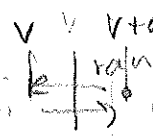
diffusion



flux $\propto \rho(v+dv) - \rho(v) \propto \frac{\partial \rho}{\partial v}$ v v+dv

$d\rho\, dv \propto dt \left\{ \left[\frac{\partial \rho}{\partial v}(v+dv) - \frac{\partial \rho}{\partial v}(v) \right] \right.$ ⇆ ⇆

Stationary solution $\rho \propto \exp(-\beta(V(x) + \frac{1}{2}mv^2))$ (Boltzmann factor)

$$\frac{d}{dt}\rho(x,v) = 0 = (a(x) - \eta v)(-\beta m v)\rho - \eta\rho + v(-\beta V')\rho + \frac{\partial}{\partial v}(-\beta m v)\rho D_{vv}$$

$$[a(x) - \eta v](-\beta m v)\rho + \eta\rho + -\beta m \rho D + (-\beta m v)^2 \rho D$$

$$= \rho(\eta \beta m v^2 - \eta - \beta m D + \beta^2 m^2 v^2 D)$$

$$= 0 \quad \text{if} \quad \eta = D\beta m$$

⇒ correct ensemble averages enforced.

Nosé-Hoover — Deterministic — **Very common**

additional variable s for heat bath

$$H_{Nosé} = H' + \frac{p_s^2}{2Q} + L\frac{\log s}{\beta}$$

(L: some parameter)

$$H' \leftarrow \frac{p_i^2}{2m_i s^2} + U(r_1 \dots r_N) \qquad p' = p/s$$

$\mu(\rho)$ is micro cannonical, constant E, N, V

$\delta[H_{Nosé} - E]$ ---- algebra ... integrating out s

⇒ $\langle A(p/s, r)\rangle_{Nosé} = \langle A(p', r)\rangle_{NVT}$ canonical!

Hoover rewrote it intelligently to make it easier to implement

Not Hamilt.
$$\begin{cases} \dot{r}_i = p_i/m & \dot{p}_i = a(r_1 \dots r_N) - \xi p_i \\ \dot{\xi} = \left(\sum p_i^2/m_i - \frac{L}{\beta}\right)/Q \\ \frac{\dot{s}}{s} = \frac{d}{dt}\log s = \xi \end{cases}$$

ξp_i: effective friction

$\dot{\xi}$ ← difference to temp you want,

$\frac{\dot{s}}{s}$ ← redundant, but nice for checking: ($H_{Nosé}$ conserved)

Notes: - $\log(s)$ was necessary to get correct behaviour

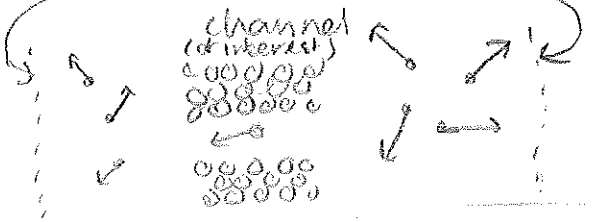
- necessary to have only one constant of motion, otherwise Nosé-Hoover chains. (due to δ function)
  ↪ thermostat coupled to more thermostats
- global dependance.

Applying thermostats

- choose carefully. What is more realistic?
- where to apply? Far away from relevant dynamics.
- careful with out-of-equilibrium systems
  $\mathcal{H}(\gamma)$ is not the only thing that needs to be ok.
- There are other options (i.e to damp phonons)

example:

periodic

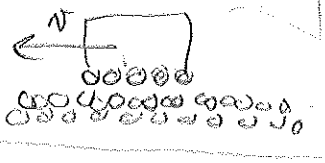


How would you thermostat this?

Will get exercises on thermostats!

How would you thermostat Ly Argon liquid?

other example



Barostats etc..

scheme similar to Nosé-Hoover: include volume as variable. read the book section 6.2.

In general: key to something-o-stat is
to produce correct $\mathcal{H}(\gamma)$

end lecture 7