Frictionless thermostats and intensive constants of motion

G. Gallavotti* and E. Presutti†
* Fisica-INFN Roma 1, † Matematica Roma 2
September 3, 2000

Abstract: Thermostats models in space dimension $d = 1, 2, 3$ for nonequilibrium statistical mechanics are considered and it is shown that, in the thermodynamic limit, the evolutions admit infinitely many constants of motion, namely the intensive observables.

I. THERMOSTATS

Extremal translation invariant DLR distributions, [1] have many constants of motion, among them all intensive observables. In fact the characterizing property of such distributions $\mu$ is that they are time invariant, [2], and since the intensive variables are measurable at infinity, [1], they are $\mu$-almost surely constant and therefore invariant at almost all times. The same property holds for all DLR distributions because they are integrals over the extreme ones.

The space-time invariance is essential: however we shall be interested in models in which such invariance properties are not satisfied, and we want also to check that the intensive variables are constant for all times (not just almost all).

The class of models that we shall investigate is when particles of a test system, in a container $\Omega_0$, and $\nu$ other particles systems, in containers $\Omega_1, \ldots, \Omega_\nu$, interact and define a model of a system in interaction with $\nu$ thermostats, if the particles in $\Omega_1, \ldots, \Omega_\nu$ can be considered at fixed temperatures $T_1, \ldots, T_{\nu}$.

A representation of the system is in Fig.1:

![Fig.1: If $d = 1, 2$ the $1 + \nu$ finite boxes $\Omega_j \cap \Lambda, j = 0, \ldots, \nu$, are marked $C_0, C_1, \ldots, C_\nu$ in the first figure and contain $N_0, N_1, \ldots, N_\nu$ particles, out of the infinitely many particles, with positions and velocities denoted $X_0, \ldots, X_\nu$, and $X_0, \ldots, X_\nu$, respectively, contained in $\Omega_j, j \geq 0$. The second figure illustrates the special geometry that will be considered for $d = 1, 2, 3$: here two thermostats, symbolized by the shaded regions, $\Omega_1, \Omega_2$ occupy half-spaces adjacent to $\Omega_0$.](image)

From the point of view of Physics the temperatures in the thermostats are fixed. A natural model, often invoked in the applications, [3], is to imagine the containers $\Omega_j, j = 1, \ldots, \nu$, as infinite and occupied by particles initially in a Gibbs distribution with given temperatures and densities $T_j, \delta_j, \ldots, T_\nu, \delta_\nu$.

To implement the physical requirement that the thermostats have well defined temperatures and densities the initial data will be imagined to be randomly chosen with a suitable Gibbs distribution.

Initial data: The probability distribution $\mu_0$ for the random choice of initial data will be, if $dx \equiv \prod_{j=0}^{\nu} \frac{dx_j}{N_j}$ the limit as $N \rightarrow \infty$ of the distributions on the configurations $x \in \mathcal{H}(\Lambda)$ with $x_j \in \mathcal{L}$ (see Fig.1),

$$ \mu_0(dx) = \text{const} \exp^{-H_0(x)} dx $$ (1.1)

with $H_0(x) = \sum_{j=0}^{\nu} \beta_j (K_j(x_j) - \lambda_j N_j + U_j(x_j))$ and $\beta_j \equiv \frac{1}{k_B T_j} > 0, \lambda_j \in \mathbb{R}, j > 0$; the values $\beta_0 = \frac{1}{k_B T_0}$, $\lambda_0 \in \mathbb{R}$ will also be fixed.

The values $\beta_0$, $\lambda_0$ bear no particular physical meaning because the test system is kept finite. Here $\Lambda = (\lambda_0, \lambda_1, \ldots, \lambda_\nu)$ and $T = (T_0, T_1, \ldots, T_\nu)$ are fixed chemical potentials and temperatures, and $\mathcal{L}$ is a ball centered at the origin and of radius $r_0$. The $K_j(x_j), U_j(x_j)$ are kinetic and potential energies of the particles in $\Omega_j$ (see below for the conditions on the potentials).

The distribution $\mu_0$ is interpreted as a Gibbs distribution $\mu_0$ obtained by taking the “thermodynamic limit $\Lambda \rightarrow \infty$. If $p_j(\beta, \lambda, \Lambda) \equiv \frac{1}{\beta(\mathcal{L})} \log Z_j(\beta, \lambda)$ with

$$ Z_j(\beta, \lambda) = \sum_{N=0}^{\infty} \frac{\int d\mathcal{L} \exp^{-\beta(\lambda N + K_j(x_N) + U_j(x_N))}}{N!} $$ (1.2)

where the integration is over positions and momenta of the $N$ particles in $\Lambda \cap \Omega_j$ then we shall say that the thermostats have pressures $p_j(\beta_j, \lambda_j)$, densities $\delta_j$, temperatures $T_j$, energy densities $e_j$, and potential energy densities $u_j, f_j > 0$, given by equilibrium thermodynamics, i.e.,

$$ p_j(\beta, \lambda) \equiv \lim_{\Lambda \rightarrow \infty} p_j(\beta_j, \lambda_j, \Lambda) $$

$$ \delta_j = -\frac{\partial p_j(\beta_j, \lambda_j)}{\partial \lambda_j}, \quad k_B T_j = \beta_j^{-1} $$ (1.3)

$$ e_j = -\frac{\partial p_j(\beta_j, \lambda_j)}{\partial \beta_j} - \lambda_j \delta_j, \quad u_j = e_j - \frac{d}{2} \delta_j \beta_j $$

which are the relations linking density $\delta_j$, temperature $T_j = (k_B \beta_j)^{-1}$, energy density $e_j$ and potential energy density $u_j$ in a grand canonical ensemble and in absence of phase transitions in correspondence of the parameters $(\beta_j, \lambda_j)$, for $j > 0$.

Remark: (1) notice that the limit defining $p_j$ does not depend on the shape of $\Omega_j$ and coincides with the usual definition of pressure in the thermodynamic limit in the sense of Van Hove, [4].

(2) An alternative definition of density, energy density and temperature could be
\[
\lim_{n \to \infty} \left( \frac{N_{j,\lambda_n}(x)}{|\Omega_n \cap \Omega_j|} \right) U_{j,\lambda_n}(x) \frac{K_{j,\lambda_n}(x)}{N_{j,\lambda_n}(x)} \right) (1.4)
\]
provided the limit exists with \( \mu_0 \)-probability 1 and is \( x \)-independent.

(3) The limits in Eq. (1.4) will exist and be equal to the values in Eq. (1.3) with \( \mu_0 \)-probability 1 if the hypotheses below hold. This is part of the result of theorem 1.

**Hypotheses:** In the geometries of Fig.1 suppose:

(1) \( \mu_0 \) satisfies the DLR equations and that

(2) the thermostats pressures \( p_j(\beta, \lambda) \) are differentiable in \( \beta, \lambda \) at \( \beta_j, \lambda_j, j = 1, \ldots, \nu \).

It is essential that the “macroscopic” property of the thermostats, of having given densities and temperatures, remains when the system evolves in time.

Evolution is defined via equations of motion: since we are dealing with infinitely many particles it will be defined by first considering the motion of the particles initially contained in some ball \( \Lambda \) keeping the particles outside \( \Lambda \) fixed. Such motion \( x \to S(\lambda)x \) is called \( \Lambda \)-regularized. Then we consider the limit as \( \lambda \to \infty \).

The regularization boxes \( \Lambda \) will be for simplicity) balls \( \Lambda_n \) centered at the origin \( O \) and with radius \( 2^n r_\varphi \), with \( r_\varphi \) equal to the range of the interparticle potential, and particles will be reflected at the boundary of \( \Lambda_n \). The limit motion reached as \( n \to \infty \) will define the thermodynamic limit motion.

The \( \Lambda_n \)-regularized equations of motion will be

\[
m_\varphi \ddot{x}_i = -\partial_i U_0(x_0) - \sum_{j>0} \partial_i U_{0,j}(x_0, x_j) + \Phi_i(x_0)
\]

\[
m_\varphi \ddot{x}_j = -\partial_j U_j(x_j) - \partial_i U_{0,j}(x_0, x_j)
\]
(1.5)

(see Fig.1) where:

(1) the first label, \( j = 0 \) or \( j = 1, \ldots, \nu \), refers (respectively) to the test system or to a thermostat, while the second indicates the derivatives with respect to the coordinates of the points located in the corresponding container and in the regularization box \( \Lambda_n \) (hence the labels \( i \) in the subscripts (\( j, i \)) have \( Nj ;) \) values).

(2) The forces \( \Phi(X_0) \) are, positional, nonconservative, smooth stirring forces, possibly vanishing; the other forces are conservative and generated by a pair potential \( \varphi \), with range \( r_\varphi \), which couples all pairs in the same containers and all pairs of particles one of which is located in \( \Omega_0 \) and the other in \( \Omega_j \) (i.e., there is no direct interaction between the different thermostats).

(3) Furthermore particles are repelled by the boundaries of the containers by a conservative force of potential energy \( \psi \), diverging with the distance \( r \) to the walls as \( r^{-\alpha} \), for some \( \alpha > 0 \), and of range \( r_\psi \ll r_\varphi \). The potential energies will be \( U_j(x_j), j \geq 0 \), and \( U_{0,j}(x_0, x_j) \), respectively denoting the internal energies of the various systems and the potential energy of interaction between the test system and the thermostats:

\[
U_j(x_j) = \sum_{q \in X_j} \psi(q) + \sum_{(q, q') \in \mathcal{E}_j, \psi' \in \mathcal{\Phi}} \varphi(q - q')
\]

\[
U_{0,j}(x_0, x_j) = \sum_{q \in X_n, q' \in X_j} \varphi(q - q')
\]

(1.6)
The potentials \( \varphi, \psi \) have been chosen \( j \)-independent for simplicity.

(4) The equations are formally defined also in the phase space \( \mathcal{H} \) of the locally finite configurations \( x = (\ldots, q_i, \ldots) \to \infty \quad i=1 \)

\[
x = (x_0, x_0, x_1, \ldots, x_n, x_n) = (X, X)
\]
(1.7)
with \( X_j \subset \Omega_j \), hence \( X \subset \Omega = U_{x=0} \Omega_j, \) and \( \Omega_i \in \mathbb{R}^4 \), in every ball \( \Sigma(x) \) of radius \( x \) and center at the origin \( O \), fall a finite number of points of \( X \).

Infinite systems are idealizations not uncommon in statistical mechanics. But we take it for granted that they must be considered as limiting cases of large yet finite systems. This leads to several difficulties: one is immediately manifest if one remarks that the equations of motion Eq. (1.5) do not even admit an obvious solution in \( \mathcal{H} \).

Dynamics is well defined with \( \mu_0 \)-probability 1 because if \( d = 1, 2, 3 \), the \( \Lambda_n \)-regularized equations with data \( x \) admit, with \( \mu_0 \)-probability 1, a limit \( S_{x, t} \in \mathcal{H} \),

\[
\lim_{n \to \infty} S_{\Lambda_n, t}(x) = S_{\Lambda_n, t}(x) \quad \text{for } t > 0; \quad \text{a precise statement is in theorem 4 below (proved in [5, theorems 6, 7], for } d = 1, 2, \text{ and in } [6, \text{ Theorem 1]} \text{ for } d = 1, 2, 3).
\]

Since the Eq. (1.5) are Newton’s equations we shall call the model a frictionless thermostats model.

An important question is whether time evolution changes the configuration \( x \) into \( S_{x, t} \) but keeps the temperatures and densities of the thermostats constant at least with \( \mu_0 \)-probability 1 and for any finite time. This is part of the more general question whether the spatial average of an intensive observable remains constant in time.

A simple, partial but quantitative formulation is in terms of the number \( N_{j,\lambda}(S_{x, t}) \) of particles of \( S_{x, t} \), of the kinetic energy \( K_{j,\lambda}(S_{x, t}) \) and of the potential energy \( U_{j,\lambda}(S_{x, t}) \) of the configuration \( S_{x, t} \) into which \( x \) evolves at time \( t \), inside a ball \( \Lambda \) centered at the origin. Consider, then, \( \forall j > 0 \), the limits (if existent)

\[
\lim_{n \to \infty} \left( \frac{N_{j,\lambda_n}(S_{x, t})}{|\Omega_n \cap \Omega_j|} \right) U_{j,\lambda_n}(S_{x, t}) K_{j,\lambda_n}(S_{x, t})
\]
(1.8)

Under the above “no phase transition” assumption on \( \mu_0 \) we shall prove:

**Theorem 1:** The limits in Eq. (1.8) exist with \( \mu_0 \)-probability 1 for all times and are time independent. The limits will be respectively \( \delta_j, u_j \) and \( \Phi_j k_B T_j \) with \( \mu_0 \)-probability 1, as in Eq. (1.3).
II. INTENSIVE OBSERVABLES

The definition of an $h_T$-particles intensive observable is in terms of a smooth function $\Gamma(q_1, q_2, \ldots, X)$ on $R^{2d_T}$ vanishing for $h \neq h_T$ and which is “translation invariant”, and with “short range” $r_T$.

This means that $\Gamma = 0$ if the diameter of $X = (q_1, \ldots, q_k)$ exceeds some $r_T > 0$ and, denoting by $\tau_X(X)$ the configuration $(q_1 + \xi, q_2 + \xi, \ldots, q_k + \xi)$, it is $\Gamma(\tau_X(X)) = \Gamma(X, X)$, $\forall \xi \in \mathbb{R}^d$.

Given a region $W$ the function $G_W$ of $x = (X, Y)$

$$G_W(x) \overset{def}{=} \sum_{Y \in \mathbb{R}^d} \Gamma(Y, Y)$$

defines a “local observable” in $W \subset R^d$ with potential $\Gamma$.

We shall say that $G_W$ is an observable of potential type if $\Gamma(Y, Y)$ depends only on $Y$, while if it depends only on $Y$ it will be called of kinetic type.

Then, if $V_n \overset{def}{=} \Omega_j \cap \Lambda_n$, $|V_n| \overset{def}{=} \text{volume}(V_n)$.

Definition 1: The “local average” of $\Gamma$ on the configuration $x = (X, Y)$ is $|V_n|^{-1} \Gamma_V(x)$. The corresponding “intensive observable” in the $j$-th thermostat is

$$g_j(x) \overset{def}{=} \lim_{n \to \infty} \frac{1}{|V_n|} \Gamma_V(x),$$

if the limit exists. Furthermore, given $\mu_0$, define the “intensive fluctuation” of $G$ (in the $j$-th thermostat)

$$\Delta g_j(x) \overset{def}{=} \lim_{n \to \infty} \left( \frac{1}{|V_n|} - \mu_0 \right) \Gamma_V(x),$$

if the limit exists.

Remark: The notation requires keeping in mind that $G_V$ depends also on $j$ (because $V_n = \Omega_j \cap \Lambda_n$); however for simplicity of notation the labels $j$ on $V_n$ and $G_V$ will not be marked.

Properties of intensive observables can be derived from various assumptions on the initial distributions of the particles in the various regions $\Omega_j$ which, we recall, are distributed independently over $j = 1, \ldots, \nu$ and depend on the $\nu$ pairs of parameters $\beta_j, \lambda_j$.

The simplest assumption is perhaps the uniqueness of the tangent plane to the graph of the pressure in various directions, which could for instance be insured by the uniqueness of the translation invariant states of our particles system with parameters $\beta_j, \lambda_j$.

Let $G$ be an observable of potential or kinetic type; and suppose that $H_{\Omega, \lambda}(x) \overset{def}{=} H_{\Omega, \lambda}(x) + \theta G(x)$ is super-perfect for $|\theta| < \text{small enough}$ (i.e. there exist constants $\alpha > 0, b > 0$ such that for all $\lambda > |\alpha - bN|$, $H_{\Omega, \lambda}(x) \geq \alpha N^2/|\lambda - bN|$ for all configurations $x = (X, X)$ for $N$ particles and with $X \in \Lambda$ and $\forall |\theta| \leq \theta_b$ for some $\theta_b > 0$.

We call $G$ an “allowed observable”. For such observables it is possible to define, for $|\theta|$ small, the “pressure”

$$P(\theta) = \lim_{\lambda \to \infty} \frac{1}{|V_n|} \log \frac{Z_\theta(\lambda)}{Z_\theta(0)},$$

with $Z_\theta(\lambda)$ given by Eq.(1.2) with the energy $\theta G(x)$ added in the exponential. It is $P(\theta) = 0$.

It is important to stress that $P(\theta)$ is, in the geometry in Fig.1 considered here, independent of the special geometry considered for the $\Omega_j$ as long as the conical containers have $d$-dimensional shape (i.e. they contain balls of arbitrary large radius).

In this context we can derive the following result:

Theorem 2: Let $G$ be an allowed observable of potential or kinetic type. If $P(\theta)$ is differentiable at $\theta = 0$, then with $\mu_0$-probability 1 the limit as $|V_n| \to \infty$ of $\frac{1}{V_n} G_V(Sx)$ exists $\mu_0$-almost everywhere and is $t$-independent.

Remarks: (1) The differentiability assumption of $P(\theta)$ has the meaning of uniqueness of the tangent plane to the graph of the pressure $p$ “in the direction of $G$”; such uniqueness is a “generic” property, see [7] for the lattice case.

(2) The super-stability of $H_{\Omega, \lambda}(x) + \theta G(x)$ is a very strong condition: it is certainly satisfied if

(i) $\Gamma(X, X) = 1$ for $|X| = 1$ and 0 otherwise, or if

(ii) $\Gamma(X, X) = \frac{1}{2} q^2$ for $|X| = 1$ and 0 otherwise, or if

(iii) $\Gamma(X, X) = 0$ unless $X = (q, q')$ and in such case

$\Gamma(q, q') = \varphi(q - q')$,

then theorem 1 is a corollary of theorem 2.

We also expect that the intensive observables will have very small probability of being appreciably different from their average values, and precisely a probability bounded above by an exponential of the volume $|\Omega_n|$. This will mean that the observable $G$ satisfies a kind of large deviations property.

Theorem 3: Under the assumptions of theorem 2 the $\mu_0$-probability that the fluctuation $\Delta G_{\Omega, \lambda}(Sx)$ differs
from 0 by more than $\varepsilon > 0$ tends to 0 exponentially fast in $\|v_n\|$ as $n \to \infty$, $\forall \varepsilon > 0$.

Remark: The assumptions in theorems 2,3 are satisfied by many observables in the Mayer expansion convergence region in the plane $\lambda_j, \beta_j$. [8]. They are also believed to be satisfied quite generally for observables generated by a potential $\Gamma$. In particular they hold generically if $\Gamma$ is a linear combination of the potentials (i),(ii),(iii) in remark (2) above.

The proof of theorems 2,3 are presented in Sec.IV.

III. TIME EVOLUTION

A quantitative existence theorem of the dynamics can be conveniently formulated in terms of the quantities $v_1 \overset{d.f.}{=} \sqrt{2\varphi(0)/m}, r_\phi$ and $W, N, v_1, \|x_1\|$ defined as

$$
W(x, \xi, R) \overset{d.f.}{=} \frac{1}{\varphi(0)} \sum_{\xi \in \Omega(R)} \left( \frac{\eta_{\xi}(2)}{2} \right) + \frac{1}{2} \sum_{j \neq i} \phi(q_j - q_j) + \psi(q_i) + \varphi(0), \quad (3.1)
$$

$$
N_\xi(x) \overset{d.f.}{=} \text{number particles within } \xi \text{ of } \xi \in \mathbb{R}^d,
$$

$$
\|x_i - x_j\| \overset{d.f.}{=} \|q_i - q_j\|/v_1 + \|q_i - q_j\|/r_\phi
$$

Let $\log_{+}z \overset{d.f.}{=} \max(\log z), g_\xi(z) = (\log_{+}z)^\xi$ and

$$
E_\xi(z) \overset{d.f.}{=} \sup_{\xi} \sup_{R > z} \frac{W(x, \xi, R)}{R^d}. \quad (3.2)
$$

Call $H_\xi$ the configurations in $H$ with

1. $E_\xi(x) < \infty$
2. $N(j, \lambda_n) \overset{d.f.}{=} \frac{U(j, \lambda_n)}{\lambda_n} \frac{K(j, \lambda_n)}{\lambda_n \cap \Omega_j} \frac{\lambda_n \cap \Omega_j}{n \rightarrow \lambda_n} \delta_{j, u_j} \frac{d\delta_j}{2\beta_j}$

with $\lambda_n$ the ball centered at the origin of radius $2n r_\phi \delta_{j, u_j}$, given by Eq.(1.8) if $N(j, \lambda_n), U(j, \lambda_n), K(j, \lambda_n)$ denote the number of particles and their internal potential or kinetic energy in $\Omega_j \cap \lambda_n$, each set $H_\xi$ has $\mu_0$-probability 1 for $\zeta \geq 1/\delta$, [2, 9-11].

Theorem 4: Let $d = 3$, then $H_{1/d}$ has $\mu_0$-probability 1 and $\forall \xi \in \mathbb{R}$ exists for $\mu_0$-almost all $x \in H_{1/d}$ and $\forall t \geq 0$.

Given (arbitrarily) a time $\Theta > 0$, if $E \overset{d.f.}{=} E_{1/d}(x)$, and $|q_0| \leq 2^k r_\phi$, there exist $c = c(E, \Theta) \leq c = c(E, \Theta) > 0$ such that $\forall n \geq k$ and $\forall t \leq \Theta$

$$
|q_0(t)| \leq c v_1 k^2,
$$

distance($q_0(t), \partial(\cup_j \Omega_j)) \geq c r_\phi k^{-\delta}

$$
N_\xi(Sx) \overset{d.f.}{=} c k^{1/2}
$$

$$
\|Sx_i - (S^{(n)}x)_i\| \leq e^{-c^{2n^{2/2}}, n > k.}
$$

This is proved in [5, theorem 7] for $d = 2$ and in [6] for $d = 3$ (the latter reference covers also the case $d = 2$ via a somewhat different approach).

Remark that the theorem does not state that the second of Eq.(3.3) holds; in [5, 6] it is however proved, in addition to theorem 4, the weaker statement that the limit of $K_{j, \lambda_n}(Sx)$ is not smaller than $1/\pi$ of the corresponding r.h.s.; and the same is true for the other two quantities in Eq.(3.3).

A corollary of the main results of this paper will be that the limit relations in Eq.(3.3) will hold for all $t > 0$.

IV. CONSTANTS OF MOTION

Let $\Gamma$ be an $h$-points local observable of potential type, $V_n = \Omega_j \cap \lambda_n$. Under the assumptions of theorem 2 we first show that $\lim_{n \rightarrow \infty} |V_n|^{-1} \langle \frac{\partial G_\lambda}{\partial \lambda} \rangle_{\mu_0} = g$ exists.

Define $P_n(\theta) \overset{d.f.}{=} \frac{1}{|\xi|} \log \langle e^{-G(V_n)} \rangle_{\mu_0}$; this is smooth and convex in $\theta$ and its unique derivative at $\theta = 0$ is $g_0 \overset{d.f.}{=} \frac{1}{|\xi|} \frac{\partial G(V_n)}{\partial \lambda}$; therefore, remarking that $P(0) = 0$, it satisfies $P_n(\theta) \geq \theta g_0$

The limit $P(\theta)$ as $n \rightarrow \infty$ of $P_n(\theta)$ is the same that would be obtained if $V_n$ was replaced by the full ball $\lambda_n$ and filled with particles at temperature $\beta_j$ and chemical potential $\lambda_j$.

Any convergent subsequence $g_{n_0}$ defines therefore a coefficient $g$ with the property $P(\theta) \geq \theta g$. Hence, by the assumed uniqueness of the tangent to $P(\theta)$ at $\theta = 0$, it follows that $g$ is uniquely determined thus implying that the limit $g \overset{d.f.}{=} \lim_{n \rightarrow \infty} g_{n_0}$ exists.

Let $g = \langle |V_n|^{-1} G_{\lambda_n} \rangle_{\mu_0}$ and, given $\gamma > 0$, let $N_{E, \gamma, n}$ to be the set of points in $H_{1/d}$ with $E(x) \leq E, G_{\lambda_n}(x) < (g + \gamma)|V_n|$ and which, under the evolution, reach in a time $T_{E, \gamma, n} \leq \Theta$ and for the first time, a point of the surface

$$
S_{E, \gamma, n} \overset{d.f.}{=} \{ x | |V_n|^{-1} G_{\lambda_n}(x) = (g + \gamma) \}. \quad (4.1)
$$

If for all $E$ and for all small $\gamma > 0$ it is $\sum_{j, \cdots, E(x), \gamma, n} \mu_0(X_{E, \gamma, n}) < +\infty$ then it will be $\lim_{n \rightarrow \infty} |V_n|^{-1} G_{\lambda_n}(Sx) \leq g$, with $\mu_0$-probability 1 (by Borel–Cantelli’s estimate), changing $\Gamma$ into $-\Gamma$ it will follow, again with $\mu_0$-probability 1, that the limit is $\geq g$; notice that the change in sign of $\Gamma$ is possible by the condition on $G$ to be an “allowed observable”, as introduced before Eq.(2.4).

This remains true if for all small $\gamma$ there is $\gamma_0 \in [\gamma, 2\gamma]$ such that $\sum_{j, \cdots, E(x), \gamma, n} \mu_0(X_{E, \gamma, n}) < +\infty$.

If $x \in N_{E, \gamma, n}$ the phase space contraction, when phase space volume is measured by $\mu_0$, within time $t$ is [5, 6],

$$
s(x, t) = \int_0^t \left( \sum_{j \geq 0} \beta_j Q_j(\tau) + \beta_0 L_0(\tau) \right) d\tau \quad (4.2)
$$
where \( Q_j(t) \stackrel{def}{=} \mathbf{X}_j(t) \cdot \mathbf{F}_j \), \( L_0(t) \stackrel{def}{=} \mathbf{X}_0 \cdot \mathbf{\Phi}(\mathbf{X}_0(t)) \).

By theorem 4, \( L_0(t) \) is uniformly bounded as \( n \to \infty \), for \( 0 \leq t \leq \Theta \), by the first of Eq. (3.2), by a quantity \( C \) (only depending on \( E, m, \theta \)).

Therefore by a quasi-invariance lemma, \([2, 12], [3, Appendix H]\), \( \mu_0(\mathcal{X}_{E, \gamma, n}) \) can be bounded \( \forall \varepsilon \in [\gamma, 2\gamma] \) by

\[
C \int \mu_0(dx) \left| \frac{\dot{G} \alpha_n(x)}{V_n} \right| (g_n + \gamma + \varepsilon) \tag{4.3}
\]

where \( \dot{G} \) denotes the time derivative (at \( t = 0 \)) of \( G_{\alpha_n}(s, x) \) (to be computed via the equations of motion) evaluated on the surface \( \Sigma_{\gamma, n} \), see Eq. (4.1).

Integrating Eq. (4.3) over \( d\gamma \), \( \mu_0(\mathcal{X}_{E, n, \gamma}) \) can be bounded by

\[
\frac{C}{\gamma} \int \mu_0(dx) \left| \frac{\dot{G} \alpha_n(x)}{V_n} \right| (\gamma \leq \frac{G_{\alpha_n}(x)}{V_n} - g_n \leq 2\gamma), \tag{4.4}
\]

with \( \dot{G} = \sum_{X \in \Sigma} \sum_{q \in \mathbb{Q}} \partial \Gamma(X) \dot{q} \). By Schwartz' inequality

\[
C_2\gamma^{-1} \mu_0 \left( \{ x : \gamma \leq \frac{G_{\alpha_n}(x)}{V_n} - g_n \leq 2\gamma \} \right)^{1/2} \tag{4.5}
\]

because from Eq. (2.1) for \( \Gamma \)

\[
\mu_0(\mathcal{G}_{\gamma}^{1/2}) \leq C_1[V_n] \tag{4.6}
\]

obtained via superstability bounds, using the Maxwellian distribution for \( q \).

The probability in Eq. (4.5) is bounded above by Chebishev inequalities (quadratic or exponential) by both averages

\[
J \stackrel{def}{=} \frac{(G_{\alpha_n}(x)/V_n - g_n)^2}{\gamma^2}, \tag{4.7}
\]

\[
I_\theta \stackrel{def}{=} \left( e^{(G_{\alpha_n}(x)/V_n - y_n + \gamma)} \right)_{\mu_0}
\]

\( \forall \theta \geq 0 \). This implies the existence of \( \gamma_n \in [\gamma, 2\gamma] \) with

\[
\mu_0(\mathcal{X}_{E, n, \gamma_n}) \leq C \gamma^{-1} J(n) \tag{4.8}
\]

Therefore we look for assumptions on the thermostats structure (i.e. on \( \lambda_j, \beta_j, \varphi \)) under which \( J(n) \) tends to zero fast enough making \( \sum_{n} \mu_0(\mathcal{X}_{E, n, \gamma_n}) < \infty \). In this case theorem 2 will follow from Borel-Cantelli’s lemma and the arbitrariness of \( \gamma \).

As a consequence of the above bounds, basically following from the uniqueness of the tangent plane in the direction \( \Gamma \), the proof of theorem 2 can be completed as follows. Fix \( \gamma > 0 \) and remark that

\[
I_\theta = \left( e^{(G_{\alpha_n}(x)/V_n - y_n + \gamma)} \right)_{\mu_0} e^{-\gamma} \leq e^{-\gamma} \tag{4.9}
\]

Continuing the argument leading to the existence of the limit of \( g_n \), at the beginning of the section, the correction term \( \eta_{\theta}(\mathbf{V}_n) \) is bounded, as follows:

(a) \( \frac{1}{\mathcal{P}} \log \left( e^{(G_{\alpha_n}(x)/V_n - y_n + \gamma)} \right)_{\mu_0} = P_0(\theta) - P_0(0) \) (notice: \( P_0(0) \equiv 0 \)) and converges to \( P(\theta) - P(0) \) as \( n \to \infty \) for \( |\theta| \leq \theta_0 \), if \( \theta_0 \) is small enough so that the potential \( \phi + \beta^2 \gamma \theta \) is superstable \( \forall \theta \leq \theta_0 \), \( j = 1, \ldots, \nu \). By superstability the limit exists for \( |\theta| \leq \theta_0 \) and it is a limit of functions \( P_0(\theta) \) which are convex for \( |\theta| \leq \theta_0 \). Hence the limit is uniform: \( |P(\theta) - P_n(\theta)| \leq \alpha(\mathbf{V}_n) \) for \( |\theta| \leq \theta_0 \).

(b) The \( g_n \) in the exponent in Eq. (4.7) has just been shown to be \( g_n[V_n] \equiv g[V_n] + \alpha(\mathbf{V}_n) \), so that \( -\theta g_n \) converges to \( -\theta g \) with an error \( \alpha(\mathbf{V}_n) \).

(c) \( P(\theta) - P(0) - \theta g \) \( V_n \) is (by the uniqueness of the tangent plane) \( \alpha(\mathbf{V}_n) \). Hence

\[
\eta_{\theta}(\mathbf{V}_n) - \gamma_n = \frac{1}{2} \eta_{\theta_n}(\mathbf{V}_n) \tag{4.10}
\]

and choosing \( \theta_n \) tending to 0 so slowly that the exponent of the l.h.s. of (4.9) tends rapidly to 0, for instance if \( \theta_n = \max\left( \frac{1}{\mathcal{P}}, \frac{1}{C(\mathcal{P})} \right) \), we see that \( I_{\theta_n} \to 0 \) so fast that \( \mu_0(\mathcal{X}_{E, \gamma, \gamma_n}) \) is summable in \( n \) implying theorem 2 and of its special case theorem 1.

Theorem 3 also follows from the existence of the limit for \( g_n \) because \( I_\theta \) yields a summable bound on \( J \), hence on \( \mu_0(\mathcal{X}_{E, \gamma, \gamma}) \).

Remarks: (1) Uniqueness of the tangent plane can be replaced by assumptions on the decays of correlations in the distribution \( \mu_0 \) somewhat stronger than just requiring its extremality among the DLR distributions in the geometry in Fig. 1.

(2) Sufficient estimates can be formulated as follows:

\[
\mu_0(\mathcal{X}_{E, \gamma, \gamma_n}) \leq C \gamma^{-1} J(n) \tag{4.8}
\]

\[
|\rho_j(x_1, \ldots, x_n; \tau_1y_1, \ldots, \tau_0y_0) - \rho_j(x_1, \ldots, x_n; \tau_0y_1, \ldots, \tau_0y_0)|_{\gamma \to 0} \tag{4.11}
\]

Assume that Eq. (4.11) holds in the stronger sense that the l.h.s. is bounded by \( \eta_{\mathbf{r}, m,n}(\varepsilon) \) if the positions of \( x_1, \ldots, x_n \) and \( y_1, \ldots, y_m \) can be enclosed in a ball of radius \( R \).

Theorem 5: If there is a constant \( C_{R,m,n} \) such that \( \eta_{\mathbf{r}, m,n}(\varepsilon) \leq C_{R,m,n} |\varepsilon|^{-a(R,m,n)} \) with \( a(R, m, n) > 0 \) and if \( \lim_{\lambda \to \infty} \frac{\mathcal{P}}{\mu_0(\mathcal{G}_{\lambda})} = g \) exists, then \( \lim_{\lambda \to \infty} \).
\(\Delta G_{V_\lambda}(x) = 0\) and \(\lim_{\lambda \to 0} \frac{1}{\lambda} G_{V_\lambda}(S_\lambda x) = g\) with \(\mu_0\) probability 1.

Remarks: (1) Thus if \(\mu_0\) has a power law cluster property all intensive observables admitting an average value, over space translations, at time 0 are constants of motion. (2) With the above assumptions we avoid use of the exponential Chebyshev inequality and we may thus drop the superstability condition in the definition of the potential \(\Gamma\). We could actually consider more general observables of the form \(f(x)\)

\[
\lim_{n \to \infty} \frac{1}{|\Omega_n|} \int_{\Omega_n} f(x) \, dx \quad (4.12)
\]

where \(f\) is a cylindrical function in \(\Delta\) (i.e. it does not depend on the particles outside \(\Delta\)) and \(\tau_r\) denotes translation by \(r\). If the power law cluster property is satisfied and \(\mu_0\) a.s. the limit in (4.12) exists at time 0, then the intensive observables \((4.12)\) are constant of motion under the assumption that \(f\) is smooth and grows at most polynomially with the number of particles.

Theorem 3. The assumption certainly holds in the cluster expansion convergence region, [4] and [13, Sec. 5.9], i.e. high temperature and low density, without extra assumptions.

Proof: Consider the first of Eq. (4.7) and choose \(\gamma = \gamma_n = \frac{1}{n}.\) The numerator tends to 0 as \(|\lambda_k|^{-a(R_n, t_n)} \frac{|\lambda_k|^{a}}{|\lambda_k|} \) if the potential \(\Gamma\) for the observable \(G_{V_\lambda}\) vanishes when the diameter of the set \(\{x_1, \ldots, x_n\}\) exceeds \(R\).

The estimate Eq. (4.8) implies that \(\lim_{n \to \infty} \frac{1}{|\Omega_n|} \Delta G_{V_\lambda}(S_\lambda x)\) tends to 0 with \(\mu_0\)-probability 1 for all \(t \leq k_0\) with \(k\) integer and \(k_0 > 0\) (arbitrarily fixed). Hence if the average \(\lim_{n \to \infty} \frac{1}{|\Omega_n|} G_{V_\lambda}(S_\lambda x)\) exists for all times and has a time-independent value.

V. ENTROPY AND THERMOSTATS

Entropy production per unit time is defined in terms of

\(Q_j = -\frac{d}{dt} \int \mathcal{L}_{x_j} U_0(x_j, X_0, X, x_j)\),

which is the work per unit time, performed by the test system on the \(j\)-th thermostat. Since \(Q_j\) is interpreted as the heat ceded by the system to the thermostat the entropy production in the configuration \(x\) is given by

\[
\sigma_0(x) = \sum_{j>0} \beta_j Q_j(x).
\]

If the volumes in phase space are measured by the distribution \(\mu_0\) this quantity differs from the contraction rate of the phase space volume by \(\beta_0 (Q_0 + U_0) \equiv \beta_0 (K_0 + U_0)\) and \(K_0 + U_0\) is expected to stay uniformly finite in time. If the statistics of the long time averages of the phase space contraction rate and of the entropy production rate will coincide (however this is not proved as the theorems above only concern what happens in an arbitrary prefixed but finite time interval).

In other words in the fractionless thermostat model and in the isoenergetic thermostat models, \([8]\), the entropy production can be identifed, possibly up to a time-derviative of a quantity expected to be uniformly finite in time, with the phase space contraction. Furthermore the entropy production is the same in both models of thermostats if the thermodynamic parameters of the thermostats \((\beta_j, T_j, j > 0)\) are the same: this follows from the equivalence theorem between fractionless and isoenergetic thermostats, \([8, \text{theorem 1}]\), which states that under such conditions the microscopic motions of the two models starting from the same initial condition remain identical forever with \(\mu_0\)-probability 1.

Other thermostats can be considered: for instance the isokinetic thermostats. At a heuristic level analogous conclusions can be reached, \([14]\).

\[\text{[14]} \ G. Gallavotti. On thermostats: Isokinetic or Hamiltonian? finite or infinite? Chaos, 19:013101 (+7), 2008.\]