On Thermostats: Isokinetic or Hamiltonian? finite or infinite?

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Abstract: *The relation between finite isokinetic thermostats and infinite Hamiltonian thermostats is studied and their equivalence in the thermodynamic limit is heuristically discussed.*

Studies on non equilibrium statistical mechanics progressed considerably after the introduction of artificial forces supposed to simulate the interaction of a "test system" with "heat reservoirs", also called "thermostats". Simulations could be developed eliminating the need of very large systems to model the action of heat reservoirs. The drawback is that the equations of motion are no longer Hamiltonian. The simulations led to developments and to many new insights into nonequilibrium, particularly with regard to the theory of large fluctuations (fluctuation theorems, work relations and attempted applications to problems ranging from biophysics to fluid turbulence). An ongoing question has been, therefore, whether such thermostat models are just devices to generate simulations that may have little to do with physical reality and, therefore, in the end not really relevant for Physics. There are, however, conjectures of equivalence between various kinds of thermostats and the often preferred "infinite thermostats" which, being Hamiltonian, are considered more fundamental (in spite of being infinite in size) or the stochastic thermostats. Here we try to substantiate, via a heuristic analysis, the equivalence conjecture between "Hamiltonian" and "isokinetic" thermostats by discussing it in precise terms. Isokinetic will mean that artificial forces are introduced whose role is to turn into an exact constant of motion the total kinetic energy of the particles identified as particles of any of the thermostats interacting with the test system. The novelty here is that a careful distinction is made between the test system particles and the particles of the thermostats in contact with it but physically located in containers outside the sytem (as in most real thermal baths). The artificial forces only act on the latter: this is a substantial difference from most cases considered in the literature in which the artificial forces act also on the test system particles (technically called "bulk thermostats"): it is convenient to call the thermostats considered here "peripheral thermostats". The test system will be kept fixed but the thermostats will be allowed to be of arbitrary size, and their behavior as the size becomes infinite is what will interest us. The conclusion is that, under a suitable assumption, a peripheral isokinetic thermostat becomes in the thermodynamic limit, when its container becomes infinite, completely equivalent to a Hamiltonian infinite thermostat: in the sense that the time evolution of the configurations (*ie* of the phase space point representing test and interaction systems) is, with probability 1, the same as that obtained by letting the isokinetic containers become infinite. In bulk thermostats there cannot be such strict equivalence because motion remains non Hamiltonian even in the limit of infinite systems. The analysis reinforces, as a byproduct, the identification (modulo an additive total time derivative) between phase space contraction and entropy production.

I. THERMOSTATS

A classical model for nonequilibrium, for instance in [1], is a *test system* in a container Ω_0, for instance a sphere of radius R_0 centered at the origin O, and several *Interaction systems* containing the *thermostats*: we denote their containers Ω_j and they can be thought (to fix ideas) as the sets Ω_j consisting of disjoint sectors $\Omega_j = \{\xi \in \mathbb{R}^3, |\xi| > R_0, \xi \cdot \mathbf{k}_j < |\xi|\,\omega_j\}$, $j = 1, \ldots, n$, $\mathbf{k}_j$ distinct unit vectors, realized, for instance, as disjoint sectors in $\mathbb{R}^3$, see Fig.1, *i.e.* as cones in $\mathbb{R}^3$ with vertex at the origin deprived of the points inside the sphere containing the test system: for precision of language we shall call such containers "sperically truncated cones"; but the actual shape could be rather arbitrarily changed, as it will appear. The terms "test" and "interaction" systems were introduced in [1]. The contact between test system and thermostats occurs only through the common boundaries (located on the boundary of the ball Ω_0) of the test system. No scaling, of time or space, will be considered here.

In the quoted reference, as well as in later related works, [2–4], the particles contained in $\Omega_0, \ldots, \Omega_n$ were quantum particles and the interaction systems were infinitely extended (and obeying a linear Schrödinger equation) and each was initially in a Gibbs state at respective temperatures $T_1, \ldots, T_n$. Here the particles will be classical, with unit mass, elastically confined in $\Omega_0, \Omega_1 \cap \Lambda_r, \ldots, \Omega_n \cap \Lambda_r$ with Λ_r a finite ball, centered at O, of radius $r > R_0$. The temperatures in the interaction systems, here called *thermostats*, will be defined by the total kinetic energies in each of them: which will be kept a constant of motion by adding a phenomenological "thermostatting force". Hence the qualification of *isokinetic* that will be given to such thermostats. More appropriately one should call such thermostats "peripherally isokinetic" because most often in the literature the term isokinetic, instead, refers to systems in which the

total kinetic energy of all particles (in the test and interaction systems) is maintained constant. The latter are called *bulk thermostats*: our models will correspond to a system in which no internal microscopic friction occurs and which exchanges energy with external systems kept at constant temperature. The properties that we discuss cannot hold for bulk thermostats. However we shall call our thermostats simply isokinetic except in the last section. The arrangement is illustrated in Fig.1 below.

Remark: peripherally isokinetic thermostats have been considered in the literature in simulations, [5], and their physically correct behavior was immediately remarked sparking investigations about the equivalence problem. See also [6, 7]. Recently a case of a model in which only hard core interactions between particles were present, and the test system was thermostatted peripherally, has been studied in [8] showing the thermostat action being efficient and measurable even in such extreme situation.

Phase space: *Phase space $\mathcal{H}$ is the collection of locally finite particle configurations $x = (\ldots, q_i, \dot{q}_i, \ldots)_{i=1}^{\infty}$*

$$x = (\mathbf{X}_0, \dot{\mathbf{X}}_0, \mathbf{X}_1, \dot{\mathbf{X}}_1, \ldots, \mathbf{X}_n, \dot{\mathbf{X}}_n) = (\mathbf{X}, \dot{\mathbf{X}}) \quad (1.1)$$

with $\mathbf{X}_j \subset \Omega_j$, hence $\mathbf{X} \subset \Omega = \cup_{j=0}^{n} \Omega_j$, and $\dot{q}_i \in \mathbb{R}^3$; and in every ball $\mathcal{B}(r, O)$, of radius r and center at the origin O, fall a finite number of points of $\mathbf{X}$.

The space $\mathcal{H}(\Lambda_r)$ will be the space of the finite configurations with $\mathbf{X} \subset \Lambda_r$. It will be convenient to imagine a configuration x as consisting of a configuration $(\mathbf{X}_0, \dot{\mathbf{X}}_0) \in \mathcal{H}(\mathcal{B}(R_0, O))$ and by n configurations $(\mathbf{X}_j, \dot{\mathbf{X}}_j) \in \mathcal{H}(\Omega_j \cap \mathbb{R}^3 / \mathcal{B}(R_0, O))), j = 1, \ldots, n$.

Interaction: *The interparticle interaction φ will be a pair potential with finite range r_φ and superstable in the sense that φ is non negative, decreasing in its range (i.e. "repulsive"), smooth and positive at the origin.*

Remark: Singularities like hard core could be also considered (at the heuristic level of this paper) but are left out for brevity. For more general cases, like Lennard-Jones interparticle potentials or for modeling by external potentials the containers walls, see [9].

The potential and kinetic energies of the configuration $x \in \mathcal{H}(\Lambda_r)$ are $U(x) = \sum_{q', q'' \in \mathbf{X} \cap \Lambda_r}^{*} \varphi(q' - q'')$, $K(x) = \sum_{q_i \in \mathbf{X} \cap \Lambda_r} \frac{\dot{q}_i^2}{2}$ where the $*$ means that the sum is restricted to the pairs q', q'' which are either in the same Ω_j or consist of two elements q', q'' of which one is in Ω_0: this means that particles in Ω_0 interact with all the others but the particles in Ω_j interact only with the ones in $\Omega_j \cup \Omega_0$. The φ's will be, for simplicity, the same for all pairs.

The system in Ω_0 interacts with the thermostats but the thermostats interact only with the system, see Fig.1.

$$x = (\mathbf{X}_0, \dot{\mathbf{X}}_0, \mathbf{X}_1, \dot{\mathbf{X}}_1, \ldots, \mathbf{X}_n, \dot{\mathbf{X}}_n)$$
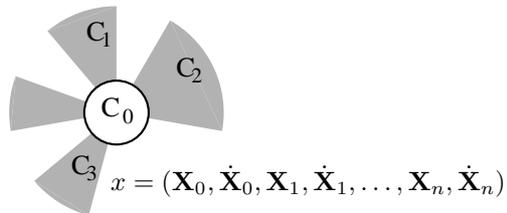
Fig.1: *The $1 + n$ boxes $\Omega_j \cap \Lambda_r$, $j = 0, \ldots, n$, are marked $C_0, C_1, \ldots, C_n$ and contain $N_0, N_1, \ldots, N_n$ particles, mass $m = 1$, with positions and velocities denoted $\mathbf{X}_0, \mathbf{X}_1, \ldots, \mathbf{X}_n$, and $\dot{\mathbf{X}}_0, \dot{\mathbf{X}}_1, \ldots, \dot{\mathbf{X}}_n$, respectively. The $\mathbf{E}$ are external, positional, non conservative, forces; the multipliers α_j are so defined that the kinetic energies $K_j = \frac{1}{2}\dot{\mathbf{X}}_j^2$ are exact constants of motion.*

Hence, if $x \in \mathcal{H}(\Lambda_r)$, the energy $U(x)$ can be written as

$$U(x) = U_0(\mathbf{X}_0) + \sum_{j=1}^{n} \left(U_j(\mathbf{X}_j) + U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) \right) \quad (1.2)$$

and the kinetic energies will be $K_j(\dot{\mathbf{X}}_j) = \frac{1}{2}\dot{\mathbf{X}}_j^2$. The equations of motion will be (see Fig.1)

$$\ddot{\mathbf{X}}_{0i} = -\partial_i U_0(\mathbf{X}_0) - \sum_{j>0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \mathbf{E}_i(\mathbf{X}_0)$$

$$\ddot{\mathbf{X}}_{ji} = -\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) - \alpha_j \dot{\mathbf{X}}_{ji} \quad (1.3)$$

where the first label, $j = 0, \ldots, n$, denotes the thermostat (or system) and the second the derivatives with respect to the coordinates of the points in the corresponding thermostat (hence the labels i in the subscripts (j, i) have $3N_j$ values); the multipliers α_j are, for $j = 1, \ldots, n$,

$$\alpha_j \stackrel{def}{=} \frac{Q_j - \dot{U}_j}{2K_j}, \qquad Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j), \quad (1.4)$$

and the "walls" (*i.e.* the boundaries $\partial\Omega_i, \partial\Lambda_r$) delimiting the different containers will be supposed elastic. A more general model to which the analysis that follows also applies is in [10].

It is also possible to imagine thermostats acting in the bulk of the test system by adding a further force $-\alpha_0 \dot{\mathbf{X}}_0$: this is, for instance, of interest in electric conduction models, [11], where the dissipation is due to energy exchanges with oscillations ("phonons") of an underlying lattice of obstacles. Such bulk thermostatted systems will not be discussed because, for physical reasons, their dynamics cannot be expected to be equivalent to the Hamiltonian one in the strong sense that will be considered here. The thermostat forces would introduce an effective friction on the system motion not disappearing as the size of the systems grows, as it is always the case in bulk thermostatted systems.

Other thermostats considered in the literature, [12, 13], could be studied and be subject to a similar analysis, which would be interesting, *e.g.* the Nosé-Hoover or the isoenergetic thermostats. Note that even the isoenergetic thermostat does not conserve Gibbs states (in presence of a test system).

The equations of motion will be called *isokinetically thermostatted* because the multipliers α_j are so defined to keep the K_j exactly constant for $j > 0$. The forces $\mathbf{E}_i(\mathbf{X}_0)$ are positional *nonconservative*, smooth, forces. The numbers N_j of particles in the intial data may be random but will be picked with a distribution giving them average values of $\frac{N_j}{|\Omega_j \cap \Lambda_r|}$ within positive and asymptotically Λ_r-independent bounds as $r \to \infty$.

Initial data: *The probability distribution μ_0 for the random choice of initial data will be, if $dx \stackrel{def}{=} \prod_{j=0}^{n} \frac{d\mathbf{X}_j \, d\dot{\mathbf{X}}_j}{N_j!}$, the limit as $\Lambda_r \to \infty$ of*

$$\mu_{0,\Lambda_r}(dx) = const \, e^{-H_0(x)} \, dx \qquad (1.5)$$

with $H_0(x) = \sum_{j=0}^{n} \beta_j(K_j(\dot{\mathbf{X}}_j) - \lambda_j N_j + U_j(x))$ *and* $\beta_j \stackrel{def}{=} \frac{1}{k_B T_j}$, $j > 0$ *and* $\beta_0 > 0$ *arbitrary.*

Here $\boldsymbol{\lambda} = (\lambda_0, \lambda_1, \dots \lambda_n)$ and $\mathbf{T} = (T_0, T_1, \dots, T_n)$ are fixed *chemical potentials* and *temperatures* (k_B being Boltzmann's constant).
The limit μ_0 as $\Lambda_r \to \infty$ of the distribution in Eq.(1.5) makes sense (with particles allowed to be located in the infinite containers Ω_j, $j > 0$) provided it is interpreted as a Gibbs distribution μ_0 obtained by taking the "thermodynamic limit" $\Lambda_r \to \infty$, supposing for simplicity that the parameters λ_j, T_j, $j > 0$ do not correspond to phase transition points (which would require care to consider boundary conditions which generate pure phases, [14]).

It will be convenient to think always the initial data chosen with respect to the latter distribution: if $\Lambda_r < \infty$ the particles positions and velocities outside Λ_r will, however, be imagined fixed in time ("frozen", see [15, 16]). Therefore, defining

$$Z_j(\lambda, \beta) = \sum_{N=0}^{\infty} \int_{(\Lambda_r \cap \Omega_j) \times \mathbb{R}^3} e^{-\beta(K_j + U_j - \lambda N_j)} \frac{d\mathbf{X} \, d\dot{\mathbf{X}}}{N!}$$
$$(1.6)$$

and $\beta p_j(\beta, \lambda) = \lim_{\Lambda_r \to \infty} \frac{1}{|\Lambda_r \cap \Omega_j|} \log Z_j(\beta, \lambda)$, the thermostats density and average potential energy will be

$$\delta_j = \frac{\partial \lambda_j p_j}{\partial \beta_j}, \qquad u_j = -\frac{\partial \beta_j p_j}{\partial \beta_j} - \frac{3}{2} k_B T_j \delta_j - \lambda_j \delta_j \quad (1.7)$$

and $\delta_j, u_j, \frac{3}{2} k_B T_j$ will be suppposed to be the average density, average potential energy density and average kinetic energy per particle in the initial configurations: without loss of generality because this holds *with μ_0- probability* 1 (by the no-phase-transitions assumption).

II. DYNAMICS

In general time evolution with the thermostatted dynamics changes the measure of a volume element in phase space by an amount related to (but different from) the variation of the Liouville volume.

Minus the change per unit time of a volume element measured via Eq.(1.5) is, in the sectors of phase space containing $N_j > 0$ particles inside $\Lambda_r \cap \Omega_j$, $j = 0, 1, \dots, n$, with kinetic energy $K_{j,\Lambda_r}(x)$,

$$\sigma(x) = \sum_{j>0} \frac{Q_j}{k_B T_j(x)} \left(1 - (3N_j)^{-1}\right) + \beta_0(\dot{K}_0 + \dot{U}_0)$$

$$- \sum_{j>0} \dot{U}_j \Big(\frac{1}{k_B T_j}(1 - \frac{1}{3N_j}) - \beta_j \Big) \qquad (2.1)$$

where $k_B T_j(x) = \frac{2}{3} \frac{K_{j,\Lambda_r}}{N_j}$, and $k_B T_j(x) \to \beta_j^{-1}$ for $\Lambda_r \to \infty$, at least for the initial data, with μ_0 probability 1.

Remarks: (1) The dynamics given by the equations of motion Eq.(1.5) or by the same equations with $\alpha_j \equiv 0$ are of course different. We want to study their difference.
(2) The choice of the initial data with the distribution μ_0 regarded as obtained by a thermodynamic limit of Eq.(1.5) rather than (more naturally) with $\mu'_{0,\Lambda_r}(dx)$

$$\frac{\mu'_{0,\Lambda_r}(dx)}{dx} = const \, e^{-H_0(x)} \prod_{j=1}^{n} \delta(K_j - \frac{3N_j k_B T_j}{2}) \quad (2.2)$$

with $N_0, N_1, \dots, N_n$ fixed, $\frac{N_j}{|\Omega_j \cap \Lambda_r|} = \delta_j$, $j > 0$, and no particles outside Λ_r is done to refer, in the following, to [15, 16]. A heuristic analysis would be possible also with this, and others, alternative choice.
(3) The Eq.(2.2) is natural, although less convenient notationally, because in the case $n = 1, \mathbf{E} = \mathbf{0}$ and $\beta_0 = \beta_1 = \beta$ with $\beta^{-1} = k_B T_1 (1 - \frac{1}{3N_1})^{-1}$ it is *exactly stationary* (a minor extension of [12]), if multiplied by the density $\rho(x) = e^{-\beta \sum_{j>0} U(\mathbf{X}_0, \mathbf{X}_j)}$, which is the "missing" Boltzmann factor in Eq.(1.5), and therefore can be called an equilibrium distribution.

Choosing initial data with the distribution μ_0 let $x \to x^{(\Lambda_r, a)}(t) \stackrel{def}{=} S_t^{(\Lambda_r, a)} x$, $a = 0, 1$ be the solution of the equations of motion with $\alpha_j = 0$ ($a = 0$, "Hamiltonian thermostats") or α_j given by Eq.(1.3) ($a = 1$, "isokinetic thermostats") and ignoring the particles initially outside Λ_r, [16]; and let $S_t^{(0)} x$ be the dynamics $\lim_{\Lambda_r \to \infty} S^{(\Lambda_r, 0)} x$.

Existence of a solution to the equations of motion is a problem only if we wish to study the $\Lambda_r \to \infty$ limit, *i.e.* in the case in which the thermostats are infinite (thermodynamic limit).

It is a very difficult problem even in the case in which $\alpha = 0$ and the evolution is Hamiltonian. For $n = 1$, $\alpha_1 = 0$, $\beta = \beta_0 \stackrel{def}{=} \beta$ and $\mathbf{E} = \mathbf{0}$, a case that will be

called *equilibrium*, it was shown, [15], that a solution to the (Hamiltonian) equations of motion exists for almost all initial data x chosen with a distribution obtained by multiplying $\mu_0(dx)$ by an arbitrary density function $\rho(x)$; and it is defined as the limit as $\Lambda_r \to \infty$ of the finitely many particles evolutions $S_t^{(\Lambda_r,0)}x$ in $\Omega \cap \Lambda_r$.

Recently, the related problem of a single infinite system and no thermostat forces has been solved in [15, 16] where it has been shown that, for a set of initial data which have probability 1 with respect to all distributions like Eq.(1.5), the Hamiltonian equations make sense and admit a unique solution, but the general nonequilibrium cases remain open.

Therefore in the following I shall suppose, heuristically, a property (called below "locality of evolution") of the equations of motion Eq.(1.3) *with and without* the thermostatting forces $\alpha_j \dot{\mathbf{X}}_j$.

The question will then be: *are the two kinds of thermostats equivalent?*

This is often raised because the isokinetically thermostatted dynamics is considered "unphysical" on grounds that are viewed, by some, sufficient to ban isokinetic thermostats from use in physically meaningful problems, like their use to compute transport coefficients, [12]. The following heuristic considerations show that the latter would be too hasty a conclusion.

III. HEURISTIC DISCUSSION AND EQUIVALENCE ISOKINETIC VERSUS HAMILTONIAN

The first paper dealing with equivalence issues is [6]: its ideas are taken up here, somewhat modified, and extended. A detailed comparison with [6] is in the last section.

In the Hamiltonian approach the thermostats are infinite systems with no thermostatting forces ($\alpha_j \equiv 0$) the initial data are still chosen with the distribution μ_0 discussed above. Let

$$x^{\Lambda_r,1}(t) = (\mathbf{X}_i^{\Lambda_r,1}(t), \dot{\mathbf{X}}_i^{\Lambda_r,1}(t))_{i=0,\ldots,n} = S_t^{(\Lambda_r,1)}x,$$

$$x^{\Lambda_r,0}(t) = (\mathbf{X}_i^{\Lambda_r,0}(t), \dot{\mathbf{X}}_0^{\Lambda_r,i}(t))_{i=0,\ldots,n} = S_t^{(\Lambda_r,0)}x,$$

$$x^0(t) = (\mathbf{X}_i^0(t), \dot{\mathbf{X}}_i^0(t))_{i=0,\ldots,n} = S_t^{(0)}x. \qquad (3.1)$$

Then a particle $(q_i, \dot{q}_i)$ located at $t=0$ in, *say*, the j-th thermostat evolves, see Eq.(1.3), as

$$q_i(t) = q_i + \int_0^t \dot{q}_i(t')dt' \qquad (3.2)$$

$$\dot{q}_i(t) = e^{-\int_0^t \alpha_j(t')dt'}\dot{q}_i + \int_0^t dt'' e^{-\int_{t''}^t \alpha_j(t')dt'} F_i(t'')dt''$$

where $F_i(t) = -\partial_{q_i}(U_j(\mathbf{X}_j(t)) + U_{j,0}(\mathbf{X}_0(t), \mathbf{X}_j(t)))$. The above relations hold up to the first collision of the i-th particle with the containers walls, afterwards they hold until the next collision with a new initial condition given by the elastic collision rule; they hold for the three dynamics considered in Eq.(3.1) provided $\alpha_j = 0$ in the second and third case and Λ_r is finite in the first and second cases.

The first difficulty with infinite dynamics is to show that the speeds and the number of particles in a finite region of diameter $r > R_0$ remain finite and bounded in terms of the region diameter (and the initial data) for all times or, at least, for any prefixed time interval.

Therefore we shall suppose that the configurations evolve in time keeping the "same general statistical properties" that certainly occur with probability 1 with respect to the equilibrium distributions or the distributions like μ_0 in Eq.(1.5): *i.e.* density and velocity that grow at most logarithmically with the size of the region in which they are observed, [15, 16] and average kinetic energy, average potential energy, average density having, asymptotically as $\Lambda_r \to \infty$, values $\frac{3}{2}k_B T_j, \delta_j, u_j$ depending only on the thermostats parameters $(\lambda_j, T_j, j > 0)$, see Eq.(1.7).

More precisely let the *local energy* in $\Omega \cap \mathcal{B}(\xi, R)$, $\xi \in \mathbb{R}^3, R > R_0 + r_\varphi$ be

$$W(x; \xi, R) = \sum_{q_i \in \mathbf{X} \cap \mathcal{B}(\xi, R)} \left(\frac{\dot{q}_i^2}{2} + \frac{1}{2}\sum_{j \neq i} \varphi(q_i - q_j) + F r_\varphi \right)$$
$$(3.3)$$

with $F = \max|\partial_q \varphi|$, and its "logarithmic scale" average

$$\mathcal{E}(x) = \sup_{\xi, |\xi| > r_\varphi} \sup_{R > r_\varphi \log \frac{2|\xi|}{r_\varphi}} \frac{W(x; \xi, R)}{R^3} \qquad (3.4)$$

and call $\mathcal{H}_0$ the configurations in $\mathcal{H}$ with

$$\mathcal{E}(x) < \infty \qquad \text{and}$$

$$\lim_{\Lambda_r \to \infty} \frac{N(j, \Lambda_r)}{|\Lambda_r \cap \Omega_j|} = \delta_j, \qquad \lim_{\Lambda_r \to \infty} \frac{U(j, \Lambda_r)}{|\Lambda_r \cap \Omega_j|} = u_j, \quad (3.5)$$

with $\delta_j > 0, u_j$ given by Eq.(1.7), if $N(j, \Lambda_r), U(j, \Lambda_r)$ denote the number of particles and their internal potential energy in $\Omega_j \cap \Lambda_r$).

The set of configurations $x \in \mathcal{H}_0$ has μ_{0,Λ_r}-probability 1, [16].

The discussion in this paper relies on the assumptions 1–3 below, motivated by the partial results in [15, 16], as it will appear shortly. It is to be expected that the probability distributions $\mu^{(\Lambda_r,a,t)}, \mu_t^{(0,t)}$ obtained by the evolution of μ_0 with $S_t^{(\Lambda_r,a)}$, $S_t^{(0)}$ ($a = 0, 1$), and all configurations in $x \in \mathcal{H}_0$ share the following properties.

Local dynamics assumption *With μ_0-probability 1 for for $x \in \mathcal{H}_0$ the number of collisions $\nu(i, t, \Lambda_r, a)$ that the*

i-th particle of $x^{(\Lambda_r,a)}(t')$ has with the containers walls for $0 \le t' \le t$, is bounded uniformly in Λ_r, a, and

(1) there is $B(x,t) > 0$, continuous and non decreasing in $|t|$, such that $\mathcal{E}(x^{(\Lambda_r,a)}(t)) \le B(x,t)$, $a = 0,1$.

(2) The limits $x^{(a)}(t) = \lim_{\Lambda_r \to \infty} x^{(\Lambda_r,a)}(t)$ exist and are in $\mathcal{H}_0$ for all t, with $\mathcal{E}(x^{(0)}(t)) \le B(x,t)$.

(3) $x^{(0)}(t)$ solve the Hamiltonian equations and the latter admit a unique solution in $\mathcal{H}_0$.

Remarks: (a) The limits of $x^{(\Lambda_r,a)}(t)$, as $\Lambda_r \to \infty$, are understood in the sense that for each i the limits $(q_i^{(0,a)}(t), p_i^{(0,a)}(t))$ of $(q_i^{(\Lambda_r,a)}(t), p_i^{(\Lambda_r,a)}(t))$ exist together with their first two derivatives; and $(q_i^{(0,a)}(t), p_i^{(0,a)}(t))$ are twice continuously differentiable in t for each i. It can be shown that, in the Hamiltonian case $a = 0$, the uniform bounds in (2) imply the existence of the limits, however they do not imply that $x^{(0)}(t) \in \mathcal{H}_0$, *i.e.* they do not imply the second of Eq.(3.5).

(b) The number of points of $x^{(\Lambda_r,a)}(t)$, $a = 0,1$, in a ball $\mathcal{B}(R,\xi)$ is bounded by $B(x,t)\,R^3$, for all R,ξ with $R > r_\varphi \log \frac{2|\xi|}{r_\varphi}$ and $|t'| < t$.

(c) The speed of a particle located in $q \in \mathbb{R}^3$ is bounded by $B(x,t)(2\log \frac{2|q|}{r_\varphi})^3$ for $|t'| \le t$.

(d) Comments (b,c) say that locally the particles keep a finite density and reasonable energies and momentum distributions.

(e) An implication is that Eq.(3.2) has a meaning with probability 1 on the choice of the initial data x. It is very important that the assumption that dynamics develops within $\mathcal{H}_0$ implies that at all times Eq.(3.5) will hold with δ_j, u_j *time independent*: physically reflecting the infinite sizes of the thermostats whose density and enegry cannot change in any finite time.

(f) The analysis of the nonequilibrium cases can be partially performed *in similar Hamiltonian cases* as done in the detailed and constructive analysis in Ref. 16, but dropping the requirement in Eq.(3.5).

(g) It seems reasonable that by the method in [16] the restriction of satisfying Eq.(3.5) can be removed in the Hamiltonian model. New ideas seem needed to obtain the local dynamics property in the case of the thermostatted dynamics.

The multipliers α_j are sums of two terms. The first is

$$\frac{|\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)|}{\dot{\mathbf{X}}_j^2} \qquad (3.6)$$

see Eq.(1.4) and the short range of the potential implies that the force $-\partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$ is a sum of contributions bounded by $F \overset{def}{=} \max |\partial \varphi(q)|$ times the number of pairs of particles in the band of width r_φ around the boundary of the container Ω_0 (because, by Eq.(3.5), $\mathcal{E}(x) < +\infty$: this is of order $O((R_0^2 r_\varphi F\delta)^2)$ if δ is an upper bound on the densities near $\partial\Omega_0$. Note that such a bound exists and is time independent, by the local evolution hypothesis (above), but of course it is not uniform in the choice of the initial data x.

Applying Schwartz' inequality $B_1 > 0$ exists with:

$$\frac{|\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)|}{\dot{\mathbf{X}}_j^2} \le B_1 \frac{R_0^2 r_\varphi F \delta}{\sqrt{3N_j k_B T_j \delta'}} \qquad (3.7)$$

for Λ_r large and $\delta' = \min_{j>0} \delta_j$, having used the first of Eq.(3.5).

The second term in α_j, with $\dot{U}_j = U(j, \Lambda_r \cap \Omega_j)$, contributes to the integrals in the exponentials Eq.(3.2) as

$$\int_{t'}^{t} \frac{\dot{U}_j}{2K_j} dt'' \simeq \frac{u_j(t) - u_j(t')}{3k_B T_j} \qquad (3.8)$$

where $u_j(t)$ is the *specific* energy at time t and the $\simeq$ reflects the use of the second equation in Eq.(3.6) to estimate $\frac{U_j}{2K_j}$ as $\frac{U_j}{k_B T_j N(j, \Lambda_r \cap \Omega_j)}$: it means equality up to quantities tending to 0 as $r \to \infty$.

By the above hypothesis the r.h.s tends to 0 as $\Lambda_r \to \infty$ because the configurations (initial and after evolution) are in $\mathcal{H}_0$, hence have the same specific potential energies u_j (by Eq.(3.5), see also comment (e) above)), while the contribution to the argument of the same exponentials from Eq.(3.6) also tends to 1 by Eq.(3.7).

Taking the limit of Eq.(3.2) *at fixed i*, this means that, for initial data in $\mathcal{H}_0$, hence *with μ_0–probability 1*, the limit motion as $\Lambda_r \to \infty$ (with β_j, λ_j, $j > 0$, constant) satisfies Hamilton's equations

$$q_i(t) = q_i + \int_0^t \dot{q}_i(t')dt', \; \dot{q}_i(t) = \dot{q}_i + \int_0^t F_i(t'')dt'' \quad (3.9)$$

and the solution to such equations is unique with probability 1.

The conclusion is that in the thermodynamic limit the thermostatted evolution becomes identical, in any prefixed time interval, to the Hamiltonian evolution on a set of configurations which have probability 1 with respect to the initial distribution μ_0, in spite of the non stationarity of the latter.

In other words. Suppose that the initial data are sampled with the Gibbs distributions of the thermostats particles (with given chemical potentials and temperatures) and with an *arbitrary distribution* for the finite system in Ω_0 (with density with respect to the Liouville volume, for instance with a Gibbs distribution at temperature T_0 and chemical potential λ_0, as in Eq.(1.5)). Then, *in the thermodynamic limit $\Lambda_r \to \infty$, the time evolution is the same* that would be obtained, in the same limit, via a isokinetic thermostat acting in each container $\Omega_j \cap \Lambda_r$ to keep the total kinetic energy constant and equal to $\frac{3}{2}N_j k_B T_j$.

IV. ENTROPY PRODUCTION

It is important to stress that *while, in the thermodynamic limit, the dynamics becomes the same for isoki-*

netic and Hamiltonian thermostats, because the thermo-stat force on each particle tends to 0, *the phase space con-traction in the isokinetic dynamics does not go to zero*, by Eq.(3.7),(3.8). Instead it becomes, up to an additive time derivative, see Eq.(2.1), $\sigma = \sum_{j>0} \frac{Q_j}{k_B T_j}$. This is possible because σ is a sum of many quantities (the α_j's) each of which tends to 0 in the thermodynamic limit while their sum does not.

The interest of the remark is that $\sum_{j>0} \frac{Q_j}{k_B T_j}$ is the natural definition of entropy production in both cases: but in the literature it is often stated (correctly so in the contexts) that entropy production is the phase space contraction, raising eyebrows because the latter vanishes in Hamiltonian models.

However in finite thermostat models the phase space contraction rate depends on the metric used to measure volume in phase space: and it has been stressed that the ambiguity affects the phase space contraction only by an additive quantity which is a time derivative of some function on phase space. Such ambiguity will not affect the fluctuations of the long time averages of the phase space contraction which, therefore, has an intrinsic phys-ical meaning for this purpose, [17].

In both the isokinetic and Hamiltonian cases the above σ (which is, physically, the physical entropy production) differs, by a time derivative $\dot{H}_{tot}$, from

$$\overline{\sigma} = \sum_{j>0} \left(\frac{Q_j}{k_B T_j} - \frac{Q_j}{k_B T_0} \right) - \frac{\mathbf{E}(\mathbf{X}_0) \cdot \dot{\mathbf{X}}_0}{k_B T_0}. \qquad (4.1)$$

The time derivative in question here is the derivative of the total energy $H_{tot} = \beta_0(\sum_{j\geq 0}(K_j(x) + U_j(x)) + \sum_{j>0} U_{0,j}(x))$, [17]. And $\overline{\sigma}$ generates the matter and heat currents, [17].

For this reason the equivalence conjectures, of which the isokinetic-Hamiltonian is a prominent example, see [6], [18, Sec.8],[19],[11, Sec.6],[20],[14, Sec.9.11], to quote a few, are relevant for the theory of transport and es-tablish a connection between the fluctuation dissipation theorem and the fluctuation theorem, [17, 21].

The works [15, 16] bring the present analysis closer to a mathematical proof for repulsive interaction and I hope to show in a future work that they actually lead to a full proof of the locality of the dynamics, at least in dimension $d = 1, 2$, for other thermostat models.

V.   COMPARISON WITH [6] & COMMENTS

(1) Equivalence between different thermostats is widely studied in the literature and it is *surprising* that there are so many questions still raised about the very founda-tions, while little attention is devoted at trying to expand the analysis of the early works. A clear understanding of the problem was already set up in comparing isoki-netic, isoenergetic and Nosé-Hoover bulk thermostats in

[6], where a history of the earlier results is presented as well, see also [22].

(2) Finite thermostats acting on the boundary were stud-ied already in [5], in special cases, and were recognized to be equivalent to thermostats acting on the bulk of the test system. More recently, [23], isokinetic versus isoen-ergetic thermostats equivalence has been analyzed and the splitting of the phase space contraction into an en-tropy part and an "irrelevant" additive time derivative has been first stressed (see also the later [10, 24]) and related to the interpretation and prediction of numerical simulations.

(3) The basic idea in [6] for the equivalence is that the multipliers defining the forces that remove the heat in finite thermostat models have equal average ("equal dis-sipation") in the thermodynamic limit, [6, Eq.(15)]: thus making all evolutions equivalent. In [6] the expectation of observables in two thermostatted evolutions is rep-resented via Dyson's expansion of the respective Liou-ville operators starting from an equilibrium distribution: equivalence follows order by order in the expansion (in the joint thermodynamic limit and infinite time limit) if a mixing property, [6, Eq.(23)], of the evolution with respect to *both* the equilibrium and the stationary dis-tributions is assumed. The method is particularly suit-able for bulk thermostatted systems close to equilibrium where application of Dyson's expansion can be justified, at least in some cases, [25].

(4) The main difference between the present work and [6] is that here, even far out of equilibrium, we discuss equiv-alence between the boundary thermostatted dynamics and Hamiltonian dynamics: therefore we compare a situ-ation in which the average value of the dissipation (ana-logue of [6, Eq.(32)]) is $\neq 0$ with one in which it is 0 exactly, at least formally.

This is achieved by showing that the multipliers in the models in Fig.1 vanish in the thermodynamic limit not only in average but also pointwise with probability 1; this is in agreement with the results in [5] and provides more theoretical grounds to explain them.

It also means that in boundary thermostatted systems the analogue of [6, Eq.(32)] does not tend to 0 when $N \to \infty$ although the analogue of the average of the multipliers, corresponding to [6, Eq.(33)], does.

(5) In bulk thermostatted systems there *cannot be equiva-lence between the Hamiltonian and the isokinetic dynam-ics* in the sense discussed in this paper, *i.e.* identity of the dynamics of individual particles. However, as dis-cussed already in [6], the expectation values of extensive observables could hold. On the other hand the analy-sis in [6] should be extendible to cover also the bound-ary thermostatted systems because, while the dissipation (*i.e.* entropy production) does not vanish in the thermo-dynamic limit, the average of the multipliers still does, see (3) above, and this is what is really needed in [6].

(6) Neither Dyson's expansion convergence questions nor time-mixing properties, on which [6] is based, enter into the present analysis: but the assumptions needed on the

dynamics (local dynamics) are still strong and are only under partial control via the theory in [15, 16].

(7) An important question is whether taking the time $t \to \infty$ limit after the thermodynamic limit $\Lambda_r \to \infty$ (when, therefore, the dynamics are identical) the probability distribution $S_t^{(0)} \mu_0$ tends to a limit μ, and μ still attributes probability 1 to $\mathcal{H}_0$: this is an apparently much harder question related to the difference between the transient results and the, deeper, steady state results, [26].

(8) Finally: the choice, made here, of dimension 3 for the ambient space is not necessary for the analysis. Dimension $d = 1, 2, 3$ would be equally suited. However it is only if the thermostats containers dimension is $d = 3$ that the system with infinite thermostats is expected to reach a stationary state: if $d = 1, 2$ the equalization of the temperatures is expected to spread from the system to the reservoirs and proceed indefinitely tending to establish a constant temperature over larger and larger regions of size growing with a power of time, [27].

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