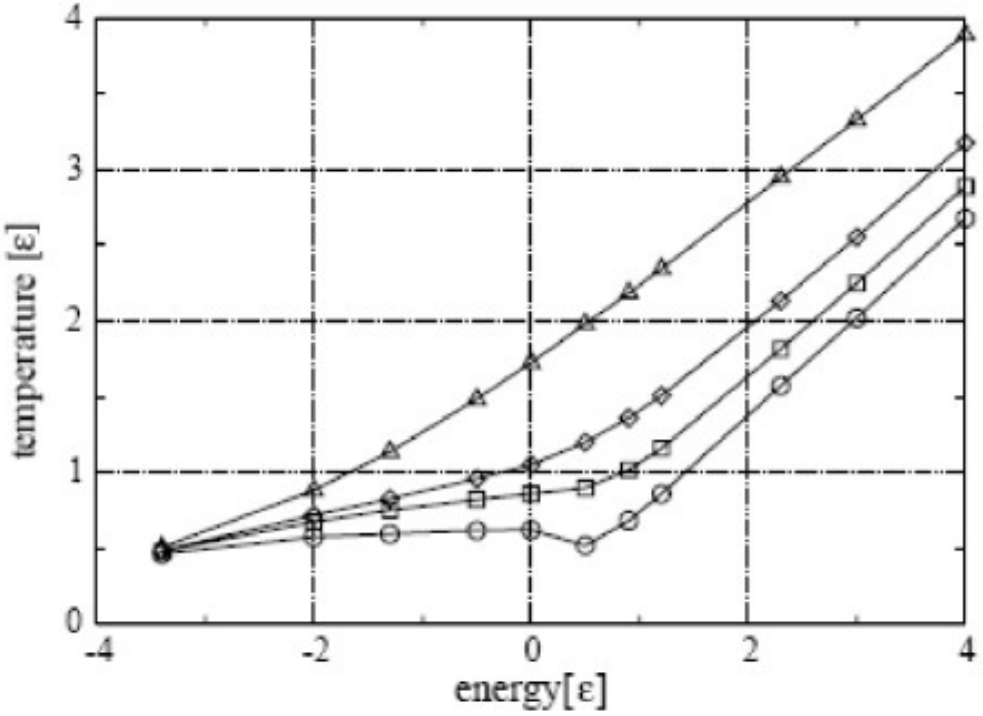


Fig. 1. In this figure we show the caloric curve for 147 Lennard-Jones particles for different sizes of the constraining volumes. Circles denote the CC corresponding to a constraining volume of radius $R = 15\sigma$, squares for $R = 8\sigma$, diamonds for $R = 6\sigma$ and finally triangles denote the CC for $R = 4\sigma$.

Once the caloric curve is known it is easy to calculate the entropy S as a function of the energy and the density:

$$S = \int \frac{\mathrm{d}E}{T(E)} \,. \tag{3}$$

In fig. 3 we show S for a dilute system (see caption for details). It is immediate that a convex intruder appears which has been proposed to be a signature of a first-order phase transition in non-extensive systems [4] (*i.e.* the formation of surfaces turns the entropy into a non-extensive function in small systems).

The next step is to calculate the behavior of the thermal response function (TRF) of such a system:

$$\mathrm{TRF} = \left(\frac{\mathrm{d}E}{\mathrm{d}T}\right) \,. \tag{4}$$

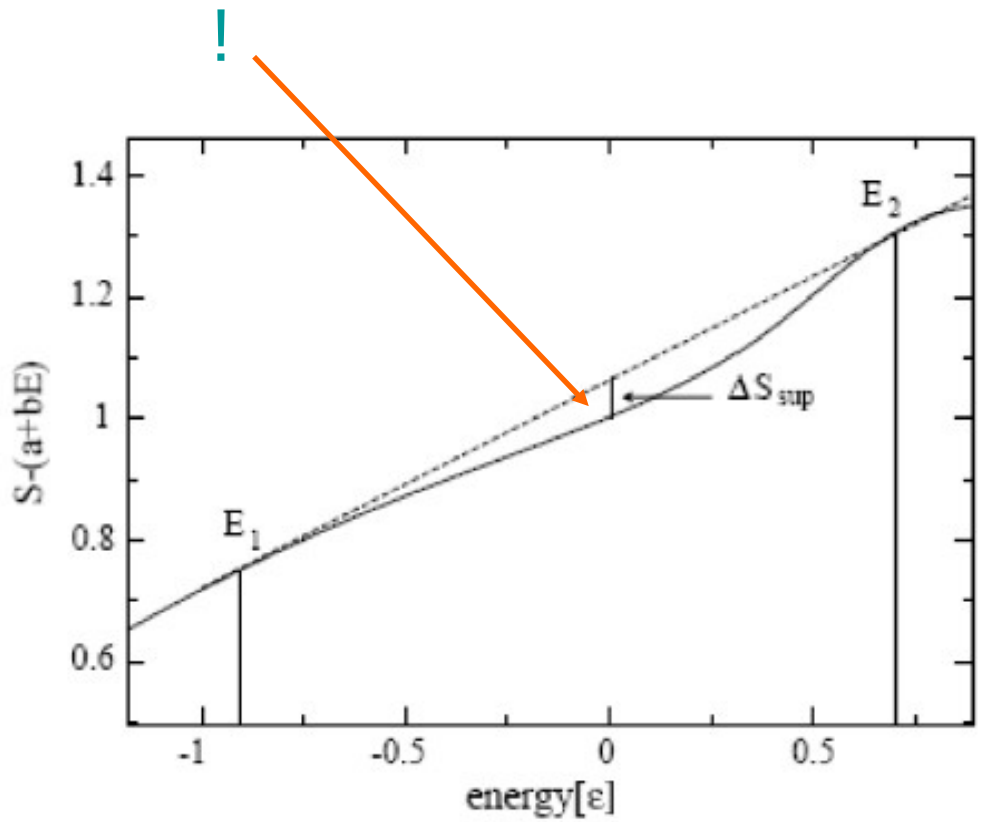


Fig. 3. In this figure we display the resulting value of the entropy as a function of the energy for a constraining volume of radius $R = 15\sigma$. The curve displays a convex intruder between E_1 and E_2 which has been associated with a first-order phase transition, ΔS being the entropy lost in the formation of surfaces. In order to visualize the convex intruder a lineal function $a + b\,E$ has been substracted to the entropy. Here $a = 4.3$, $b = 1.4$.

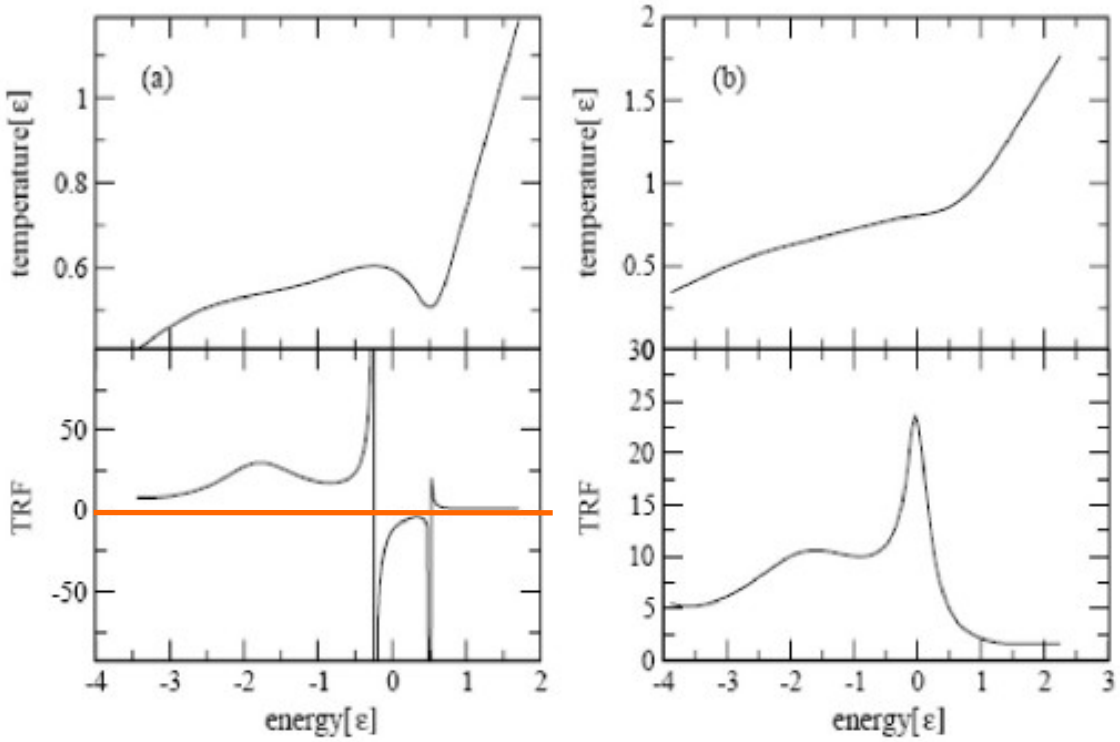
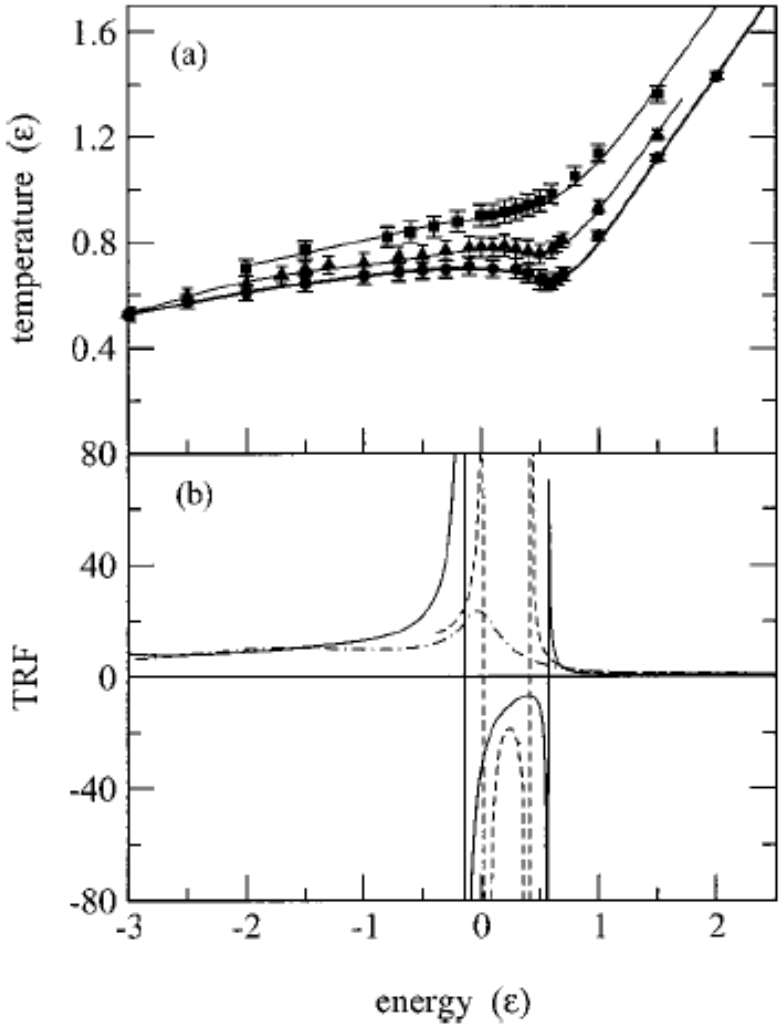


Fig. 4. Here we show the CC (upper panels) and the associated TRF (lower panels) for two values of the volume. The left-hand side corresponds to $R = 15\sigma$ (dilute case) and the right-hand side to $R = 8\sigma$ (transition to dense state). It can be seen that for the dilute case two poles are present which limit the region of negative TRF. On the other hand, at $R = 8\sigma$ the TRF is always positive and displays a maximum.



$$\mathrm{TRF} = \left(\frac{\partial T}{\partial E}\right)^{-1}.$$

FIG. 4. Caloric curve for the constrained system (a) and the respective thermal response functions (b) for three different densities $\rho = \rho_{fo}^{-}$, ρ_{fo}^{0}, and ρ_{fo}^{+} [circle, triangle, and square symbols in (a) and full, dashed, and dot-dashed lines in (b), respectively].

One of the main tools to study a chaotic system is the maximum Lyapunov exponent [14], which is a measure of the sensitivity of the system to initial conditions and also gives an idea of the velocity at which the system explores the available phase space. Given two very close initial conditions in phase space, the MLE, $\hat{\lambda}$, is given by the following relation:

$$\lambda = \lim_{t \to \infty} \lim_{d(0) \to 0} \left[\frac{1}{t} \ln \frac{d(t)}{d(0)} \right], \tag{5}$$

where $d(t)$ is the distance in phase space between two trajectories (1 and 2) which initially differs each other in a very small quantity $d(0)$.

In order to calculate this quantity we must define a metric

$$d_{12}(t) = \sqrt{\sum_{i=1,N} \left[a \left(r_1(t) - r_2(t) \right)^2 + b \left(p_1(t) - p_2(t) \right)^2 \right]}. \tag{6}$$

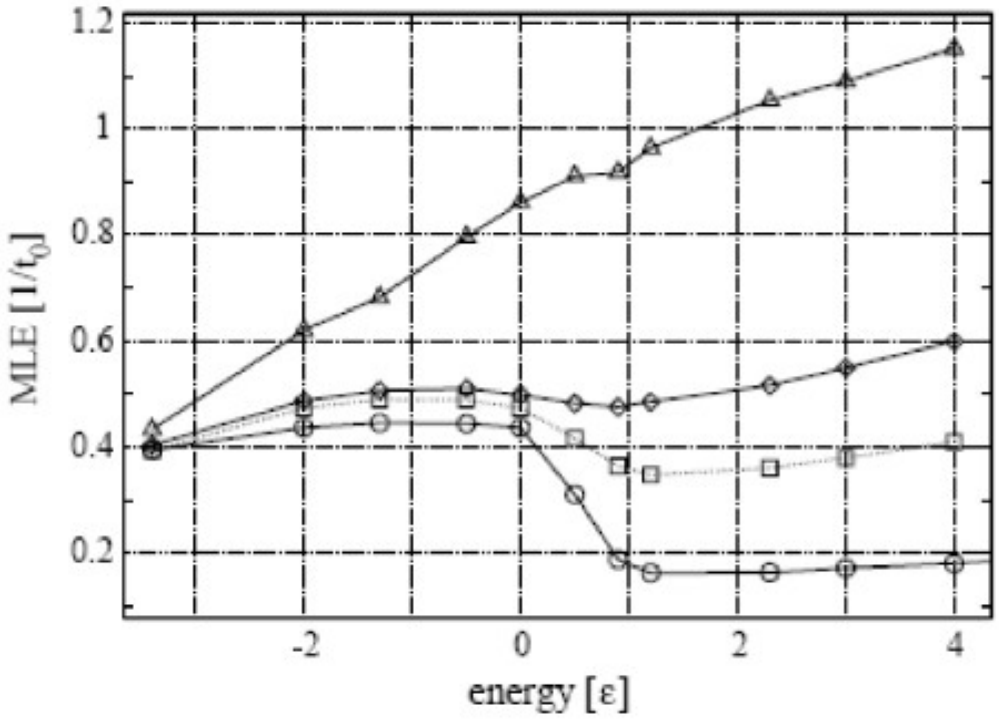
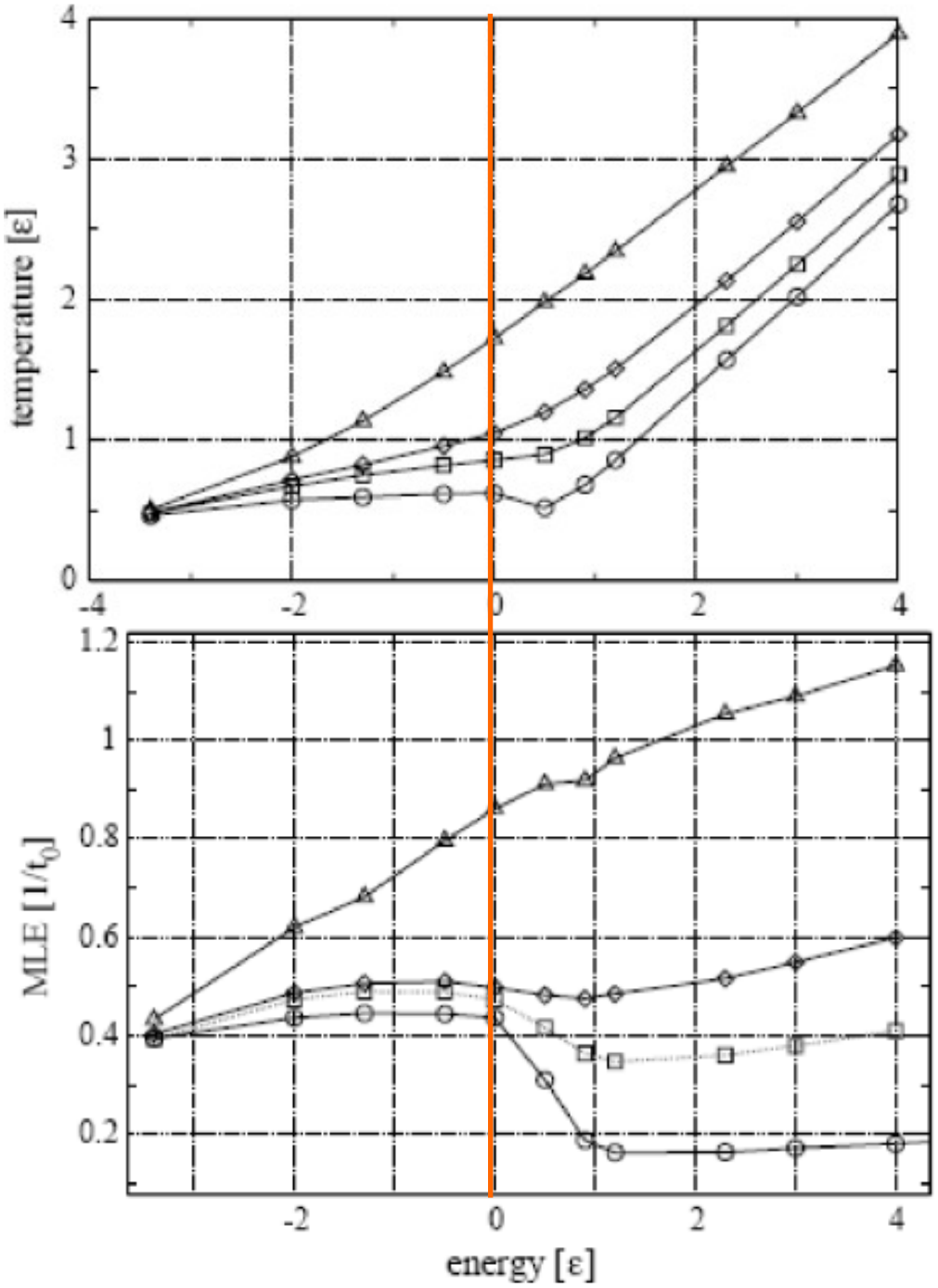


Fig. 5. In this figure we plot the MLE as a function of the energy deposited in the system for the four values of the constraining volume considered in this work. Symbols have the same meaning as in fig. 1). It can be seen that the MLE clearly signals the transition from a liquid-like regime to a vapor-like regime (according to the ECRA analysis).


temperature [ε]
MLE [1/t0]
energy [ε]

Explosiones

y diversas sorpresas que te da la vida

System under analysis

a) We study drops of size 147 particles interacting via a truncated Lennard Jones potential

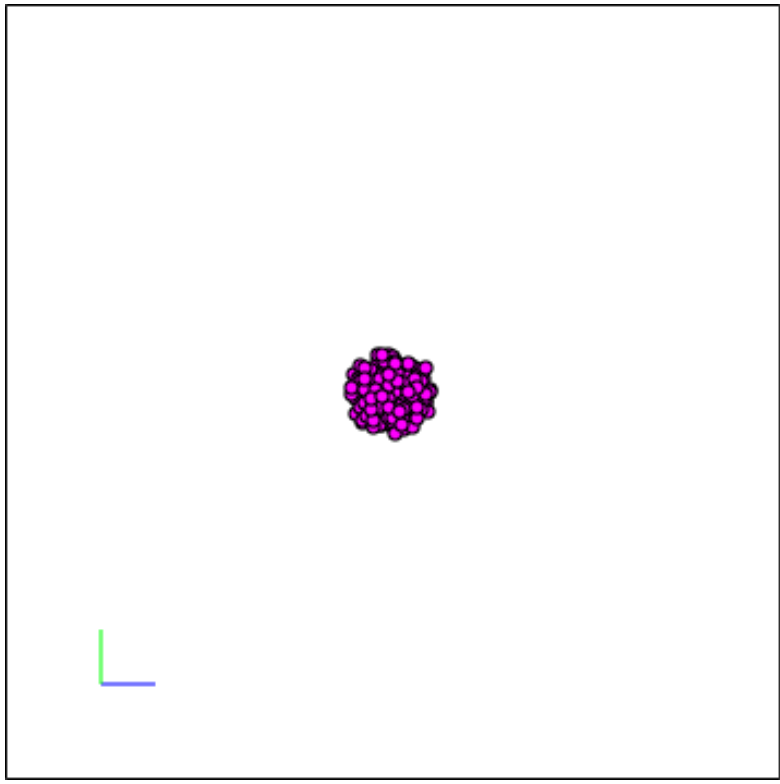
$$v(r_{ij}) = \left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6} - \left(\frac{1}{3}\right)^{12} + \left(\frac{1}{3}\right)^{6}\right] 4\varepsilon \qquad \mathbf{r_{ij} \leq 3}$$

$$v(r_{ij}) = 0 \qquad \textbf{otherwise}$$

b) We work in units of and m

c) We use velocity Verlet algorithm

d) Initial conditions are constructed by cutting a “sphere” of 147 particles out of a equilibrated PBC system



Fragment Recognition Algorithms

One of the main observables in Fragmentation experiments are the asymptotic fragment mass distributions.

In order to extract this information from numerical simulations we need fragment recognition algorithms.

The ones we use are :

- ***MST*** → ***correlations in q space***
- ***MSTE*** → ***correlation in qp space (aprox.)***
- ***ECRA*** → ***most bound partitions in phase space***

A.Strachan & C.O.Dorso Phys.Rev.C 56(1997)995

Fragment recognition algorithms

MST algorithm

Given a set of particles i,j,k,…, clusters are defined such that :

$$i \in C \Leftrightarrow \exists j \in C / (r_i - r_j) < r_{clust}$$

With r_{clust} the clusterization radius ($r_{clust}=3\sigma=r_c$ in our case)

MSTE algorithm

In this case clusters are defined in the following way:

$$i \in C \Leftrightarrow \exists j \in C / (\frac{p_{ij}^2}{4\mu} - v_{ij}) < r_{clust}$$

With μ the reduced mass and p_{ij} the relative momentum

Early Cluster Formation Model

Given a set of particles (i,j,k..) clusters are defined as those partitions C_i that minimize the following expression:

$$E = \sum_{C_i} \left[\left(\sum_{i \in C_i} \frac{p_{ij}^2}{2m} \right)_{c.m.C_i} + \sum_{i<j, \in C_i} v(r_{ij}) \right]$$

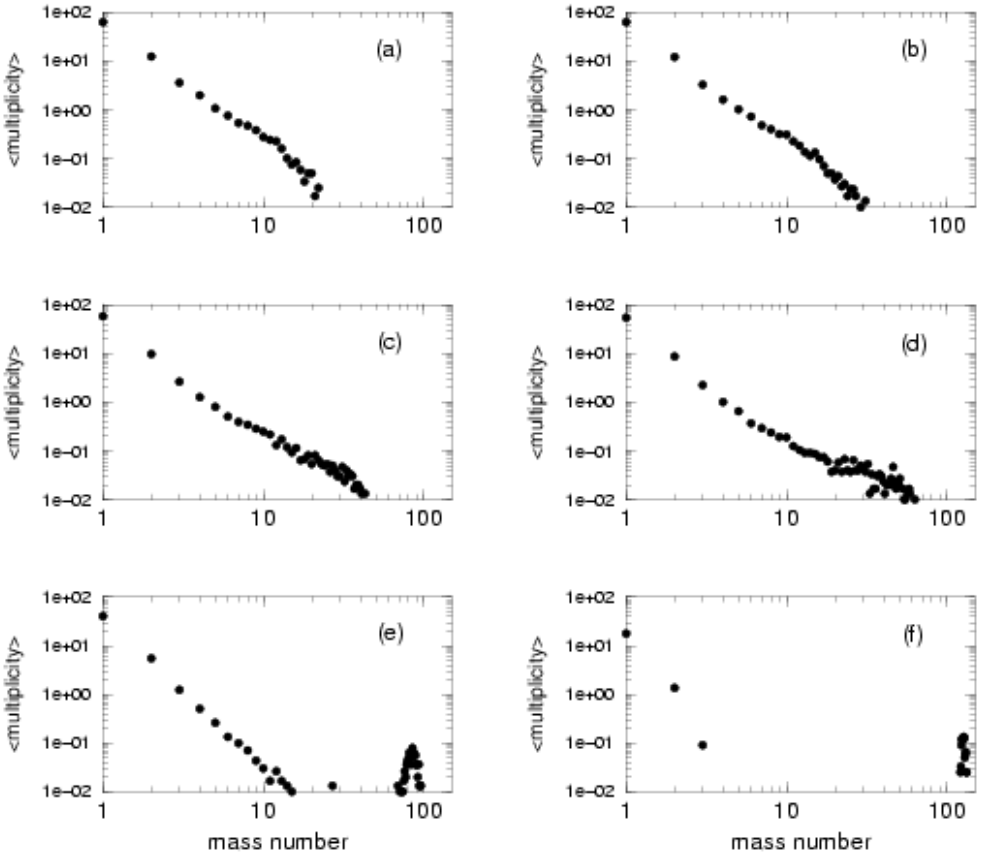
This is a highly self consistent problem that has been solved by devising a method in the spirit of simulated annealing (ECRA).

For such a problem a Markov chain in the space of partitions is constructed

C.O.Dorso & J.Randrup Phys.Lett. B 301 (1993) 328

Asymptotic Mass spectra

Asymptotic Mass spectra for exploding systems at 6 different energies
The spectra evolves from a exponetialy decaying to a "U" shaped (low energies)
In between a power law like mass spectrum is found.



This results are independent of the fragment recognition algorithm used

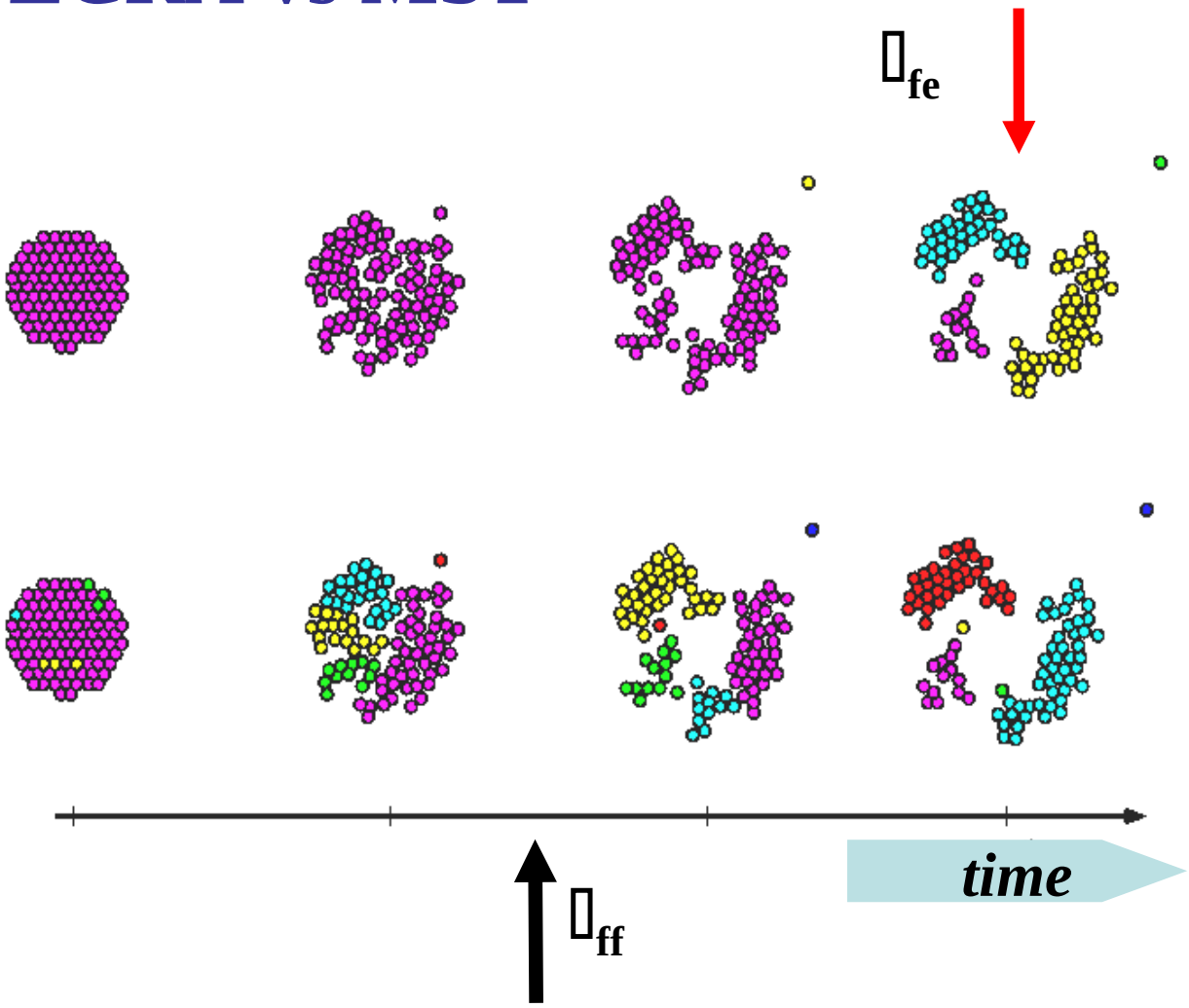
a) E=2.2 b) E=1.8 c) E=.9 d) E=.5 e) E=-0.5 f) E=-0.9

A.Stracha & C.O.Dorso Phys.Rev.C. 55(1997) 79

ECRA vs MST

MST

ECRA



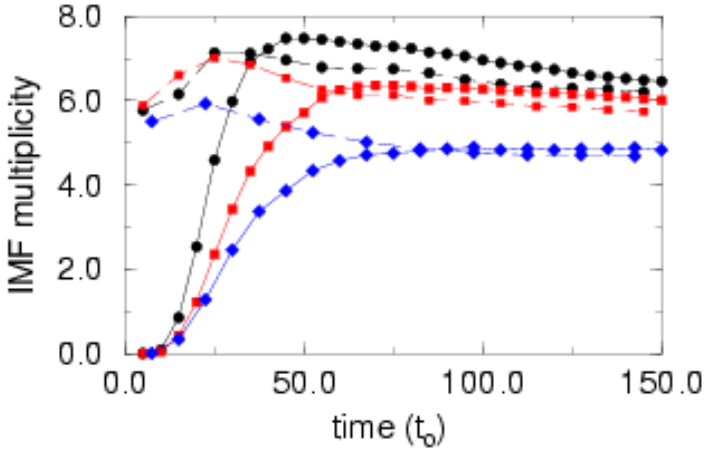
MST vs ECRA

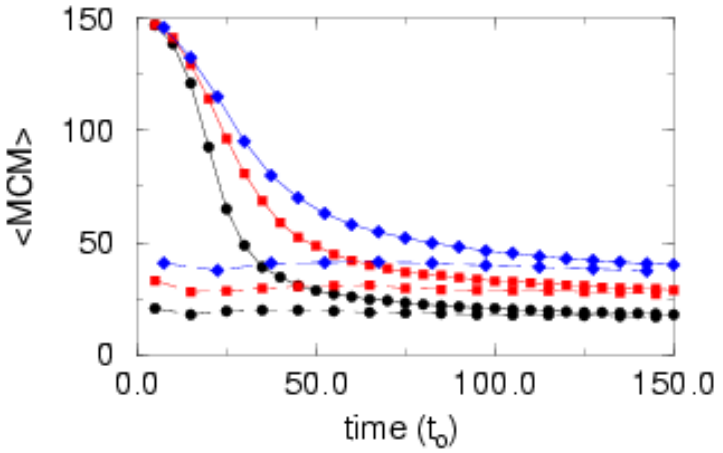
In this figures we show the multiplicity of intermediate mass fragments and the size of the biggest fragment according to MST and ECRA analysis, as a funtion of time, for different values of the total energy.

ECRA results show that fragments are formed early in the evolution

3≤IMF≤15

E=1.8
E=0.9
E=0.5





Microscopic stability of partitions

The persistence P(t) is given by:

$$P(t) = \frac{1}{N_{ev}} \sum_{ev} \frac{1}{\sum_{cl} m_i(t)} \sum_{cl} m_i(t) \frac{a_i(t)}{b_i(t)}$$

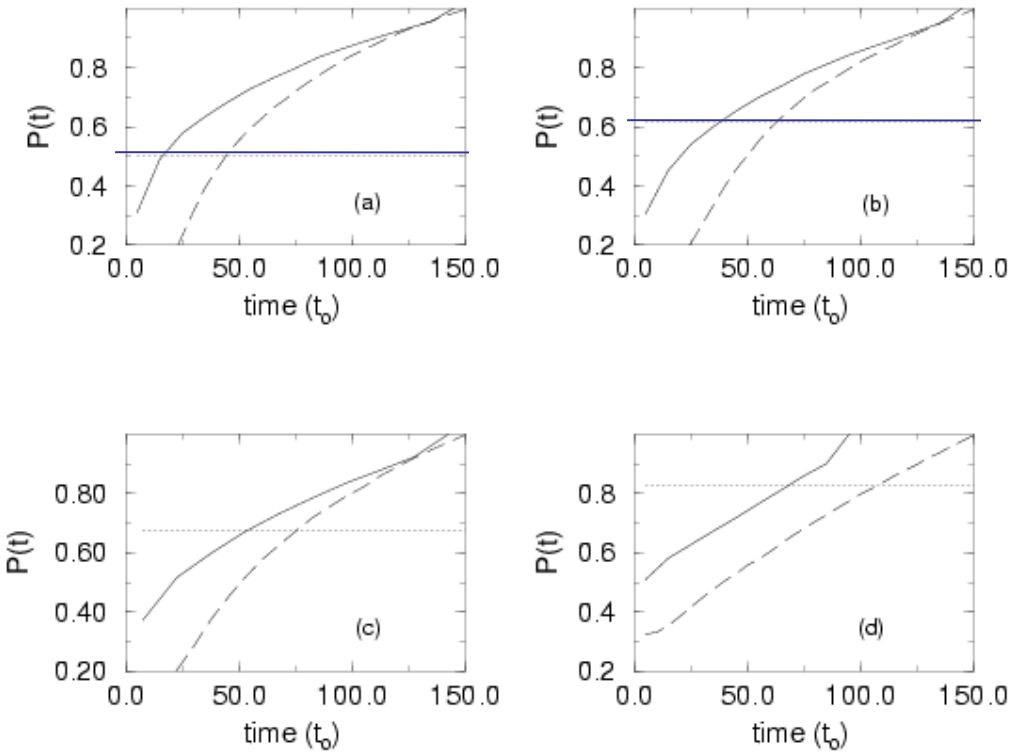
with

$$b_i(t) = n_i(t)(n_i(t) - 1)/2$$

The number of pairs of particles belonging to cluster i at time t

$$a_i(t)$$

The number of pairs of particles that remain together in asymptoyic clusters



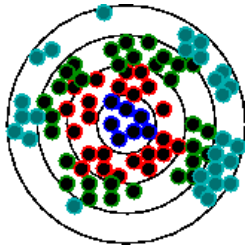
a) E=1.8, b) E=.9 , c) E=.5, d) E=-0.5

C.O.Dorso & P.Balonga Phys.Rev.C. 50(1994) 991

Energies

We divide the drop in concentrical shells

For each cell we calculate the mean radial velocity.



$$v_{rad}^{i}(t) = \sum_{ev} \frac{1}{N_i(t)} \sum_{j \in i} \frac{v_j(t) \cdot r_j(t)}{|r_j(t)|}$$

We then factorize the kinetic energy in $K(t) = K_{coll}(t) + K_{\text{int}}(t)$

with

$$K_{coll}(t) = \frac{1}{n_{ev} N} \sum_{shells} N_i(t) \frac{m}{2} (v_{rad}^{i}(t))^2$$

and

$$K_{\text{int}}(t) = \frac{1}{n_{ev} N} \sum_{shells} \sum_{j \in i} \frac{m}{2} (v_j(t) - v_{rad}^{i}(t))^2$$

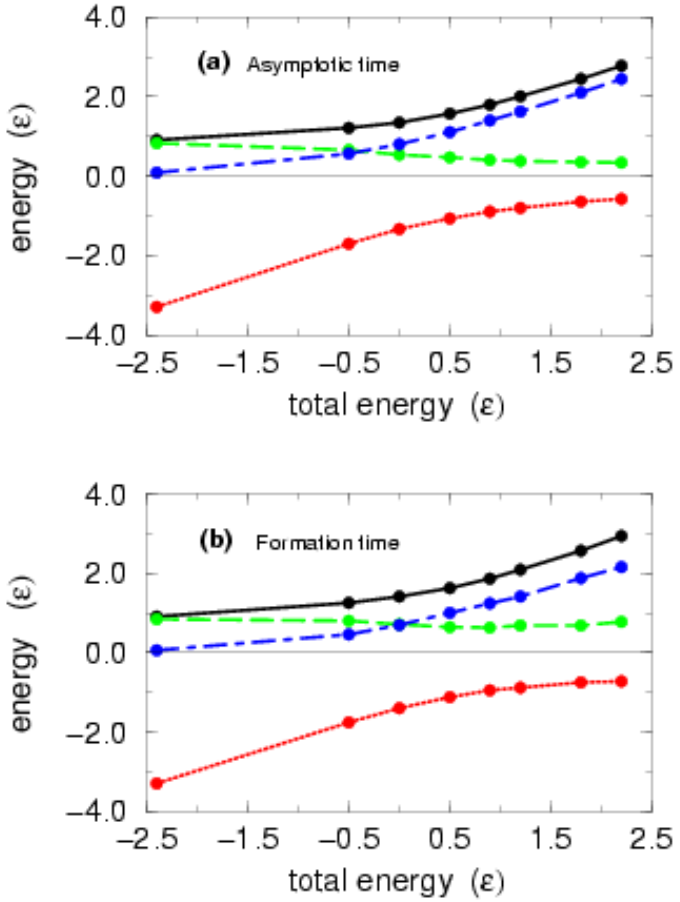
Energy Partition at different times

Total kinetic energy

Radial kinetic energy

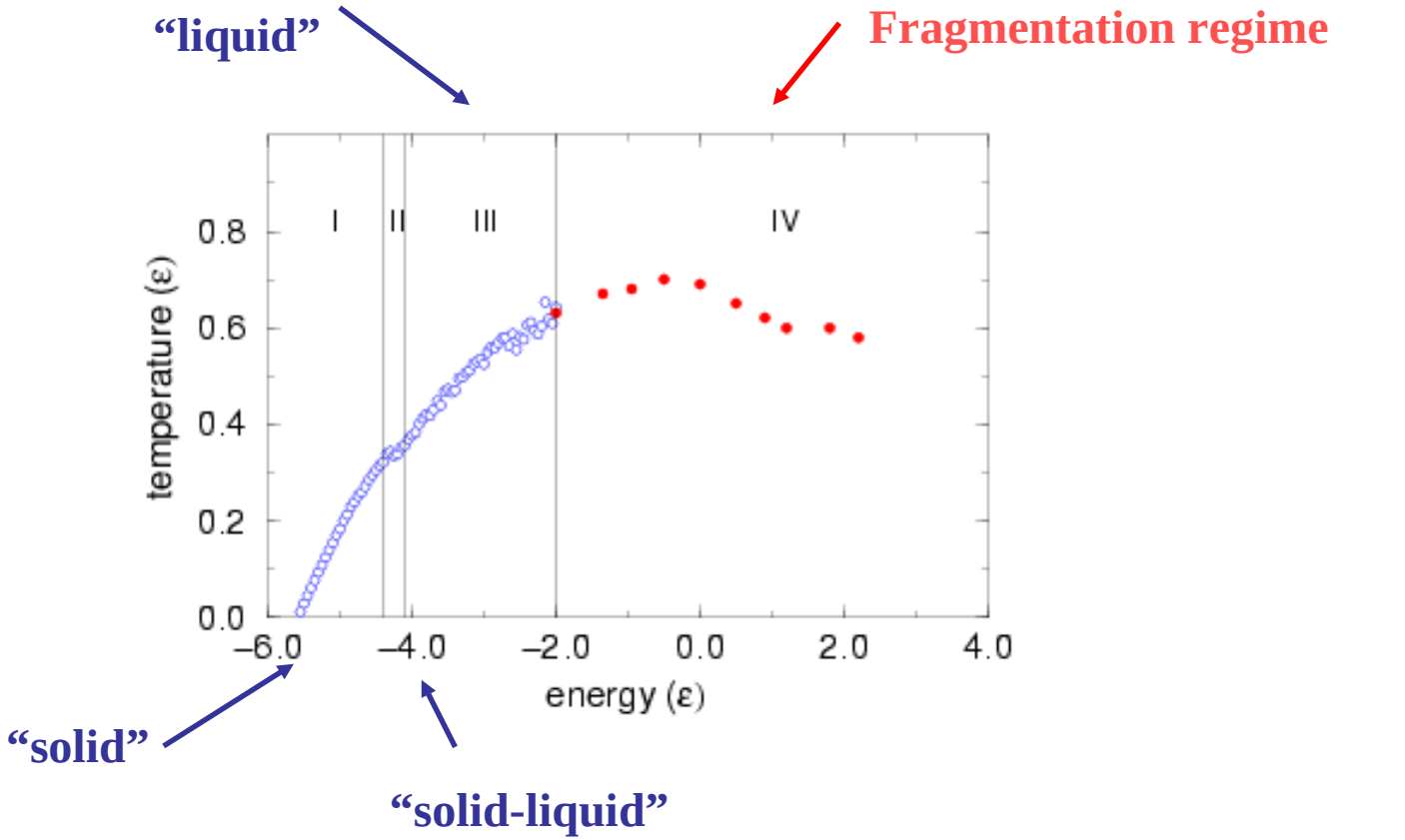
Intrisic kinetic energy

Potential energy



Extended CC expanding system

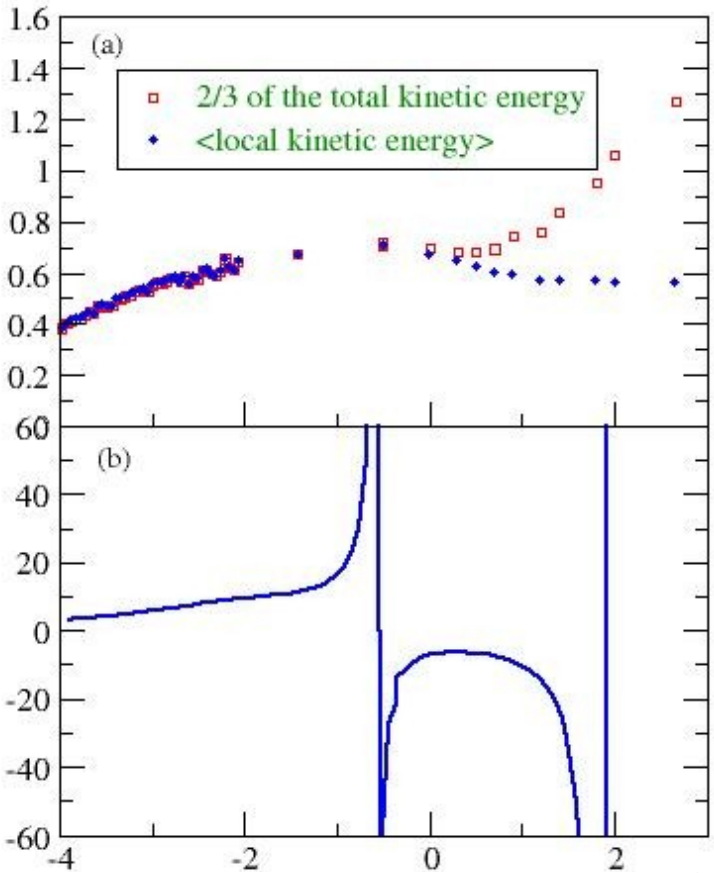
CC= functional relationship between the temperature and the energy at ε_{ff}



A.Strachan & C.O.Dorso PRC59 (1999)285

Free System CC and TRF

Temperature(T)



“Fake” CC

True CC

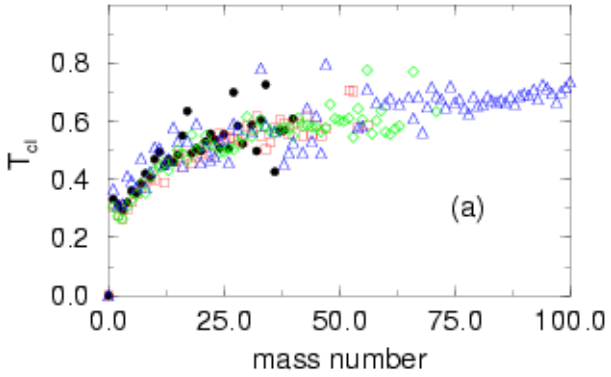
TRF

Temperatures

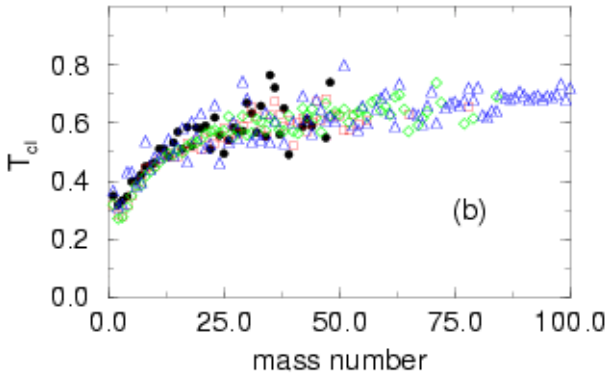
Intrinsic cluster Temperature

$$T_{\mathrm{int}}(n,t) = \frac{1}{N_n} \sum_i \frac{2}{n_l} \sum_{j \in i} \frac{1}{2} m (v_j^{(cm)})^2$$

Average Temperature of asymptotic clusters for all the energies considered as a function of the cluster mass



Average temperatures of MBDF at ρ_{ff} for all the energies considered



The information about the temperature of fragment formation is in the asymptotic clusters