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# MD Nose



# Dinamica Molecular a Temperatura cte.

Si estamos a temperatura T la distribucion de velocidades esta dada por la distribucion de Maxwell Boltzmann

$$P(p) = \left( \frac{\beta}{2\pi m} \right)^{3/2} \exp\left[ \frac{-\beta p^2}{2m} \right]$$

Se satisface tambien

$$kT = m\langle v_a^2 \rangle$$

donde  $v_a$  es una componente de la velocidad

En que sistema estamos calculando este valor medio?

De aqui, sigue que para calcular las fluctuaciones de la Temperatura es suficiente calcular las fluctuaciones de energia cinetica.

notamos que

$$\langle p^2 \rangle = \int dp p^2 P(p) = \frac{3m}{\beta}$$

$$\Rightarrow T_k = \frac{1}{2m} \langle p^2 \rangle = \frac{1}{2m} 3m kT = \frac{3}{2} kT$$

del mismo modo

$$\langle p^4 \rangle = \int dp p^4 P(p) = 15\left(\frac{m}{\beta}\right)^2$$

de donde

$$\frac{\sigma_p^2}{\langle p^2 \rangle^2} = \frac{\langle p^4 \rangle - \langle p^2 \rangle^2}{\langle p^2 \rangle^2} = \frac{15\left(\frac{m}{\beta}\right)^2 - 9\left(\frac{m}{\beta}\right)^2}{9\left(\frac{m}{\beta}\right)^2} = \frac{2}{3}$$

de donde

La energia cinetica es tal que

$$T_k = \frac{1}{2m} \langle p^2 \rangle = \frac{1}{2m} 3mkT = \frac{3}{2} \frac{1}{\beta}$$

$$T_k = \frac{1}{2m} \langle p^2 \rangle = \frac{3}{2} kT$$

$$\frac{\sigma_p^2}{\langle T_k \rangle_{NVT}^2} = \frac{\langle T_k^2 \rangle - \langle T_k \rangle^2}{\langle T_k \rangle^2}$$

$$\langle T_k \rangle^2 = \frac{1}{m^2} N^2 \langle p^2 \rangle^2$$



$$\langle T_k^2 \rangle = \langle T_k T_k \rangle = \langle [\sum p_i^2][\sum p_k^2] \rangle = N \langle p^4 \rangle + N(N-1) \langle p^2 \rangle \langle p^2 \rangle$$

entonces

$$\frac{\sigma_p^2}{\langle T_k \rangle_{NVT}^2} = \frac{N\langle p^4 \rangle + N(N-1)\langle p^2 \rangle \langle p^2 \rangle - N^2 \langle p^2 \rangle^2}{N^2 \langle p^2 \rangle^2}$$

$$= \frac{1}{N} \frac{\langle p^4 \rangle - \langle p^2 \rangle^2}{\langle p^2 \rangle^2} = \frac{2}{3N}$$

Luego, solo si  $N \rightarrow \infty$  las fluctuaciones se van 0

# Berendsen

Sea la ecuacion de Langevin (para cada  $i$  del sistema)

$$m \dot{v} = F - m\gamma v + R(t)$$

Donde  $\gamma$  es un termino de friccion y  $R$  es una fuerza estocastica

$$\langle R_i(t)R_j(t+\tau) \rangle = 2m_i\gamma_i kT_0\delta(\tau)\delta_{ij}$$

Como se comporta la Temperatura ante este acoplamiento

A partir de la energia cinetica (con  $m_i = m$  )

$$\frac{dE_k}{dt} = \lim_{\Delta t \rightarrow 0} \left\{ \left[ \sum \frac{1}{2} m v_i^2(t + \Delta t) - \sum \frac{1}{2} m v_i^2(t) \right] / \Delta t \right\}$$

Con

$$\Delta v = v(t + \Delta t) - v(t)$$

$$= \frac{1}{m} \int_t^{t+\Delta t} [F(t') - m\gamma v(t') + R(t')] dt$$

Como  $R_i(t')$  esta descorrelacionada con  $v_i(t)$  y  $R_i(t)$ , para  $t' > t$

$$\sum \int_t^{t+\Delta t} dt' \int_t^{t+\Delta t} dt'' R_i(t') R_j(t'') = 6Nm\gamma kT_0 \Delta t$$

de donde

$$\frac{dE_k}{dt} = \sum v_i F_i + 2\gamma \left( \frac{3N}{2} k T_0 - E_k \right)$$

el segundo termino se puede escribir como

$$\left( \frac{dT}{dt} \right)_{baño} = 2\gamma(T_0 - T)$$

De esta forma es suficiente considerar

$$m \dot{v}_i = F_i + m\gamma \left( \frac{T_0}{T} - 1 \right) v_i$$

pues de aqui se obtiene

$$\frac{dE_k}{dt} = \sum v_i F_i + 3N\gamma k(T_0 - T)$$

Como debe ser

Las ecuaciones de movimiento resultantes corresponden a una escala de las velocidades en cada paso de la evolucion de  $v$  a  $\lambda v$

con

$$\lambda = 1 + \frac{\Delta t}{2\tau_T} \left( \frac{T_0}{T} - 1 \right)$$

Pero no se ha encontrado a que ensemble corresponde la evolucion correspondiente

# Andersen

Supongamos que tenemos nuestro sistema descripto por un Hamiltoniano dado

$$H = \sum_i \frac{p_i^2}{2m} + \sum_i \sum_{j>i} v_{ij}$$

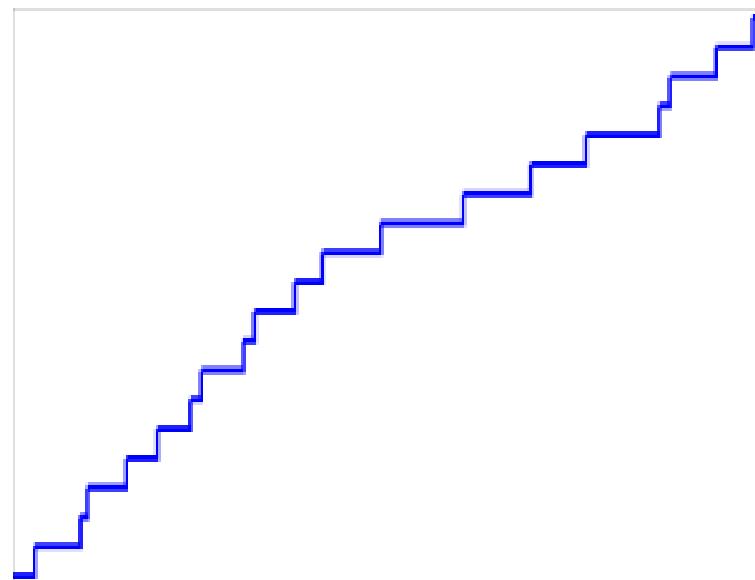
La evolucion ocurre sobre el hiperplano caracterizado por  $E$

- a) se considera que existe un sistema "fantasma"
- b) el sistema de interes sobrelleva colisiones con partculas del sistema "fantasma"
  - instantaneas,
  - no correlacionadas
  - de acuerdo con un proceso de Poisson

Entre colision y colision el sistema evoluciona segun las ecuaciones de Hamilton o sea se mueve en "su" hiperplano

la probabilidad de que el intervalo entre dos eventos sea  $t$  es

$$P(t) = \lambda \cdot \exp(-\lambda t)$$



# Proceso segun Andersen

- a) elegimos los tiempos a los cuales se produciran las colisiones  
 $(t_1, t_2, \dots, t_i, \dots, t_j, \dots)$
- b) Entre  $t_i$  y  $t_{i+1}$  el sistema evoluciona Hamiltonianamente
- c) Se eligen condiciones iniciales arbitrarias
- c) A  $t_{i+1}$  se produce la colision, entonces
  - Se elige una particula al azar
  - El nuevo momento de la particula se sortea de una MB a temperatura  $T$  (direccion aleatoria)

O sea:

$$\bar{F} = F_{NVT}(N, V, T)$$

Recordemos que En el caso de cadenas de Markov , si las probabilidades de transicion son tales que

son estacionarias

son aperiodicas

irreducibles

tendran una distribucion asintotica estacionaria

Resulta que la distribucion que es invariante para este caso es

$$\frac{1}{N!} \frac{\exp(-H\beta)}{Q(N, V, T)}$$

# Nose-Hoover

## Bibliografia

W.G.Hoover *Phys.Rev.A* **31** (1985) 1695 , *Phys.Rev.A* **34** (1986)  
2499

recordemos algunas propiedades de la  $\delta$

$$\int_{-\infty}^{\infty} \delta(ax) dx = \int_{-\infty}^{\infty} \delta(u) du \frac{1}{|a|} = \frac{1}{|a|}$$

Scaling property  $\Rightarrow$

$$\delta(ax) = \frac{\delta(x)}{|a|}$$

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$$\delta(ax) = \frac{\delta(x)}{|a|}$$

Que se puede generalizar a

$$\delta(g(x)) = \sum \frac{\delta(x - x_i)}{|g'(x_i)|}$$

Donde  $x_i$  son las raíces reales de  $g(x)$

Por ejemplo

$$\delta(x^2 - a^2) = \frac{1}{2|a|} [\delta(x + a) + \delta(x - a)]$$

Ademas

$$\int_{-\infty}^{\infty} f(x) \delta(g(x)) dx = \sum \frac{f(x_i)}{|g'(x_i)|}$$

Sea un Lagrangiano

$$L = T - V.$$

$$\dot{L}(\vec{x}, \dot{\vec{x}}) = \frac{1}{2} m \dot{\vec{x}}^2 - V(\vec{x})$$

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_i} \right) - \frac{\partial L}{\partial x_i} = 0$$

$$\frac{\partial L}{\partial x_i} = - \frac{\partial V}{\partial x_i}$$

$$\frac{\partial L}{\partial \dot{x}_i} = \frac{\partial}{\partial \dot{x}_i} \left( \frac{1}{2} m \dot{\vec{x}}^2 \right) = \frac{1}{2} m \frac{\partial}{\partial \dot{x}_i} (\dot{x}_i \dot{x}_i) = m \dot{x}_i$$

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_i} \right) = m \ddot{x}_i$$

$$m \ddot{\vec{x}} + \nabla V = 0$$

$$\cdot p_i(x_i,\dot{x}_i,t)=\frac{\partial \textbf{L}}{\partial \dot{x}_i}$$

$$\textbf{H}=\sum_i\dot{q}_i\frac{\partial \textbf{L}}{\partial \dot{q}_i}-\textbf{L}=\sum_i\dot{q}_ip_i-\textbf{L}$$

$$\textbf{L}\,=\,T-V\,=\,\frac{1}{2}m\,\dot{\vec{x}}^2\,-V\left(\vec{x}\right)$$

$$\cdot p_i(x_i,\dot{x}_i,t)=m\dot{x}\quad\Rightarrow\dot{x}=\frac{p_i(x_i,\dot{x}_i,t)}{m}$$

Sea el siguiente Lagrangiano

$$L_{Nose} = \sum \frac{m_i}{2} s^2 \dot{r}_i^2 - V(r^N) - \frac{Q}{2} \dot{s}^2 - \frac{g}{\beta} \ln s$$

Q es una masa efectiva asociada a s

Esto da lugar a las siguientes ecuaciones:

$$p_i = \frac{\partial L}{\partial \dot{r}_i} = m_i s^2 \dot{r}_i$$

$$p_s = \frac{\partial L}{\partial \dot{s}} = Q \dot{s}$$

y al siguiente Hamiltoniano:

$$H_{Nose} = \sum \frac{p_i^2}{2m_i s^2} + V(r^N) + \frac{p_s^2}{2Q} + \frac{g}{\beta} \ln s$$

Sea

$$p' = p/s$$

$$H_{Nose} = H' + \frac{p_s^2}{2Q} + \frac{g}{\beta} \ln s$$

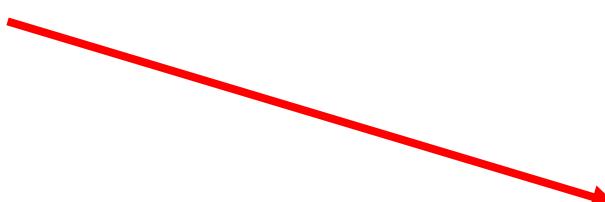
y

$$H' = \sum \frac{p_i'^2}{2m_i} + V(r)$$



Este es un Hamiltoniano genuino

El Microcanonico asociado es



$$\Gamma_{nose} = \frac{1}{N!} \int dp_s ds dp^{3N} dr^{3N} [\delta(E - H_{Nose})]$$

$$= \frac{1}{N!} \int dp_s ds dp^{3N} dr^{3N} \cdot s^{3N} \cdot \left[ \delta \left( H' + \frac{p_s^2}{2Q} + \frac{g}{\beta} \ln s - E \right) \right]$$

Que puede ser reescrita como

$$\Gamma_{nose} = \frac{1}{N!} \int dp_s ds dp^{3N} dr^{3N} \cdot s^{3N} \cdot \left[ \delta \left( \frac{g}{\beta} \ln s - (E - H' - \frac{p_s^2}{2Q}) \right) \right]$$

Pero entonces usando la relación de la  $\delta$   
obtenemos

$$\Gamma_{nose} = \frac{1}{N!} \int dp_s ds dp^{3N} dr^{3N} \cdot s^{3N} \cdot \left[ \delta\left(\frac{g}{\beta} \ln s - (E - H' - \frac{p_s^2}{2Q})\right) \right]$$

Sea

$$\ln s_0 = \frac{\beta}{g} \left[ E - \left( H' + \frac{p_s^2}{2Q} \right) \right]$$

de donde

$$s_0 = \exp \left\{ \frac{\beta}{g} \left[ E - \left( H' + \frac{p_s^2}{2Q} \right) \right] \right\}$$

Entonces aparece

$$\delta(h(s)) = \frac{\delta(s - s_0)}{h'(s)}$$

$$\Gamma_{nose} = \frac{1}{N!} \int dp_s \, ds \, dp^{3N} \, dr^{3N} \cdot s^{3N} \cdot \left[ \delta\left(\frac{g}{\beta} \ln s - (E - H' - \frac{p_s^2}{2Q})\right) \right]$$

$$\ln s_0 = \frac{\beta}{g} \left[ E - \left( H' + \frac{p_s^2}{2Q} \right) \right]$$

$$\left[ \delta\left(\frac{g}{b} \ln s - \frac{g}{b} \ln s_0\right) \right]$$

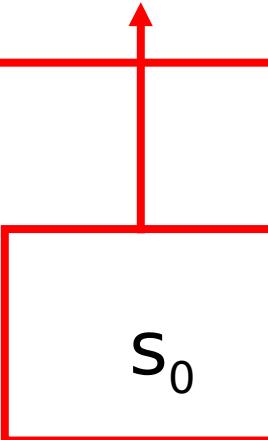
$$\delta(h(s)) = \frac{\delta(s - s_0)}{h'(s)}$$

$$h'(s) = \frac{g}{\beta s}$$

$$\delta(h(s)) = \frac{\beta}{g} \frac{1}{s} \delta(s - s_0)$$

resulta (aqui usamos  $Q$  pero en realidad es el  $\Gamma$  de Nose)

$$Q_{Nose} = \frac{1}{N!} \int dp_s ds dp^{3N} dr^{3N} \cdot s^{3N+1} \cdot \frac{\beta}{g} \cdot$$
$$\cdot \delta \left\{ s - \exp \left[ \underbrace{\frac{\beta}{g} \left[ E - \left( H' + \frac{p_s^2}{2Q} \right) \right]}_{\text{---}} \right] \right\}$$



de donde

$$Q_{Nose} = \frac{1}{N!} \frac{\beta}{g} \exp[E(3N+1)/g] \left\{ \int dp_s \exp \left[ -\beta \frac{3N+1}{g} \frac{p_s^2}{2Q} \right] \right\}.$$

$$\cdot \left\{ \int dp'^{3N} dr^{3N} \exp \left[ \beta \frac{3N+1}{g} H'(p', r) \right] \right\}$$

de donde

$$Q_{Nose} = C \frac{1}{N!} \int dp^{3N} dr^{3N} \cdot \exp \left[ -\frac{\beta(3N+1)}{g} H' \right]$$

Si tomamos  $g = 3N + 1$ ....

Obtenemos el canonico genuino!!!!!!

$$Q_{Nose} = C \frac{1}{N!} \int dp^{3N} dr^{3N} \cdot \exp[-\beta H']$$

## Calculando valores medios

$$\overline{A} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt A[p(t)/s(t), r(t)] = \langle A(p/s, r) \rangle_{Nose}$$

$$\langle A(p/s, r) \rangle_{Nose} = \frac{\int dp^N dr^N A(p^N, r) \exp[-\beta H(p^N, r)(3N+1)/g]}{\int dp^N dr^N \exp[-\beta H(p^N, r)(3N+1)/g]}$$

Hacemos la elección  $g = 3N + 1$

$$\begin{aligned}
\langle A(p/s, r) \rangle_{Nose} &= \frac{\int dp^N dr^N A(p^N, r) \exp[-\beta H(p^N, r)]}{\int dp^N dr^N \exp[-\beta H(p^N, r)]} = \\
&= \frac{\int dp^N dr^N A(p^N, r) \exp[-\beta H(p^N, r)]}{Q(N, V, T)} \\
&= \langle A(p/s, r) \rangle_{NVT}
\end{aligned}$$

Entonces

$\langle A(p/s, r) \rangle_{Nose} = \langle A(p/s, r) \rangle_{NVT}$

$$\begin{aligned}
\langle A(p/s, r) \rangle_{Nose} &= \frac{\int dp' dr^N A(p', r) \exp[-\beta H(p', r)]}{\int dp' dr^N \exp[-\beta H(p', r)]} = \\
&= \frac{\int dp' dr^N A(p', r) \exp[-\beta H(p', r)]}{Q(N, V, T)} \\
&= \langle A(p/s, r) \rangle_{NVT}
\end{aligned}$$

En este caso el espacio de fases esta asociado a las coordenadas  $r$  y a los momentos escaleados  $p'$ . A estos momentos se los llaman reales.

## Que cosa es que?

Sea  $p'$  el "momento real"

Sea  $p$  el "momento virtual"

Estan relacionadas por

$$r' = r$$

$$p' = p/s$$

$$s' = s$$

$$\Delta t' = \Delta t/s$$

Luego  $s$  es un escaleo del tiempo y por lo tanto el tiempo fluctua durante la simulacion.

Luego al samplear

$$\bar{A} = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t dt A[p(t)/s(t), r(t)] = \langle A(p/s, r) \rangle_{Nose}$$

Lo hacemos a pasos (virtuales)  $\Delta t$  corresponderá  
a pasos fluctuantes al **escalear** por  $s$

Para samplear a intervalos constantes en el tiempo real:

Sea

$$\tau' = \int_0^{\tau} dt \frac{1}{s(t)}$$

Calculamos

$$\lim_{\tau' \rightarrow \infty} \frac{1}{\tau'} \int_0^{\tau'} dt' A \left[ \frac{p(t')}{s(t')}, r(t') \right] =$$

$$= \lim_{\tau' \rightarrow \infty} \frac{\tau}{\tau'} \frac{1}{\tau} \int_0^{\tau} dt A \left[ \frac{p(t)}{s(t)}, r(t) \right] \frac{1}{s(t)}$$

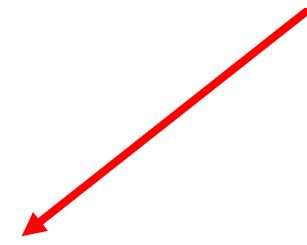
$$= \frac{\lim_{\tau' \rightarrow \infty} \frac{1}{\tau} \int_0^{\tau} dt A \left[ \frac{p(t)}{s(t)}, r(t) \right] \frac{1}{s(t)}}{\lim_{\tau' \rightarrow \infty} \frac{1}{\tau'} \int_0^{\tau'} dt \frac{1}{s(t)}}$$

$$= \langle \int A \left[ \frac{p(t)}{s(t)}, r(t) \right] \frac{1}{s(t)} \rangle \frac{1}{\langle s(t) \rangle}$$

Entonces

$$Q_{Nose} = C \frac{1}{N!} \int dp^{3N} dr^{3N} \cdot \exp\left[-\frac{\beta(3N+1)}{g} H'\right]$$

$$= \left\langle A \left[ \frac{p(t)}{s(t)}, r(t) \right] \frac{1}{s(t)} \right\rangle \frac{1}{\langle s(t) \rangle} =$$



$$= \frac{\left\{ \int dp'{}^N dr^N A(p/s, r) \exp[-\beta H(p', r) 3N/g] \right\}}{\left\{ \int dp'{}^N dr^N \exp[-\beta H(p', r) 3(N+1)/g] \right\}} =$$
$$= \frac{\left\{ \int dp'{}^N dr^N \exp[-\beta H(p', r) 3N/g] \right\}}{\left\{ \int dp'{}^N dr^N \exp[-\beta H(p', r) 3(N+1)/g] \right\}}$$

$$\cancel{i} \frac{\int dp'{}^N dr^N A(p/s, r) \exp[-\beta H(p', r) 3N/g]}{\int dp'{}^N dr^N \exp[-\beta H(p', r) 3N/g]} =$$

$$\cancel{i} \langle A(p/s, r) \rangle_{NVT}$$

$$g = 3N$$

Las ecuaciones de movimiento son (usando  $H_{Nose} = \sum \frac{p_i^2}{2m_i s^2} + V(r^N) + \frac{p_s^2}{2Q} + \frac{g}{\beta} \ln s$ )  
 (para las variables virtuales)

$$\frac{dr_i}{dt} = \frac{p_i}{(m_i s)}$$

$$\left[ \frac{d \vec{r}_i}{dt} = \frac{\partial H_{Nose}}{\partial \vec{p}_i} \right]$$

$$\frac{dp_i}{dt} = -\frac{\partial V(r)}{\partial r_i}$$

$$\frac{ds}{dt} = \frac{p_s}{Q}$$

$$\frac{dp_s}{dt} = \left[ \sum p_i^2 / (m_i s^2) - g/\beta \right] / s$$

Para las variables reales

$$\frac{dr'_i}{dt} = \frac{p_i}{(m_i s)} = \frac{p_i'}{m_i}$$

$$\frac{dp'_i}{dt} = -\frac{\partial V(r')}{\partial r'_i} - \left[ \frac{s' p'_s}{Q} \right] p'_i$$

$$\frac{1}{s} \frac{ds'}{dt} = \frac{s' p'_s}{Q}$$

$$\frac{d(s' p'_s / Q)}{dt} = \left[ \sum p_i'^2 / m_i - g/\beta \right] / Q$$

# Implementacion

Lo mas conveniente es trabajar con variables reales pues entonces los intervalos de tiempo son ctes.

Segun Hoover

Sea  $s'p'_s/Q = \xi$

W.G. Hoover. Canonical dynamics: Equilibrium phase-space distributions. *Phys. Rev. A*, 31:1695–1697, 1985.

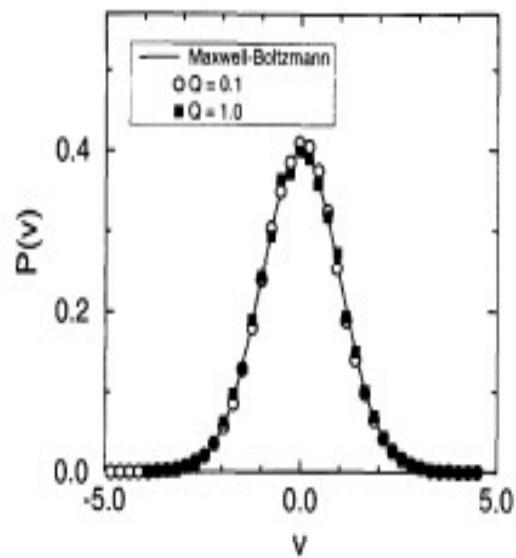
W.G. Hoover. Constant pressure equations of motion. *Phys. Rev. A*, 34:2499–2500, 1986.

Dejando de lado las primas

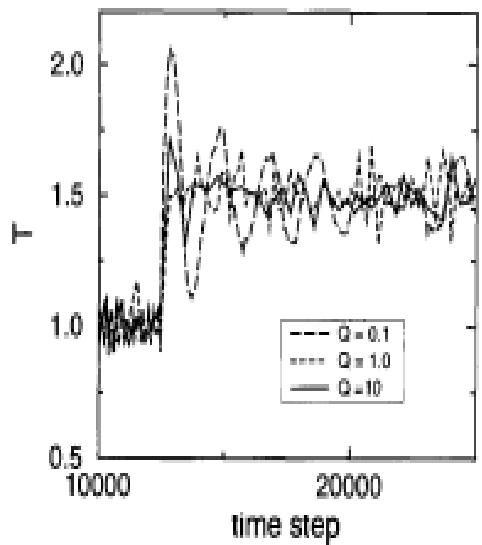
$$\frac{dr_i}{dt} = \frac{p_i}{m_i}$$

$$\frac{dp_i}{dt} = -\frac{\partial V(r)}{\partial r_i} - \xi_i p_i$$

$$\frac{d\xi}{dt} = \left[ \sum p_i^2/m_i - g/\beta \right] / Q$$



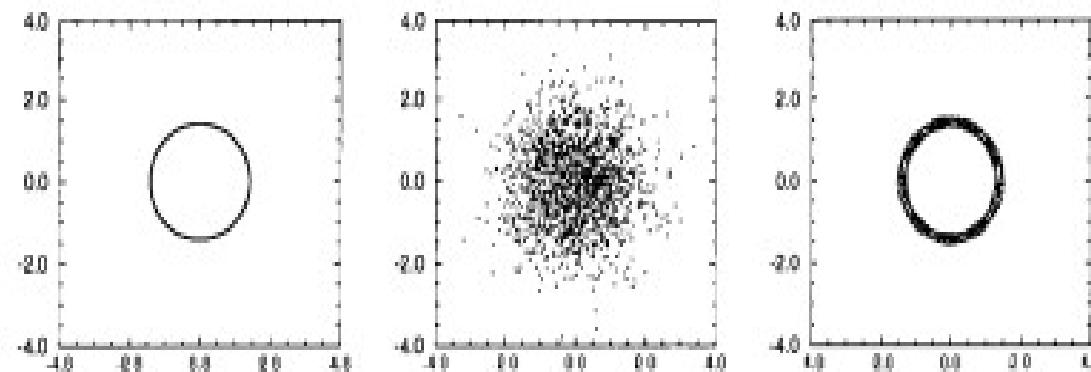
**Figure 6.4:** Velocity distribution in a Lennard-Jones fluid ( $T = 1.0$ ,  $\rho = 0.75$ , and  $N = 256$ ). The solid line is the Maxwell-Boltzmann distribution (6.1.1) the symbols were obtained in a simulation using the Nosé-Hoover thermostat.



**Figure 6.5:** Response of the system to a sudden increase of the imposed temperature. The various lines show the actual temperature of the system (a Lennard-Jones fluid  $\rho = 0.75$ , and  $N = 256$ ) as a function of the number of time steps for various values of the Nosé-Hoover coupling constant  $Q$ .

## Atencion

Estas ecuaciones no funcionan por ejemplo para el oscilar armonico pues no son "lo suficientemente caoticas"



**Figure 6.7:** Trajectories of the harmonic oscillator: (from left to right) in the microcanonical ensemble, using the Andersen method, and using the Nosé-Hoover method. The y axis is the velocity and the x axis is the position.

To alleviate the restriction for the Nosé-Hoover thermostat, Martyna *et al.* [136] proposed a scheme in which the Nosé-Hoover thermostat is coupled to another thermostat or, if necessary, to a whole chain of thermostats. As we show in Appendix B.2.2 these chains take into account additional conservation laws. In [136] it is shown that this generalization of the original Nosé-Hoover method still generates a canonical distribution (provided that it is ergodic).

The equations of motion for a system of  $N$  particles coupled with  $M$  Nosé-Hoover chains are given (in real variables, hence  $L = 3N$ ) by

$$\dot{r}_i = \frac{\dot{p}_i}{m_i} \quad (6.1.29)$$

$$\dot{p}_i = F_i - \frac{p_{L_1}}{Q_1} p_i \quad (6.1.30)$$

$$\dot{\xi}_k = \frac{p_{L_k}}{Q_k} \quad k = 1, \dots, M \quad (6.1.31)$$

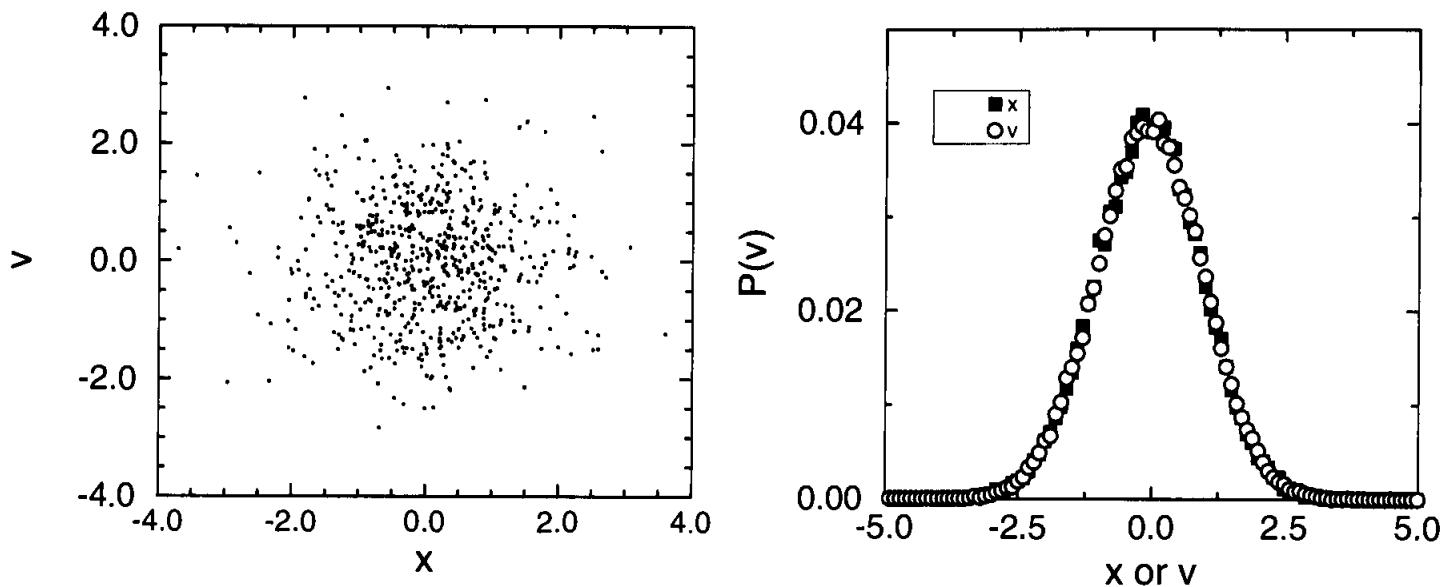
$$\dot{p}_{L_1} = \left( \sum_i \frac{p_i^2}{m_i} - L k_B T \right) - \frac{p_{L_2}}{Q_2} p_{L_1} \quad (6.1.32)$$

$$\dot{p}_{L_k} = \left[ \frac{p_{L_{k-1}}^2}{Q_{k-1}} - k_B T \right] - \frac{p_{L_{k+1}}}{Q_{k+1}} p_{L_k} \quad (6.1.33)$$

$$\dot{p}_{L_M} = \left[ \frac{p_{L_{M-1}}^2}{Q_{M-1}} - k_B T \right]. \quad (6.1.34)$$

For these equations of motion the conserved energy is

$$H_{NH\!C} = \mathcal{H}(r, p) + \sum_{k=1}^M \frac{p_{L_k}^2}{2Q_k} + L k_B T \xi_1 + \sum_{k=2}^M k_B T \xi_k. \quad (6.1.35)$$



**Figure 6.8:** Test of the phase space trajectory of a harmonic oscillator, coupled to a Nosé-Hoover chain thermostat. The left-hand side of the figure shows part of a trajectory: the dots correspond to consecutive points separated by 10,000 time steps. The right-hand side shows the distributions of velocity and position. Due to our choice of units, both distributions should be Gaussians of equal width.



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# Microscopic dynamics of pedestrian evacuation

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## THE ROLE OF PANIC IN THE ROOM EVACUATION PROCESS

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# Morphological and dynamical aspects of the room evacuation process

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## Room evacuation in the presence of an obstacle

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### EVACUATION UNDER LIMITED VISIBILITY

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# Detection of community structures in networks via global optimization<sup>☆</sup>

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## Alternative approach to community detection in networks

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## COMMUNITY DETECTION IN NETWORKS

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# Memory effects induce structure in social networks with activity-driven agents

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