Frictionless thermostats and intensive constants of motion

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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

Systems in nonequilibrium statistical mechanics have to be thermostatted, and the most realistic thermostats are infinite (i.e., very large) systems initially in equilibrium. The present paper discusses a small (classical) system interacting with fairly realistic infinite (classical) thermostats of dimension $d = 1, 2, 3$. This can be attacked via recent difficult results on the time evolution of infinite systems in dimension $d = 1, 2, 3$. It is assumed that the initial equilibrium states of the thermostats are away from phase transitions. Some technical assumptions on the interactions are also made. The result obtained here may then be expressed physically as follows: at any finite time each thermostat remains close to equilibrium in the sense that its global temperature remains the same, and this is also true for other intensive thermodynamic variables. If an infinite time limit were taken the situation would probably be quite different (and nontrivial only in dimension $d = 3$) but this is a hard problem, and not tackled in the present paper.

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 $\Omega_1, ..., \Omega_\nu$, interact and define a model of a system in interaction with $\nu$ thermostats, if the particles in $\Omega_1, ..., \Omega_\nu$ can be considered at fixed temperatures $T_1, ..., T_\nu$.

A representation of the system is in Fig.1:

![Diagram](image)

Fig.1: If $d = 1, 2$ the 1 + $\nu$ finite boxes $\Omega_j \cap \Lambda$, $j = 0, ..., \nu$, are marked $C_0, C_1, ..., C_\nu$ in the first figure and contain $N_0, N_1, ..., N_\nu$ particles, out of the infinitely many particles, with positions and velocities denoted $X_0, X_1, ..., X_\nu$, and $X_0, X_1, ..., X_\nu$, 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 $\Omega_0$.

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

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 $dx \equiv \prod_{j=0}^\nu dX_j / N_j!$, the limit as $\Lambda \to \infty$ of the distributions on the configurations $x \in \mathcal{H}(\Lambda)$ with $X_j \in \Lambda$ (see Fig.1),

$$\mu_0(\mathcal{X}) = \text{const} \, e^{-H_0(x)} \, dx \quad (1.1)$$

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

The values $\beta_0, \lambda_0$ bear no particular physical meaning because the test system is kept finite. Here $\Lambda = (\lambda_0, \lambda_1, ..., \lambda_\nu)$ and $T = (T_0, T_1, ..., T_\nu)$ are fixed chemical potentials and temperatures, and $\Lambda$ 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” $\Lambda \to \infty$. At time 0 we switch on the interaction between the particles in $\Omega_0$ and those in the thermostats $\Omega_j, j > 0$. The measure $\mu_0$ is not time invariant under the corresponding dynamics (existence of dynamics in infinite systems is not at all a trivial issue, as already revealed by the theory of the evolution in the infinite space [2] and as it will be discussed later) and we need to:

(i) define the temperatures of the thermostats (which are outside equilibrium);

(ii) prove that the “macroscopic” property of the thermostats of having given densities and temperatures remains when the system evolves in time.

If $p_j(\beta, \lambda; \Lambda) \equiv \frac{1}{\beta |\Omega_j \cap \Lambda|} \log Z_j(\beta, \lambda)$ with

$$Z_j(\beta, \lambda) = \sum_{N=0}^\infty \int \frac{dx_N}{N!} e^{-\beta(\lambda N + K_j(x_N) + U_j(x_N))} \quad (1.2)$$

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

$$p_j(\beta, \lambda) \equiv \lim_{\Lambda \to \infty} p_j(\beta_j, \lambda_j, \Lambda)$$
\[
\delta_j = -\frac{\partial p_j(\beta_j, \lambda_j)}{\partial \lambda_j}, \quad k_B T_j = \beta_j^{-1}
\]
\[
e_j = -\frac{\partial p_j(\beta_j, \lambda_j)}{\partial \beta_j} - \lambda_j \delta_j, \quad u_j = e_j - \frac{d}{2} \delta_j^{-1}
\]

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, [3].

(2) As usual in Physics we could define density, energy density and temperatures in single configurations \(x\) as

\[
\lim_{n \to \infty} \left( \frac{N_j, \Lambda_n(x)}{[\Lambda_n \cap \Omega_j]} \right) \left( \frac{U_j, \Lambda_n(x)}{[\Lambda_n \cap \Omega_j]} \right) \left( \frac{K_j, \Lambda_n(x)}{N_j, \Lambda_n(x)} \right)
\]

provided the limit exists.

(3) By the Birkhoff theorem applied to systems in the full space \(\mathbb{R}^d\), the limits exist with probability 1 for any translational invariant infinite-volume Gibbs measure (i.e. a DLR distribution, [4]). Moreover under an additional assumption of “extremality” the limits are almost surely the same for all \(x\). By suitable assumptions on the parameters \(\beta_j\) and \(\lambda_j\), stated later in this section, we shall see that the limits in Eq.(1.4) exist with probability 1 and are equal to the values in Eq.1.3.

Time independence of the intensive observables (in particular those in Eq.(1.4)) is the central issue in this paper. Even if the evolution is defined with only \(H_0\), i.e. no interaction between \(\Omega_0\) and the thermostats so that \(\mu_0\) is time-invariant, yet, in general, one can only conclude that along “typical trajectories” the intensive observables are constant at countably many times (for instance at all rational times).

However under our assumptions on \(\beta_j\) and \(\lambda_j\) (essentially absence of phase transitions) and in the interesting case when the interaction between \(\Omega_0\) and the thermostats is switched on then, by choosing the initial configurations with \(\mu_0\) probability 1, we shall prove that the intensive observables keep the same initial value at all finite times. This justifies our terminology to call thermostat the systems \(\Omega_j\), \(j > 0\).

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 \(x \to \delta_x(\Lambda) x\) is called \(\Lambda\)-regularized: then we shall 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

\[
m\dot{X}_{0j} = -\partial q_0(X_0) - \sum_{j > 0} \partial q_{0,j}(X_0, X_j) + \Phi_j(X_0)
\]

\[
m\dot{X}_{jj} = -\partial q_j(X_j) - \partial q_{0,j}(X_0, X_j)
\]

(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 \(N_j d\) 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:

\[
U_j(X) = \sum_{q \in X_j} \psi(q) + \sum_{(q, q') \in X_j, q' \in \Lambda} \varphi(q - q')
\]

\[
U_{0,j}(X_0, X_j) = \sum_{q \in X_0, q' \in X_j} \varphi(q - q')
\]

(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 \(x = (\ldots, q_1, q_1, \ldots)\) with \(\hat{q}_i \in \mathbb{R}^d\); in every ball \(\Sigma(r')\) of radius \(r'\) 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 $S_t x \overset{\text{def}}{=} \lim_{\Lambda_n \rightarrow \infty} S_t^{(\Lambda_n)} x$ for all $t > 0$: a precise statement is in theorem 4 below (proved in [5, theorems 6,7], for $d = 1, 2$, and in [6, Theorem 1] for $d = 1, 2, 3$).

Since the Eq.1.5 are Newton’s equations we shall call the model a frictionless thermostats model: this is to contrast it with other thermostats models in which artificial “frictional” forces are introduced to make it possible for the system to reach a stationary state. In models with friction entropy production (generated in the thermostats by their interaction with the system) due to the evolution is naturally defined in terms of the phase space contraction: it is therefore interesting to see that even in absence of friction entropy production occurs and actually it can be identified, in the thermodynamic limit, with the same quantity that would arise in thermostats realized via artificial frictional forces. The latter are widely studied in the numerical simulations as approximations to infinite systems in a thermodynamic limit, because it is not possible to simulate really infinite systems. See Sec.V

An important question is whether time evolution changes the configuration $x$ into $S_t x$ 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 $N_j (S_t x)$ of particles of $S_t x$, of the kinetic energy $K_j (S_t x)$ and of the potential energy $U_j (S_t x)$ of the configuration $S_t x$ into which $x$ evolves at time $t$, inside a ball $\Lambda$ centered at the origin. Consider, then, $\forall j > 0$ the limits (if existent)

$$
\lim_{n \rightarrow \infty} \left( \frac{N_j (\Lambda_n) (S_t x)}{[\Lambda_n \cap \Omega_j]}, \frac{U_j (\Lambda_n) (S_t x)}{[\Lambda_n \cap \Omega_j]}, \frac{K_j (\Lambda_n) (S_t x)}{[\Lambda_n \cap \Omega_j]} \right). \quad (1.8)
$$

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 $\delta_j, \nu_j$ and $\delta_j k_B T_j$ with $\mu_0$-probability 1, as in Eq.1.3.

**Remark:** This shows that the thermostats keep, in the thermodynamic limit, the same temperature and density that they had in the initial state: a property that has to be required for the model to adhere to the physical intuition behind the empirical notion of thermostats. Hence density and temperature of the thermostats are constants of motion. We shall show that more generally many other intensive observables are also constants of motion.

## II. INTENSIVE OBSERVABLES

The definition of an $h_\Gamma$-particles intensive observable is in terms of a smooth function $G(q_1, q_1, \ldots, q_n)$ on $\mathbb{R}^{2dn}$ vanishing for $h \neq h_\Gamma$ and which is “translation invariant”, and with “short range" $\tau_T$.

This means that $\Gamma = 0$ if the diameter of $X = (q_1, \ldots, q_n)$ exceeds some $\tau_T > 0$ and, denoting by $\tau_\Gamma (X, \tilde{X})$ the configuration $(q_1 + \xi, q_1 + \xi, \ldots, q_n + \xi, \tilde{q}_n)$, it is $\Gamma (\tau_\Gamma (X, \tilde{X})) = \Gamma (X, \tilde{X}), \forall \xi \in \mathbb{R}^d$.

Given a region $W$ the function $G_W$ of $x = (X, \tilde{X})$

$$
G_W (x) \overset{\text{def}}{=} \sum_{Y \subset X \cap W} \Gamma (Y, \tilde{Y}) \quad (2.1)
$$
defines a “local observable" in $W \subset \mathbb{R}^d$ with potential $\Gamma$.

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

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

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

$$
g(x) \overset{\text{def}}{=} \lim_{n \rightarrow \infty} \frac{1}{|V_n|} G_{V_n} (x), \quad (2.2)
$$

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

$$
\Delta G(x) \overset{\text{def}}{=} \lim_{n \rightarrow \infty} \left( \frac{1}{|V_n|} G_{V_n} (x) - \mu_0 \left( \frac{1}{|V_n|} G_{V_n} \right) \right) \quad (2.3)
$$

if the limit exists.

**Remark:** The notation requires keeping in mind that $G_{V_n}$ depends also on $j$ (because $V_n = \Omega_j \cap \Lambda_n$): however for simplicity of notation the labels $j$ on $V_n$ and $G_{V_n}$ 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 $H_{0,\Lambda}(x) \overset{def}{=} H_{0,\Lambda}(x) + \theta G_{\Lambda}(x)$ is superstable for $|\theta|$ small enough (i.e. there exist constants $a > 0, b \geq 0$ such that for all balls $\Lambda$ it is $H_{0,\Lambda}(x) \geq aN^2/|\Lambda| - bN$ for all configurations $x = (X, \dot{X})$ with $N$ particles and with $X \subset \Lambda$ and $\forall |\theta| \leq \theta_0$ for some $\theta_0 > 0$). We call $G$ an “allowed observable”. For such observables it is possible to define, for $|\theta|$ small, the “pressure”

$$ P(\theta) = \lim_{\lambda \to \infty} \frac{1}{|V|} \log \frac{Z_\lambda(\theta)}{Z_\lambda(0)} \quad (2.4) $$

with $Z_\lambda(\theta)$ given by Eq.1.2 with the energy $\theta G_{\lambda}(x)$ added in the exponential. It is $P(0) \equiv 0$.

It is important to stress that $P(\theta)$ is, in the geometries in Fig.1 considered here, independent of the special geometry considered for the $\Omega$ as long as the conical containers have $d$-dimensional shape (i.e. they contain balls of arbitrarily 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 $1/|V_n| G_{V_n}(S_\theta x)$ 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 gas case.

(2) The superstability of $H_{0,\Lambda}(x) + \theta G_{\Lambda}(x)$ is a very strong condition: it is certainly satisfied if

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

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

(iii) $\Gamma(X, \dot{X}) = 0$ unless $X = (q, q')$ and in such case $\Gamma(q, q') = \phi(q - q')$, therefore 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 $|\Lambda_n|$. 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 $\Delta G_{\Lambda_n}(S_\theta x)$ 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 $v_1 \overset{def}{=} \sqrt{2\phi(0)/m}, r_\varphi$ and $W, N, v_1, ||x||$ defined as

$$ W(x; \xi, R) \overset{def}{=} \frac{1}{\varphi(0)} \sum_{q_i \in B(\xi, R)} \left( \frac{m q_i^2}{2} + \frac{1}{2} \sum_{j, j' \neq i} \varphi(q_i - q_j) + \psi(q_i + \varphi(0)) \right), $$

$$ N_\varphi(x) \overset{def}{=} \text{number particles within } r_\varphi \text{ of } \xi \in \mathbb{R}^d, \quad (3.1) $$

Let $\log_+ z \overset{def}{=} \text{max} \{1, \log_2 |z|\}, g_c(z) = (\log_+ z)^c$ and

$$ E_c(x) \overset{def}{=} \sup_{\xi} \sup_{R \leq g_c(\xi/\varphi)} \frac{W(x; \xi, R)}{R^d}. \quad (3.2) $$

Call $H_c$ the configurations in $H$ with

$$ (1) \quad E_c(x) < \infty \quad (3.3) $$

(2) $N(j, \Lambda_n) \overset{def}{=} U(j, \Lambda_n) \frac{K(j, \Lambda_n)}{|\Lambda_n \cap \Omega_j|} \frac{1}{|\Lambda_n \cap \Omega_j|} \sim_{n \to \infty} \delta_j, u_j, \delta_j \overset{def}{=} \frac{d \delta_j}{2\beta_j} \quad (3.4)$

with $\Lambda_n$ the ball centered at the origin and of radius $\varphi$, $\delta_j, u_j, T_j$, given by Eq.(e1.8) 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 $H_c$ has $\mu_0$-probability 1 for $\zeta \geq 1/d, [2, 9–11]$. Then:

**Theorem 4:** Let $d \leq 3$, then $H_{1/d}$ has $\mu_0$-probability 1 and $S_\varphi x$ exists for $\mu_0$-almost all $x \in H_{1/d}$ and $\forall t \geq 0$. Given (arbitrarily) a time $\Theta > 0$, if $E \overset{def}{=} E_{1/d}(x)$, and $|q_0(0)| \leq 2^k r_\varphi$ there are $c = c(E, \Theta) < \infty, c' = c'(E, \Theta) > 0$ such that $\forall n \geq k$ and $\forall t \leq \Theta$.

$$ |q_i(t)| \leq c v_1 k^+, \quad \text{distance}(q_i(t), \partial(\cup_j \Omega_j)) \geq c' r_\varphi k^{-\frac{d}{2}} $$

$$ \Delta x \leq c k^{1/2} \quad (3.4) $$

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

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 inf of $K_{E,n}(S(x)) / |\tilde{B}|$ is not smaller than $1/2$ 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 $\lim_{n \to \infty} |V_n|^{-1} (G_{\Lambda_n})_{\mu_0} = g$ exists.

Define $P_n(\theta) \overset{\text{def}}{=} \frac{1}{|V_n|} \log \langle e^{-\theta G_{V_n}} \rangle_{\mu_0}$; this is smooth and convex in $\theta$ and its unique derivative at $\theta = 0$ is $g_n = \frac{1}{|V_n|} \mu_0(G_{V_n})$; therefore, remarking that $P(0) = 0$, it satisfies $P_n(\theta) \geq \theta g_n$.

The limit $P(\theta)$ is $\lim_{n \to \infty} P_n(\theta)$ which would be obtained if $V_n$ was replaced by the full ball $\Lambda_n$ and filled with particles at temperature $\beta_j^{-1}$ and chemical potential $\Lambda_j$.

Any convergent subsequence $g_n$, 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 $g = \lim_{n \to \infty} g_n$ exists.

Let $g_n = (|V_n|^{-1} G_{\Lambda_n})_{\mu_0}$ and, given $\gamma > 0$, let $X_{E,\gamma,n}$ to be the set of points in $H_{\Lambda_j \cap \Lambda_n}$ with $E(x) \leq E, G_{\Lambda_n}(x) < (g_n + \frac{1}{2}\gamma)|V_n|$ and which, under the evolution, reach in a time $\tau_{n,\gamma}(x) \leq \Theta$ and for the first time, a point of the surface

$$
\Sigma_{n,\gamma} \overset{\text{def}}{=} \{ x | |V_n|^{-1} G_{\Lambda_n}(x) = (g_n + \gamma) \}.
$$

If for all $E$ and for all small $\gamma > 0$ it is $\sum \mu_0(X_{E,\gamma,n}) < +\infty$ then it will be $\limsup_n -|V_n|^{-1} G_{\Lambda_n}(S(x)) \leq g$, 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 inf $g$ is $\geq g$: notice that the change in sign of $G$ is possible by the condition on $\Lambda_j$.

This remains true if for all small $\gamma$ there exists $\gamma_n \in [\gamma, 2\gamma]$ such that $\sum \mu_0(X_{E,\gamma,n}) < +\infty$.

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

$$
s(x,t) = \int_0^t (\sum_{j \geq 0} \beta_j Q_j(\tau) + \beta_0 L_0(\tau)) d\tau
$$

and $Q_j(t) \overset{\text{def}}{=} \dot{X}_j(t) \cdot \mathbf{F}_j, L_0(t) \overset{\text{def}}{=} \dot{X}_0 \cdot \Phi(X_0(t))$.

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 $E, n_0, \Theta$).

Therefore by a quasi-invariance lemma, [2, 12], [5, Appendix H], the probability $\mu_0(X_{E,\gamma+\varepsilon,n})$ can be bounded $\forall \varepsilon \in [\gamma, 2\gamma]$ by

$$
C \int \mu_0(d\gamma) \frac{|\widehat{G}_n|}{|V_n|} \delta_0 \left( \frac{G_{\Lambda_n}(x)}{|V_n|} - (g_n + \gamma + \varepsilon) \right)
$$

where $\widehat{G}$ denotes the time derivative at $t = 0$ of $G_{\Lambda_n}(S(x))$ (to be computed via the equations of motion) evaluated on the surface $\Sigma_{n,\gamma+\varepsilon}$, see Eq.4.1.

Integrating Eq.4.3 over $d\gamma / \gamma$, $\mu_0(X_{E,n,\gamma,n})$ can be bounded by

$$
\frac{C}{\gamma} \int \mu_0(d\gamma) \frac{|\widehat{G}_n|}{|V_n|} \chi(\gamma \leq \frac{G_{\Lambda_n}(x)}{|V_n|} - g_n \leq 2\gamma),
$$

with $\widehat{G} = \sum_{X \subset V_n} \sum_{\eta \in X} \partial_\eta \Gamma(X) \dot{q}$. By Schwartz’ inequality

$$
C_2 \gamma^{-1} \mu_0(\{ x : \gamma \leq \frac{G_{\Lambda_n}(x)}{|V_n|} - g_n \leq 2\gamma \})^{1/2}
$$

because from Eq.2.1 for $\Gamma$

$$
\mu_0(\widehat{G}^2)^{1/2} \leq C_1 |V_n|
$$

obtained via superstability bounds, using the Maxwellian distribution for $\dot{q}$.

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

$$
I_\varepsilon \overset{\text{def}}{=} \langle |G_{\Lambda_n}(x)|^2 \rangle_{\mu_0}, \quad I_{\varepsilon,\gamma} \overset{\text{def}}{=} \langle e^{\varepsilon (G_{\Lambda_n}(x) - g_n)} \rangle_{\mu_0}
$$

$\forall \gamma \geq 0$. This implies the existence of $\gamma_n \in [\gamma, 2\gamma]$ with:

$$
\mu_0(X_{E,n,\gamma,n}) \leq C_3 \gamma^{-1} J(n), \quad J(n)^2 = I, I_{\theta}
$$

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 $\sum \mu_0(X_{E,n,\gamma,n}) < \infty$. 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

$$
I_{\theta} = \langle e^{\theta G_{V_n}} \rangle_{\mu_0} e^{-\theta (g_n + \gamma)} \leq e^{-\theta \gamma} |V_n| + \eta(\theta, V_n)
$$

Continuing the argument leading to the existence of the limit of $g_n$, at the beginning of the section, the correction term $\eta(\theta, V_n)$ is bounded, as follows:
the limit exists for \( \theta \leq \theta_0 \) if \( \theta_0 \) is small enough so that the potential \( \varphi + \beta^{-1} g \) is superstable \( \forall \theta \leq \theta_0, j = 1, \ldots, \nu \). By superstability the limit exists for \( \theta \leq \theta_0 \) if it is a limit of functions \( P_n(\theta) \) which are convex for \( \theta \leq \theta_0 \). Hence the limit is uniform: \( |P(\theta) - P_n(\theta)| \leq o(|V_n|) \) for \( \theta \leq \theta_0 \).

(b) the \( g_n \) in the exponent in Eq.4.7 has just been shown to be \( g_n \mid V_n = g \mid V_n + o(V_n) \), so that \( \theta g_n \) converges to \( -g \) with an error \( o(V_n) \).

(c) \( (P(\theta) - P(0) - \theta g) \mid V_n \) is (by the uniqueness of the tangent plane) \( o(\theta) \mid V_n \).

Hence

\[
\eta(\theta, V_n) - \gamma_n \mid V_n \leq -\frac{1}{2} \gamma \theta_n |V_n| + \frac{1}{2} \gamma a_n |V_n| + o(\theta) |V_n| \leq -\frac{1}{2} \gamma \theta_n |V_n|
\]

and choosing \( \theta_n \) tending to 0 so slowly that the exponent of the r.h.s. of 4.9 tends rapidly to \( \infty \), for instance if \( \theta_n = \max(1, \log |V_n|) \), we see that \( \eta \mid \theta \rightarrow 0 \) so fast that \( \mu_0(X_{E_n, \gamma_n}) \) 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 \( \theta \rightarrow 0 \) yields a summable bound on \( J \), hence on \( \mu_0(\Delta^2_{G, \Lambda_0}) \).

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: \( \rho_j(x_1, \ldots, x_n) \) be the \( n \)-points correlation function in the \( j \)-th container: by superstability \( \rho_j \leq C^m \), [9]. If \( x = (q, \dot{q}) \) and \( \xi \in \Omega_j \), extremality of \( \mu_0 \) implies, [4, 9], for \( x_1, \ldots, x_n \) and \( y_1, \ldots, y_m \) with positions in \( \Omega_j \):

\[
\rho_j(x_1, \ldots, x_n, \tau, y_1, \ldots, \tau, y_m) - \rho_j(x_1, \ldots, x_n) \rho_j(\tau, y_1, \ldots, \tau, y_m) \mid \xi \rightarrow 0 \text{ as } |\xi| \rightarrow \infty. \tag{4.11}
\]

Assume that Eq.4.11 holds in the stronger sense that the l.h.s. is bounded by \( \eta_{R,m,n}(\xi) \) 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 \( C_{R, m, n} < \infty \) such that \( \eta_{R,m,n}(\xi) \leq C_{R,m,n} \xi^{-a(R,m,n)} \) with \( a(R, m, n) > 0 \) and if \( \lim_{\xi \rightarrow \infty} |\xi|^{-a} \mu_0(G_{V_n}) = g \) exists, then \( \lim_{\Lambda \rightarrow \infty} \frac{1}{|V_n|} \Delta_{G,V_n}(x) = 0 \) and \( \lim_{\Lambda \rightarrow \infty} \frac{1}{|V_n|} G_{V_n}(S|x) = g \) 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 (in \( \Omega_j \))

\[
\lim_{n \rightarrow \infty} \frac{1}{\Omega_j \cap \Lambda_n} \int_{\tau \in \mathbb{R}^{d}, \tau \cdot \Delta \subseteq \Omega_j \cap \Lambda_n} \tau f(x) \, dr \tag{4.12}
\]

where \( f \) is a cylindrical function in \( \Delta \) (i.e. it does not depend on the particles outside \( \Delta \)) and \( \tau \) 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.

(3) The assumption certainly holds in the cluster expansion convergence region, [3] 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 \( \gamma = \gamma_n = 1/n \). The numerator tends to 0 as \( |V_n|^{-a(R,m,n)/d} \) if the potential \( \Gamma \) for the observable \( G_{V_n} \) vanishes when the diameter of the set \( \{x_1, \ldots, x_n\} \) exceeds \( R \).

The estimate Eq.4.8 implies that \( \frac{1}{|V_n|} \Delta_{G,V_n}(S|x) \) tends to 0 with \( \mu_0 \)-probability 1 for all \( t \leq k t_0 \) with \( k \) integer and \( t_0 > 0 \) (arbitrarily fixed). Hence if the average of \( \frac{1}{|V_n|} \mu_0(G_{V_n}) \) exists it exists for all times and has a time-independent value.

**V. ENTROPY AND THERMOSTATS**

Entropy production rate (due to the action of the system upon the thermostats and identified with the rate of their entropy increase, which is finite even though the thermostats entropy is infinite because the thermostats are infinite) is defined in terms of \( Q_j = -\dot{x}_j \cdot \partial x_j U_{0,j}(X_0, X_j) \), 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 thermostats the entropy production in the configuration \( x \) is given by \( \sigma_0(x) = \sum_j \beta_j Q_j(x) \).

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 \( \beta_0(\dot{Q}_0 + L_0) \equiv \beta_0(\dot{K}_0 + U_0) \) and \( K_0 + U_0 \) is expected to stay finite uniformly in time. If so 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 arbitrarily prefixed but finite time interval).

In other words in the frictionless thermostats model and in the isoenergetic thermostat models, [6], the entropy production can be identified with the phase space contraction, possibly up to a time derivative of a quantity expected to be uniformly finite in time. Furthermore the entropy production is the same in both models of thermostats if the thermodynamic parameters of the thermostats \( (\delta_j, T_j, j > 0) \) are the same: this follows from the equivalence theorem between frictionless and isoenergetic thermostats, [6, 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].

Considering external thermostats as correctly representing the physics of the interaction of a system in contact with external reservoirs has been introduced in [15].

Their analysis was founded on the grounds of

(1) identity, in the thermodynamic limit, of the evolution with and without thermostats
(2) identity of the phase space contraction of the thermostatted systems with the physical entropy production (up to a time derivative).

For a more mathematical view see [14].

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