On the physical significance of finite thermostats

Nonequilibrium: stationary states of particles subject to non conservative forces whose work is dissipated in thermostats.

Problem: simulations $\rightarrow$ finite systems which **however** cannot be Hamiltonnian.

"*Solution*": introduce artificial forces which absorb energy, and allow reaching stationarity

Question: is this OK ? are physical properties altered? can there be equivalence between artificial non Hamiltonian thermostats and infinite Hamiltonian thermostats?

Example: $U_j,\ U_{0,j}$ pair int., short range

$$x = (\mathbf{X}_0, \dot{\mathbf{X}}_0, \mathbf{X}_1, \dot{\mathbf{X}}_1, \ldots, \mathbf{X}_n, \dot{\mathbf{X}}_n)$$

$$\begin{aligned}
\ddot{\mathbf{X}}_{0i} &= -\,\partial_i U_0(\mathbf{X}_0) - \sum_{j>0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \mathbf{F}_i(\mathbf{X}_0)\\
\ddot{\mathbf{X}}_{ji} &= -\,\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) - a\,\alpha_j \dot{\mathbf{X}}_{ji}, \qquad a = 0, 1
\end{aligned}$$

Particles move in containers bounded by a sphere Λ of radius R and, for $a = 1$, α_j are multipliers to impose *Isokinetic* or *Isoenergetic*

$$\frac{\dot{\mathbf{X}}_j^2}{2} \equiv \frac{3N_j}{2} k_B T_j, \qquad \text{or} \qquad \frac{\dot{\mathbf{X}}_j^2}{2} + U_j(\mathbf{X}_j) \equiv E_j$$

and $a = 0$ corresponds to the Hamiltonian dynamics

Initial data chosen (for instance) w.r. to Gibbs distribution

$$\mu_0 = \lim_{\Lambda\to\infty} c\, e^{-H_0(x)} \prod_j \frac{d\mathbf{X}_j d\dot{\mathbf{X}}_j}{N_j!}, \qquad H_0(x) = \sum_{j=0}^n \beta_j \Big(\frac{\dot{\mathbf{X}}_j^2}{2} + U_j(\mathbf{X}_j) - \lambda_j N_j\Big)$$

Choosing x with μ_0 gives an infinite configuration with well defined temperature, energy density e_j, density δ_j to each thermostat.
The x evolves $x \to S_t^{(\Lambda,1)} x$ ignoring the particles outside Λ.

Idea: If Λ large a simulation with the finite thermost. dynamics gives motions very close to those of the infinite thermostats **with** μ_0**–prob.** 1. The latter is defined as $x \to S_t^{(0)} x = \lim_\Lambda S_t^{(\Lambda,0)} x$

The limits of the finite volume dynamics should exist and with and without thermostat forces and *the energy per particle, the density, and the kinetic energy per particle should be constants of motion* with probability 1.

Local dynamics $S_t^{(\Lambda,a)}x$ is such that each particle has finitely many collisions with the walls fot $t' << \leq t$ ($\leq \nu_i(x,t)$, $\forall\,\Lambda, a=0,1$). And the limits $S_t^{(a)}x$ exist with μ_0 probability 1 and the energy density and the density in a ball $B(\xi,\rho)$ is bounded if $\rho > \log_+|\xi|$ while the global quantities are **constant**, for all t,

$$\frac{N_j(x^{(\Lambda,a)}(t))}{|\Lambda\cap C_j|}\xrightarrow[\Lambda\to\infty]{}\delta_j,\ \frac{U_j(x^{(\Lambda,a)}(t))}{|\Lambda\cap C_j|}\xrightarrow[\Lambda\to\infty]{}u_j,\ \frac{K_j(x^{(\Lambda,a)}(t))}{|\Lambda\cap C_j|}\xrightarrow[\Lambda\to\infty]{}\frac{3k_BT_j\,\delta_j}{2},$$

Theorem For any fixed t the *a–independent limit* exists

$$\lim_{\Lambda\to\infty} S_t^{(\Lambda,a)}x = S_t^{(0)}x, \qquad a=0,1$$

This means that for Λ large the two dynamics become identical in spite of the fact that the thermostatted is dissipative and the Hamiltonian is conservative.
BUT: have we lost the entropy production???

If $Q_j \stackrel{def}{=} \dot{\mathbf{X}}_j \cdot \partial_{\mathbf{X}_j} U_{j.0}(\mathbf{X}_j, \mathbf{X}_0)$ is the *heat*

$$\alpha_j = \frac{Q_j - \dot{U}_j}{3k_B T_j N_j}, \ (i.k.) \qquad \alpha_j = \frac{Q_j}{3k_B T_j N_j}, \ (i.e.)$$

The entropy production is $\varepsilon = \sum_{j>0} \frac{Q_j}{k_B T_j}$ in the Hamiltonian case. The phase space contraction is 0 in the Hamiltonian case and in the therm. cases is

$$\sigma(x) = \sum_{j>0} \frac{Q_j - \dot{U}_j}{k_B T_j}, (i.k.) \qquad \sigma(x) = \sum_{j>0} \frac{Q_j}{k_B T_j}, (i.e.)$$

Hence σ and ε are identified (additive time derivatives do not count).
How is this possible: $\alpha_j \xrightarrow[\Lambda\to\infty]{} 0$ but $\sigma \simeq \sum 3N_j\alpha_j$ *does not*: like the energy in mean field models. Proof:

$$x_i^{(\Lambda,a)}(t) = x_i(0) + e^{-\int_0^t a\alpha_j(t')dt'}\dot{x}_i(0) + \int_0^t dt'' e^{-\int_{t''}^t a\alpha_j(t')dt'} F_i(t'')dt''$$

and $\alpha_i \xrightarrow[\Lambda\to\infty]{} 0$ for all $j \Rightarrow$ the limits $x_i^{(a)}(t)$ satisfy *the same equations.*

Reference:
arxiv.org: 0810.1510
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