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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.

Keywords Nonequilibrium statistical mechanics · Thermostats · Entropy · Constants of motion · Infinite particles systems

1 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 $d = 1, 2$, or 3. This can be attacked via recent difficult results on the time evolution of infinite systems in dimension $d = 1, 2$, or 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 Ω_0, and ν other particles systems, in containers $\Omega_1, \ldots, \Omega_\nu$, interact and define a model of a system in interaction with ν thermostats, if the particles in $\Omega_1, \ldots, \Omega_\nu$ can be considered at fixed temperatures $T_1, \ldots, T_\nu$.

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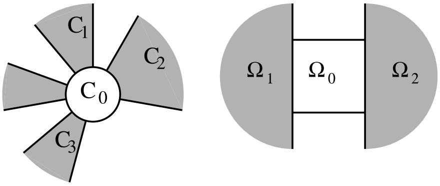

Fig. 1 If $d=1,2$ the $1+\nu$ finite boxes $\Omega_j\cap\Lambda$, $j=0,\dots,\nu$, are marked $\mathcal{C}_0,\mathcal{C}_1,\dots,\mathcal{C}_\nu$ in the *first figure* and contain $N_0,N_1,\dots,N_\nu$ particles, out of the infinitely many particles, with positions and velocities denoted $\mathbf{X}_0,\mathbf{X}_1,\dots,\mathbf{X}_\nu$, and $\dot{\mathbf{X}}_0,\dot{\mathbf{X}}_1,\dots,\dot{\mathbf{X}}_\nu$, respectively, contained in Ω_j, $j\ge 0$. The *second figure* illustrates the special geometry that will be considered for $d=1,2,3$: here two thermostats, symbolized by the *shaded regions*, Ω_1,Ω_2 occupy half-spaces adjacent to Ω_0

A representation of the system is in Fig. 1:

$$x=(\mathbf{X}_0,\dot{\mathbf{X}}_0,\mathbf{X}_1,\dot{\mathbf{X}}_1,\dots,\mathbf{X}_\nu,\dot{\mathbf{X}}_\nu)$$

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 Ω_j, $j=1,\dots,\nu$, as infinite and occupied by particles initially in a Gibbs distribution with given temperatures and densities $T_1,\delta_1,\dots,T_\nu,\delta_\nu$.

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 μ_0 for the random choice of initial data will be, if $dx\stackrel{def}{=}\prod_{j=0}^{\nu}\frac{d\mathbf{X}_j\,d\dot{\mathbf{X}}_j}{N_j!}$, the limit as $\overline{\Lambda}\to\infty$ of the distributions on the configurations $x\in\mathcal{H}(\overline{\Lambda})$ with $\mathbf{X}_j\in\overline{\Lambda}$ (see Fig. 1),

$$\mu_{0,\overline{\Lambda}}(dx)=const\,e^{-H_0(x)}\,dx \tag{1.1}$$

with $H_0(x)=\sum_{j=0}^{\nu}\beta_j(K_j(\dot{\mathbf{X}}_j)-\lambda_jN_j+U_j(\mathbf{X}_j))$ and $\beta_j\stackrel{def}{=}\frac{1}{k_BT_j}>0$, $\lambda_j\in\mathbb{R}$, $j>0$; the values $\beta_0=\frac{1}{k_BT_0}>0$, $\lambda_0\in\mathbb{R}$ will also be fixed.

The values β_0,λ_0 bear no particular physical meaning because the test system is kept finite. Here $\boldsymbol{\lambda}=(\lambda_0,\lambda_1,\dots,\lambda_\nu)$ and $\mathbf{T}=(T_0,T_1,\dots,T_\nu)$ are fixed *chemical potentials* and *temperatures*, and $\overline{\Lambda}$ is a ball centered at the origin and of radius r_0. The $K_j(\dot{\mathbf{X}}_j),U_j(\mathbf{X}_j)$ are kinetic and potential energies of the particles in Ω_j (see below for the conditions on the potentials).

The distribution μ_0 is interpreted as a Gibbs distribution μ_0 obtained by taking the "thermodynamic limit" $\overline{\Lambda}\to\infty$. At time 0 we switch on the interaction between the particles in Ω_0 and those in the thermostats Ω_j, $j>0$. The measure μ_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 $p_j(\beta,\lambda;\overline{\Lambda}) \stackrel{def}{=} \frac{1}{\beta|\Omega_j\cap\overline{\Lambda}|}\log Z_j(\beta,\lambda)$ with

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

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

$$\begin{aligned} &p_j(\beta,\lambda)\stackrel{def}{=}\lim_{\overline{\Lambda}\to\infty}p_j(\beta_j,\lambda_j,\overline{\Lambda})\\ &\delta_j=-\frac{\partial p_j(\beta_j,\lambda_j)}{\partial\lambda_j},\qquad k_BT_j=\beta_j^{-1}\\ &e_j=-\frac{\partial\beta_j p_j(\beta_j,\lambda_j)}{\partial\beta_j}-\lambda_j\delta_j,\qquad u_j=e_j-\frac{d}{2}\delta_j\beta_j^{-1}\end{aligned} \tag{1.3}$$

which are the relations linking density δ_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 (β_j,λ_j), for $j>0$.

Remark (1) notice that the limit defining p_j does not depend on the shape of Ω_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

$$\lim_{n\to\infty}\left(\frac{N_{j,\Lambda_n}(x)}{|\Lambda_n\cap\Omega_j|},\frac{U_{j,\Lambda_n}(x)}{|\Lambda_n\cap\Omega_j|},\frac{K_{j,\Lambda_n}(x)}{N_{j,\Lambda_n}(x)}\right) \tag{1.4}$$

provided the limit exists.

(3) By the Birkhoff theorem applied to systems in the full space $\mathbf{R}^d$, 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 β_j and λ_j, stated later in this section, we shall see that the limits in (1.4) exist with μ_0 probability 1 and are equal to the values in (1.3).

Time independence of the intensive observables (in particular those in (1.4)) is the central issue in this paper. Even if the evolution is defined with only H_0, *i.e.* no interaction between Ω_0 and the thermostats so that μ_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 β_j and λ_j (essentially absence of phase transitions) and in the interesting case when the interaction between Ω_0 and the thermostats is switched on then, by choosing the initial configurations with μ_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 Ω_j, $j>0$.

Hypotheses In the geometries of Fig. 1 suppose:

(1) μ_0 satisfies the DLR equations and that
(2) the thermostats pressures $p_j(\beta, \lambda)$ are differentiable in β, λ at β_j, λ_j, $j = 1, \dots, \nu$.

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 Λ keeping the particles outside Λ fixed. Such motion $x \to S_t^{(\Lambda)} x$ is called Λ-*regularized*: then we shall consider the limit as $\Lambda \to \infty$.

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

The Λ_n-regularized equations of motion will be

$$\begin{aligned} m\ddot{\mathbf{X}}_{0i} &= -\partial_i U_0(\mathbf{X}_0) - \sum_{j>0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \boldsymbol{\Phi}_i(\mathbf{X}_0), \\ m\ddot{\mathbf{X}}_{ji} &= -\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) \end{aligned} \tag{1.5}$$

(see Fig. 1) where:

(1) the first label, $j = 0$ or $j = 1, \dots, \nu$, 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* Λ_n (hence the labels i in the subscripts (j, i) have $N_j d$ values).
(2) The forces $\boldsymbol{\Phi}(\mathbf{X}_0)$ are, positional, *nonconservative*, smooth stirring forces, possibly vanishing; the other forces are conservative and generated by a pair potential φ, with range r_φ, which couples all pairs in the same containers and all pairs of particles one of which is located in Ω_0 and the other in Ω_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 ψ, 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 $U_j(\mathbf{X}_j)$, $j \geq 0$, and $U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$, respectively denoting the internal energies of the various systems and the potential energy of interaction between the test system and the thermostats:

$$\begin{aligned} U_j(\mathbf{X}) &= \sum_{q \in \mathbf{X}_j} \psi(q) + \sum_{(q,q') \in \mathbf{X}_j, q \in \Lambda} \varphi(q - q'), \\ U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) &= \sum_{q \in \mathbf{X}_0, q' \in \mathbf{X}_j} \varphi(q - q'). \end{aligned} \tag{1.6}$$

The potentials φ, ψ 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 $x = (\dots, q_i, \dot{q}_i, \dots)_{i=1}^{\infty}$

$$x = (\mathbf{X}_0, \dot{\mathbf{X}}_0, \mathbf{X}_1, \dot{\mathbf{X}}_1, \dots, \mathbf{X}_n, \dot{\mathbf{X}}_n) = (\mathbf{X}, \dot{\mathbf{X}}) \tag{1.7}$$

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

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 (1.5) do not even admit an obvious solution in $\mathcal{H}$.

Dynamics is well defined with μ_0-probability 1 because if $d = 1, 2, 3$ the Λ_n-regularized equations with data x admit, with μ_0-probability 1, a limit $S_t x \stackrel{def}{=} \lim_{\Lambda_n\to\infty} S_t^{(\Lambda_n)} x$ 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 (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 Sect. 5.

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 μ_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 $N_{j,\Lambda}(S_t x)$ of particles of $S_t x$, of the kinetic energy $K_{j,\Lambda}(S_t x)$ and of the potential energy $U_{j,\Lambda}(S_t x)$ of the configuration $S_t x$ into which x evolves at time t, inside a ball Λ centered at the origin. Consider, then, $\forall j > 0$, the limits (if existent)

$$\lim_{n\to\infty}\left(\frac{N_{j,\Lambda_n}(S_t x)}{|\Lambda_n \cap \Omega_j|}, \frac{U_{j,\Lambda_n}(S_t x)}{|\Lambda_n \cap \Omega_j|}, \frac{K_{j,\Lambda_n}(S_t x)}{|\Lambda_n \cap \Omega_j|}\right). \tag{1.8}$$

Under the above "no phase transition" assumption on μ_0 we shall prove:

Theorem 1 *The limits in* (1.8) *exist with μ_0-probability* 1 *for all times and are time independent. The limits will be respectively δ_j, u_j and $\frac{d}{2}\delta_j k_B T_j$ with μ_0-probability* 1, *as in* (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.

2 Intensive Observables

The definition of an h_Γ*-particles intensive observable* is in terms of a smooth function $\Gamma(q_1, \dot q_1, \ldots, q_h, \dot q_h)$ on R^{2dh} vanishing for $h \neq h_\Gamma$ and which is "translation invariant", and with "short range" r_Γ.

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

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

$$G_W(x) \stackrel{def}{=} \sum_{Y \subset X \cap W} \Gamma(Y, \dot{Y}) \tag{2.1}$$

defines a "*local observable*" in $W \subset R^d$ with potential Γ.

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

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

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

$$g(x) \stackrel{def}{=} \lim_{n\to\infty} \frac{1}{|V_n|} G_{V_n}(x), \tag{2.2}$$

if the limit exists. Furthermore, given μ_0, define the "intensive fluctuation" of G (in the j-th thermostat)

$$\Delta_G(x) \stackrel{def}{=} \lim_{n\to\infty} \left(\frac{1}{|V_n|} G_{V_n}(x) - \mu_0 \left(\frac{1}{|V_n|} G_{V_n} \right) \right) \stackrel{def}{=} \lim_{n\to\infty} \Delta_{G,V_n}(x), \tag{2.3}$$

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 Ω_j which, we recall, are distributed independently over $j = 1, \dots, \nu$ and depend on the ν pairs of parameters β_j, λ_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 β_j, λ_j.

Let G be an observable of potential or kinetic type; and suppose that $H_{0,\Lambda,\Gamma}(x) \stackrel{def}{=} H_{0,\Lambda}(x) + \theta G_\Lambda(x)$ is superstable for $|\theta|$ small enough (*i.e.* there exist constants $a > 0, b \geq 0$ such that for all balls Λ it is $H_{0,\Lambda,\Gamma}(x) \geq aN^2/|\Lambda| - bN$ 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"

$$P(\theta) = \lim_{\Lambda\to\infty} \frac{1}{|V|} \log \frac{Z_j(\theta)}{Z_j(0)} \tag{2.4}$$

with $Z_j(\theta)$ given by (1.2) with the energy $\theta\, G_V(x)$ 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 Ω_j 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 μ_0-probability 1 the limit as $|V_n| \to \infty$ of $\frac{1}{|V_n|} G_{V_n}(S_t x)$ exists μ_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 $H_{0,\overline{\Lambda}}(x) + \theta G_{\overline{\Lambda}}(x)$ 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) $\Gamma(X, \dot X) = \frac{1}{2}\dot q^2$ for $|X| = 1$ and 0 otherwise, or if
(iii) $\Gamma(X, \dot X) = 0$ unless $X = (q, q')$ and in such case $\Gamma(q, q') = \varphi(q - q')$, 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* μ_0*-probability that the fluctuation* $\Delta_{G,\Lambda_n}(S_t x)$ *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 λ_j, β_j, [8]. They are also believed to be satisfied quite generally for observables generated by a potential Γ. In particular they hold generically if Γ is a linear combination of the potentials (i), (ii), (iii) in remark (2) above.

The proof of Theorems 2, 3 are presented in Sect. 4.

3 Time Evolution

A quantitative existence theorem of the dynamics can be conveniently formulated in terms of the quantities $v_1 \stackrel{def}{=} \sqrt{2\varphi(0)/m}$, r_φ and $W, \mathcal{N}, v_1, \|x_1\|$ defined as

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

$$\mathcal{N}_\xi(x) \stackrel{def}{=} \text{number particles within } r_\varphi \text{ of } \xi \in \mathbb{R}^d, \tag{3.1}$$

$$\|x_i - x_i'\| \stackrel{def}{=} |\dot q_i - \dot q_i'|/v_1 + |q_i - q_i'|/r_\varphi.$$

Let $\log_+ z \stackrel{def}{=} \max\{1, \log_2 |z|\}$, $g_\zeta(z) = (\log_+ z)^\zeta$ and

$$\mathcal{E}_\zeta(x) \stackrel{def}{=} \sup_\xi \sup_{R > g_\zeta(\xi/r_\varphi)} \frac{W(x; \xi, R)}{R^d}. \tag{3.2}$$

Call $\mathcal{H}_\zeta$ the configurations in $\mathcal{H}$ with

$$\begin{aligned} &(1) \quad \mathcal{E}_\zeta(x) < \infty, \\ &(2) \quad \frac{N(j, \Lambda_n)}{|\Lambda_n \cap \Omega_j|}, \frac{U(j, \Lambda_n)}{|\Lambda_n \cap \Omega_j|}, \frac{K(j, \Lambda_n)}{|\Lambda_n \cap \Omega_j|} \xrightarrow[n \to \infty]{} \delta_j, u_j, \frac{d\, \delta_j}{2\beta_j} \end{aligned} \tag{3.3}$$

with Λ_n the ball centered at the origin and of radius $2^n r_\varphi$ δ_j, u_j, T_j, given by (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 $\mathcal{H}_\zeta$ has μ_0-probability 1 for $\zeta \ge 1/d$, [2, 9–11]. Then:

Theorem 4 *Let $d \le 3$, then $\mathcal{H}_{1/d}$ has μ_0-probability 1 and $S_t x$ exists for μ_0-almost all $x \in \mathcal{H}_{1/d}$ and $\forall t \ge 0$. Given (arbitrarily) a time $\Theta > 0$, if $\mathcal{E} \stackrel{def}{=} \mathcal{E}_{1/d}(x)$, and $|q_i(0)| \le 2^k r_\varphi$ there are $c = c(\mathcal{E},\Theta) < \infty$, $c' = c'(\mathcal{E},\Theta) > 0$ such that $\forall n \ge k$ and $\forall t \le \Theta$*

$$\begin{aligned}
&|\dot q_i(t)| \le c\, v_1\, k^{\frac12},\\
&\text{distance}\Big(q_i(t), \partial\Big(\bigcup\nolimits_j \Omega_j\Big)\Big) \ge c'\, r_\varphi\, k^{-\frac{1}{\alpha}}\\
&\mathcal{N}_\xi(S_t x) \le c\, k^{1/2}\\
&\|(S_t x)_i - (S_t^{(n)} x)_i\| \le e^{-c' 2^{n/2}}, \quad n > k.
\end{aligned} \tag{3.4}$$

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 (3.3) holds: in [5, 6] it is however proved, in addition to Theorem 4, the weaker statement that the lim inf of $\frac{K_{j,\Lambda_n}(S_t x)}{|\Omega_j \cap \Lambda_n|}$ is not smaller than $\frac12$ of the corresponding *r.h.s.*; and the same is true for the other two quantities in (3.3).

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

4 Constants of Motion

Let Γ 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 $\lim_{n\to\infty} |V_n|^{-1} \langle G_{\Lambda_n} \rangle_{\mu_0} = g$ exists.

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

The limit $P(\theta)$ as $n \to \infty$ of $P_n(\theta)$ is the same that would be obtained if V_n was replaced by the full ball Λ_n and filled with particles at temperature β_j^{-1} and chemical potential λ_j.

Any convergent subsequence g_{n_i} defines therefore a coefficient g with the property $P(\theta) \ge \theta g$. 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 $g \stackrel{def}{=} \lim_{n\to\infty} g_n$ exists.

Let $g_n = \langle |V_n|^{-1} G_{\Lambda_n} \rangle_{\mu_0}$ and, given $\gamma > 0$, let $\mathcal{X}_{E,\gamma,n}$ to be the set of points in $\mathcal{H}_{1/d}$ with $\mathcal{E}(x) \le E$, $G_{\Lambda_n}(x) < (g_n + \frac12 \gamma)|V_n|$ and which, under the evolution, reach in a time $\tau_{\gamma,n}(x) \le \Theta$ and for the first time, a point of the surface

$$\Sigma_{n,\gamma} \stackrel{def}{=} \{x \,|\, |V_n|^{-1} G_{\Lambda_n}(x) = (g_n + \gamma)\}. \tag{4.1}$$

If for all E and for all small $\gamma > 0$ it is $\sum_n \mu_0(\mathcal{X}_{E,\gamma,n}) < +\infty$ then it will be $\limsup_{n\to\infty} |V_n|^{-1} G_{\Lambda_n}(S_t x) \le g$, with μ_0-probability 1 (by Borel–Cantelli's estimate); changing Γ into $-\Gamma$ it will follow, again with μ_0-probability 1, that the lim inf is $\ge g$:

notice that the change in sign of Γ is possible by the condition on G to be an "allowed observable", as introduced before (2.4).

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

If $x \in \mathcal{X}_{E,\gamma,n}$ the phase space contraction, when phase space volume is measured by μ_0, within time t is, [5, 6],

$$s(x,t) = \int_0^t \Big(\sum_{j\ge 0} \beta_j Q_j(\tau) + \beta_0 L_0(\tau)\Big)\, d\tau \tag{4.2}$$

where $Q_j(t) \stackrel{def}{=} \dot{\mathbf{X}}_j(t)\cdot \mathbf{F}_j$, $L_0(t) \stackrel{def}{=} \dot{\mathbf{X}}_0 \cdot \boldsymbol{\Phi}(\mathbf{X}_0(t))$.

By Theorem 4, $L_0(t)$ is uniformly bounded as $n \to \infty$, for $0 \le t \le \Theta$, by the first of (3.2), by a quantity C (only depending on E, n_0, Θ).

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

$$C \int \mu_0(dx) \frac{|\widehat{G}|}{|V_n|} \delta\bigg(\frac{G_{\Lambda_n}(x)}{|V_n|} - (g_n + \gamma + \varepsilon)\bigg) \tag{4.3}$$

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

Integrating (4.3) over $d\varepsilon/\gamma$, $\mu_0(\mathcal{X}_{E,n,\gamma_n})$ can be bounded by

$$\frac{C}{\gamma} \int \mu_0(dx) \frac{|\widehat{G}|}{|V_n|} \chi\bigg(\gamma \le \frac{G_{\Lambda_n}(x)}{|V_n|} - g_n \le 2\gamma\bigg), \tag{4.4}$$

with $\widehat{G} = \sum_{X\subset V_n} \sum_{q\in X} \partial_q \Gamma(X)\, \dot{q}$. By Schwartz' inequality

$$C_2 \gamma^{-1} \mu_0\bigg(\bigg\{x : \gamma \le \frac{G_{\Lambda_n}(x)}{|V_n|} - g_n \le 2\gamma\bigg\}\bigg)^{1/2} \tag{4.5}$$

because from (2.1) for Γ

$$\mu_0(\widehat{G}^2)^{1/2} \le C_1 |V_n| \tag{4.6}$$

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

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

$$I \stackrel{def}{=} \bigg\langle \frac{(G_{\Lambda_n}(x)/|V_n| - g_n)^2}{\gamma^2} \bigg\rangle_{\mu_0}, \qquad I_\theta \stackrel{def}{=} \big\langle e^{\theta\,(G_{\Lambda_n} - |V_n|(g_n+\gamma))} \big\rangle_{\mu_0} \tag{4.7}$$

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

$$\mu_0(\mathcal{X}_{E,n,\gamma_n}) \le C_3 \gamma^{-1} J(n), \qquad J(n)^2 = I, I_\theta \tag{4.8}$$

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 arbtrariness of γ.

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

$$I_\theta = \langle e^{\theta U_{\Gamma,V_n}} \rangle_{\mu_0} e^{-\theta(g_n+\gamma)|V_n|} \le e^{-\theta\gamma|V_n|+\eta(\theta,V_n)} \tag{4.9}$$

Continuing the argument leading to the existence of the limit of g_n, at the beginning of the section, the correction term $\eta(\theta, V_n)$ is bounded as follows:

(a) $\frac{1}{|V_n|}\log\langle e^{\theta U_{\Gamma,V_n}}\rangle_{\mu_0}$ is $P_n(\theta) - P_n(0)$ (notice: $P_n(0) \equiv 0$) and converges to $P(\theta) - P(0)$ as $V_n \to \infty$ for $|\theta| \le \theta_0$, if θ_0 is small enough so that the potential $\varphi + \beta_j^{-1}\theta$ is superstable $\forall\, |\theta| \le \theta_0$, $j = 1, \ldots, \nu$. By superstability the limit exists for $|\theta| \le \theta_0$ and it is a limit of functions $P_n(\theta)$ which are convex for $|\theta| \le \theta_0$. Hence the limit is uniform: $|P(\theta) - P_n(\theta)| \le o(|V_n|)$ for $|\theta| \le \theta_0$,
(b) the g_n in the exponent in (4.7) has just been shown to be $g_n|V_n| = g|V_n| + o(|V_n|)$, so that $-\theta\, g_n$ converges to $-\theta\, g$ with an error $\theta\, o(|V_n|)$,
(c) $(P(\theta) - P(0) - \theta\, g)|V_n|$ is (by the uniqueness of the tangent plane) $o(\theta)\,|V_n|$. Hence

$$\begin{aligned}&\eta(\theta, V_n) - \gamma\theta_n|V_n| \\ &\quad\le -\frac{1}{2}\gamma\theta_n|V_n| + \left(-\frac{1}{2}\gamma\theta_n + \frac{o(|V_n|)}{|V_n|} + o(\theta_n)\right)|V_n| \le -\frac{1}{2}\gamma\theta_n|V_n|\end{aligned} \tag{4.10}$$

and choosing θ_n tending to 0 so slowly that the exponent of the *r.h.s.* of (4.9) tends rapidly to ∞, for instance if $\theta_n = \max(\frac{1}{\log n}, \frac{1}{4\gamma}\frac{o(|V_n|)}{|V_n|})$, we see that $I_{\theta_n} \xrightarrow[n\to\infty]{} 0$ so fast that $\mu_0(\mathcal{X}_{E,n,\gamma_n})$ 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 I_θ yields a summable bound on J, hence on $\mu_0(\Delta^2_{G,\Lambda_n})$.

Remarks (1) Uniqueness of the tangent plane can be replaced by assumptions on the decays of correlations in the distribution μ_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 $\rho_j \le C^n$, [9]. If $x = (q, \dot q)$ and $\xi \in \Omega_j$, extremality of μ_0, implies, [4, 9], for $x_1, \ldots, x_n$ and $y_1, \ldots, y_m$ with positions in Ω_j:

$$|\rho_j(x_1, \ldots, x_n, \tau_\xi y_1, \ldots, \tau_\xi y_m) - \rho_j(x_1, \ldots, x_n)\rho_j(\tau_\xi y_1, \ldots, \tau_\xi y_m)| \xrightarrow[\xi\to\infty]{} 0. \tag{4.11}$$

Assume that (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* $\eta_{R,m,n}(\xi) \le C_{R,m,n}|\xi|^{-a(R,m,n)}$ *with* $a(R, m, n) > 0$ *and if* $\lim_{\Lambda\to\infty}\frac{1}{|V_n|}\mu_0(G_{V_n}) = g$ *exists, then* $\lim_{\Lambda\to\infty}\frac{1}{|V_n|}\Delta_{G,V_n}(x) = 0$ *and* $\lim_{\Lambda\to\infty}\frac{1}{|V_n|}G_{V_n}(S_t x) = g$ *with* μ_0 *probability* 1.

Remarks (1) Thus if μ_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 Chebishev inequality and we may thus drop the superstability condition in the definition of the potential Γ. We could actually consider more general observables of the form (in Ω_j)

$$\lim_{n\to\infty} \frac{1}{|\Omega_j \cap \Lambda_n|} \int_{r\in\mathbb{R}^d:\tau_r\Delta\subset\Omega_j\cap\Lambda_n} \tau_r f(x)dr, \tag{4.12}$$

where f is a cylindrical function in Δ (i.e. it does not depend on the particles outside Δ) and τ_r denotes translation by r. If the power law cluster property is satisfied and μ_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, Sect. 5.9], *i.e* high temperature and low density, without extra assumptions.

Proof Consider the first of (4.7) and choose $\gamma = \gamma_n = \frac{1}{n}$. The numerator tends to 0 as $|V_n|^{-a(R,n,n)/d}$ if the potential Γ for the observable G_{V_n} vanishes when the diameter of the set $\{x_1, \ldots, x_n\}$ exceeds R.

The estimate (4.8) implies that $\frac{1}{|V_n|}\Delta_{G,V_n}(S_t x)$ tends to 0 with μ_0-probability 1 for all $t \le kt_0$ 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. □

5 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 $Q_j = -\dot{\mathbf{X}}_j \cdot \partial_{\mathbf{X}_j} U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$, 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 $\sigma_0(x) = \sum_{j>0} \beta_j Q_j(x)$.

If the volumes in phase space are measured by the distribution μ_0 this quantity differs from the contraction rate of the phase space volume by $\beta_0(\dot{Q}_0 + L_0) \equiv \beta_0(\dot{K}_0 + \dot{U}_0)$ 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 a *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 μ_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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