Thermodynamic limit of isoenergetic and Hamiltonian Thermostats

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Abstract: *The relation between isoenergetic and Hamiltonian thermostats is studied and their equivalence in the thermodynamic limit is proved in space dimension* $d = 1, 2$.

Contents

I. THERMOSTATS

In a recent paper [1] equivalence between isokinetic and Hamiltonian thermostats has been discussed heuristically, leaving aside several difficulties on the understanding of the classical dynamics of systems of infinitely many particles. Understanding it is, however, a necessary prerequisite, because strict equivalence can be expected to hold only in the thermodynamic limit. In this paper we proceed along the same lines, comparing the isoenergetic and the Hamiltonian thermostats, and study the conjectures corresponding to the ones formulated in [1] for isokinetic thermostats, obtaining a complete proof of equivalence in 1 and 2–dimensional systems.

Here the class of models to which our main result applies is described in detail. The main result is informally quoted at the end of Sec.I after discussing the physics and the equations of motion of the models; a precise statement will be theorem 1 in Sec.III and it will rely on a property that we shall call *local dynamics*: the proof is achieved by showing that in the models considered the local dynamics property holds as a consequence of the theorems 2-9, each of which is interesting on its own right, discussed in the sections following Sec.III.

A classical model for nonequilibrium statistical mechanics, *e.g.* see [2], is a *test system* in a container Ω_0, and one or more containers Ω_j adjacent to it and enclosing the *interaction systems*.

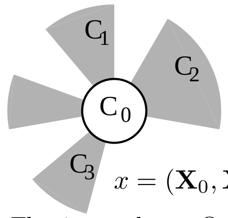

Fig.1: *The* $1+\nu$ *boxes* $\Omega_j \cap \Lambda$, $j = 0, \ldots, \nu$, *are marked* $\mathcal{C}_0, \mathcal{C}_1, \ldots, \mathcal{C}_\nu$ *and contain* $N_0, N_1, \ldots, N_\nu$ *particles with positions and velocities denoted* $\mathbf{X}_0, \mathbf{X}_1, \ldots, \mathbf{X}_\nu$, *and* $\dot{\mathbf{X}}_0, \dot{\mathbf{X}}_1, \ldots, \dot{\mathbf{X}}_\nu$, *respectively.*

To fix the ideas the geometry that will be considered can be imagined (see Fig.1, keeping in mind that it is just an example for convenience of exposition and which could be widely changed) as follows:

(1) The *test system* consists of particles enclosed in a sphere $\Omega_0 = \Sigma(D_0)$ of radius D_0 centered at the origin.

(2) The *interaction systems* consist of particles enclosed in regions Ω_j which are disjoint sectors in $\mathbb{R}^d$, *i.e.* disjoint semiinfinite "spherically truncated" cones adjacent to Ω_0, of opening angle ω_j and axis $\mathbf{k}_j$: $\Omega_j = \{\xi \in \mathbb{R}^d, |\xi| > D_0, \xi \cdot \mathbf{k}_j < |\xi|\,\omega_j\}$, $j = 1, \ldots, \nu$.

The initial configurations x of positions and velocities will be supposed to contain finitely many particles in each unit cube. Thus the *test system* will consist of *finitely many particles*, while the *interaction systems are infinitely extended*.

The motion starting from x must be defined by first *regularizing* the equations of motion (which are infinitely many and therefore a "solution" has to be shown to exist). The regularization considered here will be that only the (finitely many) particles of the initial data x inside an artificial finite ball $\Lambda = \Sigma(r)$ of radius $r > D_0$ will be supposed moving.

I.e. for the same initial data x only the particles in $\Omega_0, \Omega_1 \cap \Lambda, \ldots, \Omega_\nu \cap \Lambda$ will move and kept inside Λ by an *elastic reflection* boundary condition at the boundary of Λ, while they will never reach the boundaries of the Ω_j's because of the action of a force, modeling the walls of the Ω_j and diverging near them.

The particles of x located outside the container $\Omega_0 \cup \cup_{j>0}(\Omega_j \cap \Lambda)$ are imagined immobile in the initial positions and influence the moving particles only through the force that the ones of them close enough to the boundary of Λ exercise on the particles inside Λ.

In the "*thermodynamic limit*", which will be of central interest here, the ball Λ grows to ∞ and the particles that eventually become internal to Λ start moving: in other words we approximate the infinite volume dynamics with a finite volume one, called Λ–*regularized*, and then take an infinite volume limit.

A configuration x will be imagined to consist of a configuration $(\mathbf{X}_0, \dot{\mathbf{X}}_0)$ with $\mathbf{X}_0$ contained in the sphere $\Sigma(D_0)$, delimiting the container Ω_0 of the test systems, and by n configurations $(\mathbf{X}_j, \dot{\mathbf{X}}_j)$ with $\mathbf{X}_j \subset \Omega_j \cap \mathbb{R}^d$), $j = 1, \ldots, \nu$:

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

$$x = (\mathbf{X}_0, \dot{\mathbf{X}}_0, \mathbf{X}_1, \dot{\mathbf{X}}_1, \ldots, \mathbf{X}_\nu, \dot{\mathbf{X}}_\nu) \stackrel{def}{=} (\mathbf{X}, \dot{\mathbf{X}}) \tag{1.1}$$

with $\mathbf{X}_j \subset \Omega_j$ 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 $\mathbf{X}$. If $\Lambda = \Omega \cap \Sigma(r)$ and $x \in \mathcal{H}$ we shall denote x_Λ the positions and velocities of the particles of x located in Λ together with the positions of the particles of x outside Λ.

The particles of x located outside Λ will be regarded as immobile. The particles are supposed to interact with each other via a potential φ and with the walls with a potential ψ:

Interaction: *Interparticle interaction will be through a pair potential φ with finite range r_φ smooth, decreasing and positive at the origin. The walls of the containers Ω_j are represented by a smoooth decreasing potential $\psi \ge 0$ of range $r_\psi \ll r_\varphi$ and diverging as an inverse power of the distance to the walls.*

Hence the potential φ is *superstable* in the sense of [3]: a property that will play an important role in the following. The value of the potential φ at midrange will be denoted $\overline{\varphi}$ and $0 < \overline{\varphi} < \varphi_0 \stackrel{def}{=} \varphi(0)$; the wall potential at a point q at distance r from a wall will be supposed to be given by

$$\psi(q) = \big(\frac{r_\psi}{2r}\big)^\alpha \varphi_0, \qquad r \le \frac{r_\psi}{2} \tag{1.2}$$

with $\alpha > 0$ and r equal to the distance of q to the wall; for larger r it continues, smoothly decreasing, reaching the value 0 at $r = r_\psi$. The choice of ψ as proportional to φ_0 limits the number of dimensional parameters, but it could be made general. The restriction $r_\psi \ll r_\varphi$ is required to facilitate the interaction between particles in Ω_0 and particles in $\cup_{j>0}\Omega_j$.

The particles in Ω_0 are supposed to interact with all the others but the particles in Ω_j interact only with the ones in $\Omega_j \cup \Omega_0$: *the test system in Ω_0 interacts with all thermostats but each thermostat interacts only with the system*, see Fig.1.

The equations of the Λ–regularized motion (see Fig.1), aside from the reflecting boundary condition on the artificial boundary of Λ, concern only the particles in $\Omega_0 \cup \cup_{j>0}(\Omega_j \cap \Lambda)$ and will be

$$\begin{aligned} m\ddot{\mathbf{X}}_{0i} =& -\partial_i U_0(\mathbf{X}_0) - \sum_{j>0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \boldsymbol{\Phi}_i(\mathbf{X}_0)\\ m\ddot{\mathbf{X}}_{ji} =& -\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) - a\,\alpha_j \dot{\mathbf{X}}_{ji} \end{aligned} \tag{1.3}$$

where (1) the parameter a will be $a = 1$ or $a = 0$ depending on the model considered;

(2) the potential energies $U_j(\mathbf{X}_j)$, $j \ge 0$ and, respectively, $U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$ denote the internal energies of the various systems and the potential energy of interaction between the system and the thermostats; hence for $\mathbf{X}_j \subset \Omega_j \cap \Lambda$ the U_j's are:

$$\begin{aligned} U_j(\mathbf{X}_j) =& \sum_{q\in\mathbf{X}_j} \psi(q) + \sum_{q,q'\in\mathbf{X}_j, q\in\Lambda} \varphi(q-q')\\ U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) =& \sum_{q\in\mathbf{X}_0, q'\in\mathbf{X}_j} \varphi(q-q'); \end{aligned} \tag{1.4}$$

(3) the first label in Eq.(1.3), $j = 0$ or $j = 1, \ldots, \nu$ respectively, refers to the test system or to a thermostat, while the second indicates the derivatives with respect to the coordinates of the points in the corresponding container. Hence the labels i in the subscripts (j, i) have N_j values and each i corresponds (to simplify the notations) to d components;

(4) the multipliers α_j are, for $j = 1, \ldots, \nu$,

$$\begin{aligned} \alpha_j \stackrel{def}{=}& \frac{Q_j}{d\,N_j k_B T_j(x)/m}, \qquad \text{with}\\ Q_j \stackrel{def}{=}& -\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j), \end{aligned} \tag{1.5}$$

where $\frac{d}{2}\,N_j\,k_B\,T_j(x) \stackrel{def}{=} K_{j,\Lambda}(\dot{\mathbf{X}}_j) \stackrel{def}{=} \frac{m}{2}\dot{\mathbf{X}}_j^2$ and α_j are chosen so that $K_{j,\Lambda}(\dot{\mathbf{X}}_j) + U_{j,\Lambda}(\mathbf{X}_j) = E_{j,\Lambda}$ are *exact constants of motion if* $a = 1$: the subscript Λ will be omitted unless really necessary. A more general model to which the analysis that follows also applies is in [4].

(5) The forces $\boldsymbol{\Phi}(\mathbf{X}_0)$ are, positional, *nonconservative*, smooth "stirring forces", possibly absent.

(6) In the case of Λ-regularized thermostatted dynamics we shall consider only initial data x for which the kinetic energies $K_{j,\Lambda}(\dot{\mathbf{X}}_j)$ of the particles in the $\Omega_j \cap \Lambda$'s are > 0 for all large enough Λ. Then the time evolution is well defined for $t < t_\Lambda(x)$ where $t_\Lambda(x)$ is defined as the maximum time for which the kinetic energies remain positive (hence the equations of motion remain well defined because the denominators in the α_j stay positive). It will be important to remark that if $t_\Lambda(x) < +\infty$ the moving particles positions and velocities have a limit even as $t \to t_\Lambda(x)$ because the accelerations $\alpha_j \dot q_{ji}$ remain bounded even though $\alpha_j \to \infty$ (by the Schwartz inequality a bound on $\alpha_j \dot q_{ji}$ could be $N_\Lambda^2 \,|\max|\partial\varphi|$ if N_Λ is the number of particles in Λ).

The equations of motion with $a = 1$ will be called Λ–regularized *isoenergetically thermostatted* because the energies $E_j = K_j + U_j$ stay exactly constant for $j > 0$ and equal to their initial values E_j. The equations with $a = 0$ in Eq.(1.3) will be considered together with the above and called the Λ–regularized *Hamiltonian equations*.

The qualifier "Hamiltonian" refers to case $a = 0$ in which *no dissipation* occurs even though, strictly speaking, the equations, unless $\boldsymbol{\Phi} = 0$, are still not Hamiltonian (in spite of $\alpha_j = 0$).

Remark that Q_j is the work done, per unit time, by the test system on the particles in the j-th thermostat.

The *essential physical requirement* that the thermostats should have a well defined temperature and density is satisfied by an appropriate selection of the inital conditions. The guiding idea is that the thermostats should be so large that the energy that the test system transfers to them, per unit time in the form of work Q_j, is acquired without changing, not at least in the thermodynamic limit, the average values of the densities and kinetic energies (*i.e.* temperatures) of the thermostats in any finite observation time $\Theta > 0$..

To impose the latter requirement, in the thermodynamic limit, the values N_j, E_j will be such that $\frac{N_j}{|\Omega_j\cap\Lambda|} \xrightarrow[\Lambda\to\infty]{} \delta_j$ and, for $j > 0$, $\frac{E_j}{|\Omega_j\cap\Lambda|} \xrightarrow[\Lambda\to\infty]{} e_j$: with $\delta_j, e_j > 0$ fixed in a sense that is specified by a choice of the initial data that will be studied, and whose physical meaning is that of imposing the values of density and temperature in the termostats, for $j > 0$.

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 $\Lambda_0 \to \infty$ of the finite volume grand canonical distributions on $\mathcal{H}$*

$$\begin{aligned} &\mu_{0,\Lambda_0}(dx) = const\ e^{-H_{0,\Lambda_0}(x)}\, dx, \qquad \text{with} \\ &H_{0,\Lambda_0}(x) \stackrel{def}{=} \sum_{j=0}^{\nu} \beta_j (K_{j,\Lambda_0}(x) - \lambda_j N_{j,\Lambda_0} + U_{j,\Lambda_0}(x)) \\ &\beta_j \stackrel{def}{=} \frac{1}{k_B T_j} > 0,\ \lambda_j \in \mathbb{R}, \end{aligned} \tag{1.6}$$

Remarks: (a) The values $\beta_0 = \frac{1}{k_B T_0} > 0, \lambda_0 \in \mathbb{R}$, are also fixed, although they bear no particular physical meaning because the test system is kept finite.
(b) Here $\boldsymbol{\lambda} = (\lambda_0, \lambda_1, \ldots \lambda_\nu)$ and $\mathbf{T} = (T_0, T_1, \ldots, T_\nu)$ are fixed *chemical potentials* and *temperatures*, and Λ_0 is a ball centered at the origin and of radius r_0.
(c) The distribution μ_0 is a Gibbs distribution obtained by taking the "thermodynamic limit" $\Lambda_0 \to \infty$. Notice that μ_0 is a product of independent Gibbs distributions because H_0 does not contain the interaction potentials $U_{0,j}$.
(d) Λ_0 should not be confused with the regularization sphere Λ: it is introduced here and made, right away, ∞ only to define μ_0.
(e) The theory of the thermodynamic limit implies the existence of the limit distribution μ_0, either at low density and high temperature or on subsequences, [5]. In the second case (occurring when there are phase transitions at the chosen values of the thermostats parameters) boundary conditions have to be imposed that imply that the thermostats are in a pure phase: for simplicity such exceptional cases will not be considered; this will be referred to as a "no-phase transitions" restriction.

Main result: *In the thermodynamic limit, the thermostatted evolution, within any prefixed time interval $[0, \Theta]$, becomes the Hamiltonian evolution at least on a set of configurations which have probability 1 with respect to the initial distribution μ_0, in spite of the non stationarity of the latter.*

II. NOTATIONS AND SIZES

The initial data will be naturally chosen at random with respect to μ_0. Let the "pressure" in the j-th thermostat be defined by $p_j(\beta, \lambda; \Lambda_0) \stackrel{def}{=} \frac{1}{\beta\,|\Omega_j\cap\Lambda_0|} \log Z_{j,\Lambda_0}(\beta, \lambda)$ with

$$Z_{\Lambda_0}(\beta, \lambda) = \sum_{N=0}^{\infty} \int \frac{dx_N}{N!} \cdot e^{-\beta(-\lambda N + K_j(x_N) + U_j(x_N))} \tag{2.1}$$

where the integration is over positions and velocities of the particles in $\Lambda_0 \cap \Omega_j$. Defining $p(\beta, \lambda)$ as the thermodynamic limit, $\Lambda_0 \to \infty$, of $p_j(\beta, \lambda; \Lambda_0)$ we shall say that the thermostats have densities δ_j, temperatures T_j, energy densities e_j and potential energy densities u_j, for $j > 0$, given by equilibrium themodynamics, *i.e.*:

$$\begin{aligned} &\delta_j = -\frac{\partial p(\beta_j, \lambda_j)}{\partial \lambda_j}, \quad k_B T_j = \beta_j^{-1} \\ &e_j = -\frac{\partial \beta_j p(\beta_j, \lambda_j)}{\partial \beta_j} - \lambda_j \delta_j, \qquad u_j = e_j - \frac{d}{2}\delta_j \beta_j^{-1} \end{aligned} \tag{2.2}$$

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.

In general the Λ–regularized time evolution changes the measure of a volume element in phase space by an amount related to (but different from) the variation of the Liouville volume. The variation per unit time and unit mass of a volume element, measured via μ_0 in the sector of phase space containing $N_j > 0$ particles in $\Omega_j \cap \Lambda$, $j = 0, 1, \ldots, \nu$, can be computed and is, under the Λ–regularized dynamics,

$$\sigma(x) = \sum_{j>0} \frac{Q_j}{k_B T_j(x)} \, (1 - \frac{1}{d\, N_j}) + \beta_0(\dot{K}_0 + \dot{U}_0)) \tag{2.3}$$

as it follows by adding the time derivative of $\beta_0(K_0 + U_0)$ to the divergence of Eq.(1.3) (regarded as a first order equation for the q's and $\dot{q}$'s) using the expression in Eq.(1.5) for α_j.

Remarks: (1) The dynamics given by the Eq.(1.3) or by the same equations with $\alpha_j \equiv 0$ are different.
(2) The relation $\beta_0\,(\dot{K}_0 + \dot{U}_0) = \beta_0\,(\boldsymbol{\Phi} \cdot \dot{\mathbf{X}}_0 - \sum_{j>0}(\dot{U}_{0j} - Q_j))$ is useful in studying Onsager reciprocity and Green-Kubo formulae, [6].

(3) It is also interesting to consider *isokinetic* thermostats: the multipliers α_j are then so defined that K_j is an exact constant of motion: calling its value $\frac32 N_j k_B T_j$ the multiplier α_j becomes

$$\alpha_j \stackrel{def}{=} \frac{Q_j - \dot U_j}{d\, N_j k_B T_j/m}, \tag{2.4}$$

with Q_j defined as in Eq.(1.5). They have been studied heuristically, from the present point of view, in [1].

Choose initial data with the distribution μ_0 and let $x \to S_t^{(\Lambda,a)}x$, $a=0,1$, be the solution of the Λ–regularized equations of motion with $\alpha_j=0$ ($a=0$, "Hamiltonian thermostats") or a;ternatively α_j given by Eq.(1.5) ($a=1$, "isoenergetic thermostats"), *assuming* $t<t_\Lambda(x)$.

Let $S_t^{(a)}x$ be the infinite volume dynamics $\lim_{\Lambda\to\infty} S_t^{(\Lambda,a)}x$, $a=0,1$, *provided the limit exists.* Let

$$\begin{aligned} &x^{(\Lambda,1)}(t) \stackrel{def}{=} S_t^{(\Lambda,1)}x, \qquad x^{(\Lambda,0)}(t) \stackrel{def}{=} S_t^{(\Lambda,0)}x,\\ &x^{(0)}(t) \stackrel{def}{=} S_t^{(0)}x. \end{aligned} \tag{2.5}$$

In the Hamiltonian case the existence of a solution to the equations of motion poses a problem only if we wish to study the $\Lambda\to\infty$ limit, *i.e.* in the case in which the thermostats are infinite. For Λ finite $S_t^{(\Lambda,0)}x$ is well defined with μ_0-probability 1 as in [7].

In the thermostatted case the kinetic energy appearing in the denominator of α_j, see Eq.(1.5), can be supposed to be >0 with μ_0–probability 1. However it can become 0 at some later time $t_\Lambda(x)$ (see item (6), p.2, and the example at the end of Sec.III). In the course of the analysis it will be proved that with μ_0–probability 1 it is $t_\Lambda(x) \xrightarrow[\Lambda\to\infty]{} \infty$; therefore $S_t^{(\Lambda,1)}x$ is eventually well defined.

We shall denote $(\mathbf{X}_j^{(\Lambda,a)}(t), \dot{\mathbf{X}}_j^{(\Lambda,a)}(t))$ or $(S_t^{(\Lambda,a)}x)_j$ or $x_j^{(\Lambda,a)}(t)$ the positions and velocities of the particles of $S_t^{(\Lambda,a)}x$ in Ω_j. And by $x_{ji}^{(\Lambda,a)}(t)$ the pairs of positions and velocities $(q_i^{(\Lambda,a)}(t), \dot q_i^{(\Lambda,a)}(t))$ with $q_i\in\Omega_j$.

Then a particle with coordinates $(q_i,\dot q_i)$ at $t=0$ in, *say*, the j-th container evolves, see Eq.(1.3), as

$$\begin{aligned} q_i(t) =& q_i(0) + \int_0^t \dot q_i(t')\,dt'\\ \dot q_i(t) =& e^{-\int_0^t a\,\alpha_j(t')dt'}\,\dot q_i(0)\\ &+\int_0^t e^{-\int_{t''}^t a\,\alpha_j(t')dt'}\,\frac{F_i(t'')}{m}\,dt'' \end{aligned} \tag{2.6}$$

where $F_i(t) = -\partial_{q_i}\big(U_j(\mathbf{X}_j(t)) + U_{j,0}(\mathbf{X}_0(t),\mathbf{X}_j(t))\big) + \delta_{j0}\Phi_i(\mathbf{X}_0(t))$ and $\mathbf{X}_j(t)$ denotes $\mathbf{X}_j^{(\Lambda,a)}(t)$ or $\mathbf{X}_j^{(0)}(t)$.

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

It is convenient to work with dimensionless quantities: therefore suitable choices of the units will be made. If Θ is a prefixed time which is the maximum time that will be considered, then

$$\begin{aligned} &\varphi_0\,:\,\text{(energy scale)},\ r_\varphi\,:\,\text{(length scale)},\\ &\Theta\,:\,\text{(time scale)},\ v_1=\sqrt{\frac{2\varphi(0)}{m}}\ \text{(velocity scale)} \end{aligned} \tag{2.7}$$

are natural units for measuring energy, length, time, velocity, respectively.

It will be necessary to estimate quantitatively the size of various kinds of energies of the particles, of a configuration x, which are localized in a region Δ. Therefore introduce, for any region Δ, the following dimensionless quantities:

$$\begin{aligned} &(a)\ N_\Delta(x), N_{j,\Delta}(x) \text{ the number of particles of } x\\ &\qquad \text{located in } \Delta \text{ or, respectively, } \Delta\cap\Omega_j\\ &(b)\ E_\Delta(x) \stackrel{def}{=} \max_{q_i\in\Delta}\big(\frac{m\dot q^2}{2}+\psi(q)\big)/\varphi_0\\ &(c)\ U_\Delta(x) = \frac12 \sum_{q_i,q_j\in\Delta,\,i\ne j} \varphi(q_i-q_j)/\varphi_0\\ &(d)\ V_\Delta(x) = \max_{q_i\in\Delta}\frac{|\dot q_i|}{v_1} \end{aligned} \tag{2.8}$$

The symbol $\mathcal{B}(\xi,R)$ will denote the ball centered at ξ and with radius $R\,r_\varphi$. With the above notations the *local dimensionless energy* in $\mathcal{B}(\xi,R)$ will be defined as $W(x;\xi,R) \stackrel{def}{=} E_{\mathcal{B}(\xi,R)}(x) + U_{\mathcal{B}(\xi,R)}(x) + N_{\mathcal{B}(\xi,R)}(x)$ or, more explicitly,

$$\begin{aligned} W(x;\xi,R) \stackrel{def}{=}& \frac{1}{\varphi(0)}\sum_{q_i\in\mathcal{B}(\xi,R)}\Big(\frac{m\dot q_i^2}{2}+\psi(q_i)\\ &+\frac12\sum_{q_i,q_j\in\mathcal{B}(\xi,R),\,i\ne j}\varphi(q_i-q_j)+\varphi(0)\Big) \end{aligned} \tag{2.9}$$

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

$$\mathcal{E}_\zeta(x) \stackrel{def}{=} \sup_\xi \sup_{R>g_\zeta(\frac{\xi}{r_\varphi})} \frac{W(x;\xi,R)}{R^d} \tag{2.10}$$

If $\mathcal{H}$ is the space of the locally finite configurations (*i.e.* containing finitely many particles in any finite region) and let $\mathcal{H}_\zeta\subset\mathcal{H}$ be the configurations with

$$(1)\ \ \mathcal{E}_\zeta(x)<\infty, \qquad (2)\ \ \frac{K_{j,\Lambda}}{|\Lambda\cap\Omega_j|} > \frac12\frac{\delta_j\,d}{2\beta_j} \tag{2.11}$$

for all $\Lambda = \mathcal{B}(O,L)$ large enough and for δ_j, T_j, given by Eq.(2.2). Let $N_{j,\Lambda}$, $U_{j,\Lambda}, K_{j,\Lambda}$ denote the number of particles and their potential or kinetic energy in $\Omega_j \cap \Lambda$. Each set $\mathcal{H}_\zeta$ has μ_0-probability 1 for $\zeta \ge 1/d$, see Appendix A,B.

III. EQUIVALENCE: ISOENERGETIC VERSUS HAMILTONIAN

It can be expected (and proved here if $d = 1,2$) adapting to the present situation a conjecture proposed in [1], that the following property holds for the time evolutions $x_i^{(\Lambda,a)}(t) \stackrel{def}{=} (q_i^{(\Lambda,a)}(t), \dot q_i^{(\Lambda,a)}(t))$, $a = 0,1$, of an initial configuration x:

Local dynamics *Let* $d = 1,2,3$. *Given* $\Theta > 0$, *with* μ_0*–probability* 1 *then for* $t \in [0,\Theta]$,
(1) The limits $x^{(a)}(t) \stackrel{def}{=} \lim_{\Lambda\to\infty} x^{(\Lambda,a)}(t)$ *("thermodynamic limits") exist for all* $t \le \Theta$ *and* $a = 0,1$.
(2) For $t \le \Theta$, $x^{(\Lambda,1)}(t)$ *satisfies the second of Eq.(2.11).*
(3) The function $t \to x^{(0)}(t)$ *solves uniquely the Hamiltonian equations in a subspace of* $\mathcal{H}$ *to which also* $x^{(1)}(t)$ *belongs (explicit, sufficient, bounds are described in theorem 7).*

Remarks: (a) The limits of $x^{(\Lambda,a)}(t)$, as $\Lambda \to \infty$, are understood in the sense that for any ball Δ whose boundary does not contain a particle of $x^{(0)}(t)$ the labels of the particles of $x^{(a)}(t)$ and those of the particles in $x^{(\Lambda,a)}(t)$ which are in Δ are the same and for each i the limits $\lim_{\Lambda\to\infty}(q_i^{(\Lambda,a)}(t), \dot q_i^{(\Lambda,a)}(t))$ exist and are continuous, together with their first two derivatives for each i.

(b) Uniquess in (3) can be given several meanings. The simplest is to require uniqueness in the spaces $\mathcal{H}_\zeta$ for $\zeta \ge 1/d$ fixed: and theorem 9 shows that for $d = 1,2$ one could suppose such simpler property. However our result is more general and we have left deliberately undetermined which subspace is meant in (3) so that the determination of the subspace has to be considered part of the problem of establishing a local dynamics property. The generality might become relevant in studying the case $d = 3$, where even in equlibrium there is no proof that the evolution of data in $\mathcal{E}_\zeta$ remains in the same space.

(c) Recalling the characteristic velocity scale (namely $v_1 = \sqrt{2\varphi(0)/m}$), the initial speed of a particle located in $q \in \mathbb{R}^d$, $|q| > r_\varphi$, is bounded by $v_1\sqrt{\mathcal{E}} g_{1/d}(q/r_\varphi)^{\frac{d}{2}}$; and the distance to the walls of the particle located at q is bounded by $(\sqrt{\mathcal{E}} g_{1/d}(q/r_\varphi)^d)^{-1/\alpha}\, r_\varphi$.

(d) Hence for $|q|$ large they are, respectively, bounded proportionally to $[(\log|q|/r_\varphi)^{\frac{1}{d}}]^{\frac{d}{2}}$ and $[(\log|q|/r_\varphi)^{\frac{1}{d}}]^{\frac{1}{\alpha}}$: this says that locally the particles have, initially, a finite density and reasonable energies and velocity distributions (if measured on boxes of a "logarithmic scale"). The theorem 9 in appendix B will show that this property remains true for all times, with μ_0 probability 1.

(e) An implication is that Eq.(2.6) has a meaning at time $t = 0$ with μ_0–probability 1 on the choice of the initial data x, because $\mathcal{E}(x) < \infty$.

(f) The further property that the thermostats are *efficient*: *i.e.* the work performed by the external non conservative forces is actually absorbed by the thermostats in the form of heat Q_j, so that the system can eventually reach a stationary state, will not be needed because in a finite time the external forces can only perform a finite work (if the dynamics is local).

(g) It has also to be expected that, with μ_0–probability 1, the limits in item (2) of Eq.(2.11) should exist and be equal to $\frac{d\,\delta_j}{2\beta_j}$ for almost all $t \ge 0$ respectively: this is a question left open (as it is not needed for our purposes).

Assuming the local dynamics property, equivalence, *i.e.* the property $x^{(0)}(t) \equiv x^{(1)}(t)$ for any finite t, can be established as in [1]. This is recalled in the next few lines of this section.

In the thermostatted case, with Λ–regularized motion, it is

$$|\alpha_j(x)| = \frac{|\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)|}{\dot{\mathbf{X}}_j^2} \tag{3.1}$$

The force between pairs located in Ω_0, Ω_j is bounded by $F \stackrel{def}{=} \max|\partial\varphi(q)|$; the numerator of Eq.(3.1) can then be bounded by $F N_0 \sqrt{\overline{N}_\Theta}\sqrt{2K_j/m}$ where N_0 is the number of particles in $\mathcal{C}_0$ and $\overline{N}_\Theta$ bounds the number of thermostat particles that can be inside the shell of radii D_0, $D_0 + r_\varphi$ for $0 \le t \le \Theta$ (having applied Schwartz' inequality).

Remark that the bound on $\overline{N}_\Theta$ exists by the local evolution hypothesis (see (1) and remark (a)) but, of course, is not uniform in the initial data x).

For $0 \le t \le \Theta$ and for large enough Λ, by Schwartz' inequality,

$$|\alpha_j| \le \frac{\sqrt{m} F N_0 \sqrt{\overline{N}_\Theta}}{\sqrt{2K_{j,\Lambda}(x^{(1,\Lambda)}(t))}} \le \frac{\sqrt{m} F N_0 \sqrt{\overline{N}_\Theta}}{\sqrt{|\Omega_j \cap \Lambda| \delta_j d/2\beta_j}} \tag{3.2}$$

having used property (2) of the local dynamics assumption; letting $\Lambda \to \infty$ it follows that $\alpha_j \xrightarrow[\Lambda\to\infty]{} 0$.

Taking the limit $\Lambda \to \infty$ of Eq.(2.6) *at fixed* i, this means that, *with* μ_0*–probability* 1, the limit motion as $\Lambda \to \infty$ (with β_j, λ_j, $j > 0$, constant) satisfies

$$q_i(t) = q_i + \int_0^t \dot q_i(t')dt', \; \dot q_i(t) = \dot q_i + \int_0^t F_i(t'')dt'' \tag{3.3}$$

i.e. Hamilton's equations, see Eq.(2.6); and the solution to such equations is unique with probability 1, (having again used assumption (3) of the local dynamics). In conclusion

Theorem 1: *If the dynamics is local in the above sense then in the thermodynamic limit the thermostatted evolution, within any prefixed time interval* $[0,\Theta]$*, becomes the Hamiltonian evolution at least on a set of configurations which have probability* 1 *with respect to the initial distribution* μ_0*, in spite of the non stationarity of the latter.*

Suppose, in other words, that the initial data are sampled with the Gibbs distributions for the thermostat particles (with given temperatures and densities) and with an *arbitrary distribution* for the finite system in Ω_0 with density with respect to the Liouville volume (for instance with a Gibbs distribution at temperature T_0 and chemical potential λ_0 as in Eq.(1.6)).

Then, *in the thermodynamic limit*, the time evolution is the same that would be obtained, in the same limit $\Lambda\to\infty$, via a isoenergetic thermostat acting in each container $\Omega_j\cap\Lambda$ and keeping its total energy (in the sector with N_j particles) constant and with a density equal (asymptotically as $\Lambda\to\infty$) to e_j.

The difficulty of proving the locality property (2) cannot be underestimated, although it might seem, at first sight, "physically obvious": the danger is that evolution implies that the thermostat particles *grind to a stop* in a finite time converting the kinetic energy entirely into potential energy. The consequence would be that α_j becomes infinite and the equations even ill defined. As a consequence it is natural to expect, as stated in the local dynamics assumption, only a result in μ_0–probability. This can be better appreciated if the following *counterexample*, in the Hamiltonian case, is kept in mind.

Consider an initial configuration in which particles are on a square lattice (adapted to the geometry): regard the lattice as a set of adjacent tiles *with no common points*. Imagine that the particles at the four corners of each tile have velocities of equal magnitude pointing at the center of the tile. Suppose that the tiles sides are $> r_\varphi$. If $\varphi(0)$ is large enough all particles come to a stop in the same finite time and at that moment all kinetic energy has been converted into potential energy: at time 0 all energy is kinetic and later all of it is potential. Certainly this example, which concerns a single event that has, therefore, 0 probability in μ_0, shows that some refined analysis is necessary: the thermostatted evolution $x^{(\Lambda,1)}(t)$ might be not even be defined because the denominator in the definition of α_j might become 0.

It should be stressed that the thermostats models considered here preserve even at finite Λ an important symmetry of nature: *time reversal*: this ceertainly explains the favor that they have received in recent years in the simulations.

Finally a corollary will be that the non dissipative Hamiltonian motion and the dissipative thermostatted motions, although different at finite volume become identical in the thermodynamic limit: neither conserves phase space volume (measured with μ_0) but in both cases the entropy production rate coincides with the phase space μ_0–volume contraction.

IV. FREE THERMOSTATS

The need for interaction between the particles in order to have a physically sound thermostat model has been stressed in [8, 9] and provides a measure of the importance of the problems met above.

The above discussion is heuristic because the local dynamics assumption is not proved. However if the model is modified by keeping only the interaction φ between the test particles and between test particles and thermostat particles, but suppressing the interactions between particles in the same Ω_j, $j>0$, and, furthermore, replacing the wall potentials by an elastic collision rule. *I.e.* supposing $U_j(\mathbf{X}_j)\equiv 0$, $j>0$, together with the collision rule, the analysis can be further pursued and completed. This will be referred as the "*free thermostats*" model.

It can be remarked that in the Hamiltonian case this is the classical version of the Hamiltonian thermostat models that could be completely treated in quantum mechanics, [2].

Let Λ_n be the ball $\mathcal{B}(O,2^n)$ of radius $2^n r_\varphi$ and $n\ge n_0$ be such that $2^{n_0}r_\varphi\ge D_0+r_\varphi$; if $\overline{N}$ bounds the number of particles in the ball D_0+r_φ up to an arbitrarily prefixed time Θ, the first inequality Eq.(3.2) and the supposed isoenergetic evolution (which in this case is *also* isokinetic)

$$|\alpha_j|\le N_0F\sqrt{\frac{\overline{N}}{2K_j/m}}\le\frac{N_0F}{\sqrt{d\,k_BT_j/m}}\stackrel{def}{=}\ell. \tag{4.1}$$

It follows that, for $\zeta\ge1$, the speed of the particles initially in the shell Λ_n/Λ_{n-1} with radii $2^nr_\varphi, 2^{n+1}r_\varphi$ will remain within the initial speed by, at most, a factor $\lambda^{\pm1}=e^{\pm\ell\Theta}$. The initial speed of the latter particles is bounded by, see Eq.(2.10),

$$V_n=v_1\sqrt{\mathcal{E}_\zeta(x)}\,n^{\frac12\zeta d} \tag{4.2}$$

Hence if $n(\Theta)$ is the smallest value of n for which the inequality $2^nr_\varphi-V_n\,\lambda\,\Theta<D_0+r_\varphi$ *does not hold* no particle at distance $>2^{n(\Theta)+1}r_\varphi$ can interact with the test system.

This means that $\overline{N}\le\mathcal{E}_\zeta(x)\,2^{\,(n(\Theta)+1)\,d}$ and the dynamics $x^{(n,a)}(t)$ becomes a finitely many particles dynamics involving $\le N_0+\overline{N}$ particles at most.

From the equations of motion for the $N_0+\overline{N}$ particles we see that their speed will never exceed

$$V_\Theta=(\overline{V}+F\,N_0\,\overline{N}\,\Theta)\,\lambda \tag{4.3}$$

if $\overline{V}$ is the maximum of their initial speeds. In turn this means that for n large enough a better bound holds on α_j,

$$|\alpha_j\dot q_i|\le\frac{N_0\overline{N}V_\Theta^2F}{\omega_{j,n}2^{dn}r_\varphi^d\delta k_BT/m}\xrightarrow[n\to\infty]{}0 \tag{4.4}$$

with $T = \min_{j>0} T_j$ and $\delta = \min_{j>0} \delta_j$ and $\omega_{j,n} 2^{dn} r_\varphi^d$ bounds below (for suitable $\omega_{j,n}$) the volume of $\Omega_j \cap \Lambda_n$.

Hence, for $a = 0, 1$, it is $\lim_{n\to\infty} x^{(n,a)}(t) = x^{(0)}(t)$, and *also* the dynamics is local in the above sense. This completes the analysis of free thermostats and proves:

Theorem 2: *Free isoenergetic and Hamiltonian thermostats are equivalent in the thermodynanic limit*

Notice that essential use has been made of the property that, in absence of interaction among pairs of thermostat particles and in presence of perfectly elastic walls, isokinetic and isoenergetic dynamics coincide: so the denominators in Eq.(4.1) are constant.

It would be possible to consider non rigid walls, modeled by a soft potential ψ diverging near them. We do not perform the analysis because it is a trivial consequence of the analysis that follows. We have chosen the example of this section because it pedagogically illustrates well the simplest among the ideas of the coming analysis.

V. KINEMATICS

The proof of the local dynamics property will require controlling the maximal particles speeds, the number of particles interacting with any given one as well as their number in any finite region. This will be achieved by proving bounds on the local energies $W(x;\xi,R)$, Eq.(2.9).

In this section we shall prove bounds at time 0, see Eq.(5.3) below as a preparation to the next section where we shall use energy conservation to extend the bounds to positive time.

To study general thermostats in dimension d consider the dimensionless sum of the energy, measured in units of φ_0, and the particle number in the ball $\mathcal{B}(\xi,R)$, with center ξ and radius $r_\varphi R$ as defined in Eq.(2.9) and denoted $W(x;\xi,R)$.

The potential φ is superstable so that the number N of points in a region Δ can be bounded in terms of the potential energy U in the same region and of $\varphi_0 = \varphi(0)$ and $\overline{\varphi} > 0$ (defined after Eq.(1.4)). This is checked below.

In fact, by the dimensionless energy definition in Eq.(2.9), $W \ge (\frac{U}{\varphi_0} + N) \ge \frac{\overline{\varphi}}{2\varphi_0} \sum_p N_p^2$ with the sum running over labels p of disjoint boxes of diameter $\frac{r_\varphi}{2}$ covering Δ and containing $N_p \ge 0$ particles (in particular: $N = \sum_p N_p$), hence over $\ell \le |\Delta|(2\sqrt{d}/r_\varphi)^d$ terms. By the Schwartz' inequality $\sqrt{\overline{\varphi}/2\varphi_0} N \le \sqrt{W\,\ell}$ gives a bound of the total number of particles in a region Δ in terms of the local dimensionless energy W:

$$N_\Delta \le C \frac{\sqrt{W}}{\sqrt{|\Delta|}}, \qquad C \stackrel{def}{=} \Big(\frac{2\varphi_0}{\overline{\varphi}}\Big)^{\frac12} \tag{5.1}$$

This is the well known "superstability estimate" (derived in our simplifying assumptions of $\varphi \ge 0$ and finite range).

Calling $\mathcal{E} \stackrel{def}{=} \mathcal{E}_{1/d}(x)$, Eq.(2.10), consider a sequence of balls $\Lambda_n = \mathcal{B}(O, 2^n)$, of radii $L_n = 2^n r_\varphi$ with $n \ge n_0$: so that $2^{n_0} r_\varphi > D_0 + r_\varphi$ and all Λ_n enclose the test system and the particles interacting with it. Given a configuration x define $N(x;\xi,R)$ the number of particles in the ball of radius $R\,r_\varphi$ centered at ξ and, given x,

$$\begin{aligned} &(1)\ V_n = \ \text{the maximum velocity in } \Lambda_n \\ &(2)\ \rho_n = \ \text{the minimum distance to } \partial(O_j \cap \Lambda_n) \\ &(3)\ \mathcal{N}_n = \max_{q_i \in \Lambda_n} N(x; q_i, 1) \end{aligned} \tag{5.2}$$

After the definition of $W, \mathcal{E}$, the *initial speed* of a particle in the ball Λ_n, $n \ge 1$, and its distance to the walls will be bounded above and respectively below by v_n, ρ_n with, see definitions Eq.(2.7),

$$V_n = v_1\,(n\mathcal{E})^{\frac12}, \quad \rho_n = \frac{r_\psi}{(n\,\mathcal{E})^{1/\alpha}}, \quad \mathcal{N}_n \le C(n\mathcal{E})^{\frac12} \tag{5.3}$$

under the assumption that the wall potential has range r_ψ and is given by Eq.(1.2); the last inequality is a consequence of the definition of W and of the above mentioned superstability.

Constant convention: From now on we shall encounter various constants that are all computable in terms of the data of the problem (geometry, mass, potentials, densities, temperatures and the (arbitrarily) prefixed time Θ) as in the above Eq.(5.1) which gives a simple example of a computation of a constant. To avoid proliferation of labels all constants will be positive and denoted $C, C', C'', \ldots, B, B', \ldots$ or $c, c', c'', \ldots, b, b', b'', \ldots$: they have to be regarded as functions of the order of appearance, non decreasing the ones denoted by capital letters and non increasing the ones with lower case letters; furthermore the constants $C, \ldots, c, \ldots$ may also depend on the parameters that we shall name $\mathcal{E}$ or, in Sec.IX, E and will be again monotonic non decreasing or non increasing, respectively, as functions of the order of appearance and of $\mathcal{E}$ or E.

Consider motions, evolving for times $0 \le t \le \Theta$, or in the thermostatted case for $0 \le t \le \min\{t_{\Lambda_n}(x), \Theta\}$, from an initial configuration x following the Λ_n-*regularized* evolution of Sec.2 with n fixed (see comment (6), p.2). Define

$$R_n(t) \stackrel{def}{=} n^{\frac1d} + \int_0^t V_n(s) \frac{ds}{r_\varphi}, \tag{5.4}$$

where $R_n(0) = g_{1/d}(2^n) = n^{1/d}$ and $V_n(s)$ is the maximum speed that a moving particle can acquire in the time interval $[0, s]$ under the Λ_n-regularized evolution.

The choice of $R_n(0) = n^{\frac1d}$ is made so that it will be possible to claim that $W(x(0); O, R(0)) \le \mathcal{E}(x(0))n$ with μ_0–probability 1, see Eq.(2.9),(2.10) and appendix A.

The dimensionless quantity $R_n(t)$ will also provide a convenient upper bound to the maximal distance a moving particle can travel during time t, in units of r_φ, following the Λ_n–regularized motion.

It will be necessary to estimate the total energy and number of particles in a ball of radius $R_n(t)r_\varphi$ around ξ assuming the particles to move with the Λ_n–regularized equations. Consider the ball around $\xi\in\mathbb{R}^d$ of radius

$$R_n(t,s)\stackrel{def}{=}R_n(t)+\int_s^t\frac{V_n(s)}{r_\varphi}\,ds\ge 1. \tag{5.5}$$

This is a ball whose radius shrinks as s increases between 0 and t at speed $V_n(s)$: therefore no particle can enter it. Abridging $x^{(\Lambda_n,a)}(\tau)$ by $x(\tau)$, this can be used to obtain a bound on the size of $W(x(\tau);\xi,R_n(t))$ in terms of the initial data $x(0)=x$ and of

$$W_n(x,R)\stackrel{def}{=}\sup_\xi W(x_n;\xi,R). \tag{5.6}$$

if x_n denotes the particles of x in $\widetilde\Lambda_n\stackrel{def}{=}\mathcal{B}(O,2^n+r_\varphi)$, *i.e* at distance $\le r_\varphi$ from Λ_n.

The analysis in the following Sec. VI, VII is taken, with a minor adaptation effort, from the version in [10, p.34] *of an idea in* [11, p.72] *and is repeated here only for completeness.*

Let $\chi_\xi(q,R)$ be a smooth function of $q-\xi$ that has value 1 in the ball $\mathcal{B}(\xi,R)$ and decreases radially to reach 0 outside the ball $\mathcal{B}(\xi,2R)$ with gradient bounded by $(r_\varphi R)^{-1}$. Let also

$$\begin{aligned}\widetilde W_n(x;\xi,R)\stackrel{def}{=}&\frac{1}{\varphi_0}\sum_{q\in\widetilde\Lambda_n}\chi_\xi(q,R)\\ &\cdot\big(\frac{m\dot q^2}{2}+\psi(q)+\frac12\sum_{q'\in\widetilde\Lambda_n}\varphi(q-q')+\varphi_0\big).\end{aligned} \tag{5.7}$$

Denoting B an estimate of how many balls of radius 1 are needed to cover a ball of radius 3 (a multiple of the radius large enough for later use in Eq.(6.3)) in $\mathbb{R}^d$ so that every pair of points at distance <1 is inside at least one of the covering balls, it follows that $W(x;\xi,2R)\le B\,W(x,R)$, see Eq.(5.5), so that for $\xi\in\Lambda_n$:

$$\begin{aligned}&W(x_n;\xi,R)\le\widetilde W_n(x;\xi,R)\le W(x_n;\xi,2R),\\ &\widetilde W_n(x;\xi,R)\le\ B\,W_n(x,R)\end{aligned} \tag{5.8}$$

Although W has a direct physical interpretation $\widetilde W$ turns out to be mathematically more convenient and, for our purposes, equivalent by Eq.(5.8).

VI. ENERGY BOUND

A. Hamiltonian systems

Considering $\widetilde W(x(s);\xi,R_n(t,s))$, for $0\le s\le t\le\Theta$, it follows that

$$\begin{aligned}\frac{d}{ds}\widetilde W_n(x(s);\xi,R_n(t,s))\le&\frac{1}{\varphi_0}\sum_{q\in\widetilde\Lambda_n}\chi_\xi(q(s),R_n(t,s))\\ \cdot\frac{d}{ds}\big(&\frac{m\dot q(s)^2}{2}+\psi(q(s))+\frac12\sum_{q'\in\widetilde\Lambda_n}\varphi(q(s)-q'(s))\big)\end{aligned} \tag{6.1}$$

because the s–derivative of $\chi_\xi(q(s),R_n(t,s))$ is ≤0 since no particle can enter the shrinking ball $\mathcal{B}(\xi,R(r,s))$ as s grows: *i.e.* $\chi_\xi(q(s),R_n(t,s))$ cannot increase.

In the Hamiltonian case a computation of the derivative in Eq.(6.1) leads, with the help of the equations of motion and setting $\chi_\xi(q(s),R_n(t,s))\equiv\chi_{\xi,q,t,s}$, to

$$\begin{aligned}\frac{d}{ds}\widetilde W_n(x(s);\xi,R_n(t,s))\le&\sum_{q\in\Omega_0}\dot q(s)\Phi(q(s))\chi_{\xi,q,t,s}\\ -\sum_{\substack{q\in\Lambda_n\\ q'\in\widetilde\Lambda_n}}&\big(\chi_{\xi,q,t,s}-\chi_{\xi,q',t,s}\big)\frac{\dot q(s)\partial_q\varphi(q(s)-q'(s))}{2\varphi_0}\end{aligned} \tag{6.2}$$

where the dot indicates a s–derivative and it has been kept in mind that positions and velocities of the particles outside Λ_n are considered, in the Λ_n–regularized dynamics, to be time independent.

Since the non zero terms have $|q(s)-q'(s)|<r_\varphi$ and the derivatives of χ are $\le(r_\varphi R_n(t,s))^{-1}$ and $|\dot q|,|\dot q'|\le V_n(s)=r_\varphi|\dot R_n(t,s)|$ it follows, setting $F=\max(|\partial\varphi|+|\Phi|)$,

$$\begin{aligned}\frac{d}{ds}\widetilde W_n(x(s);\xi,R_n(t,s))\le&\frac{Fv_1}{\varphi_0}\widetilde W_n(x(s);\xi,\frac{D_0}{r_\varphi})\\ +&\frac{Fr_\varphi}{\varphi_0}\frac{|\dot R_n(t,s)|}{R_n(t,s)}B\,\widetilde W_n(x(s);\xi,2R_n(t,s)+1)\\ \le&B^2\frac{Fv_1}{\varphi_0}(\frac{r_\varphi}{v_1}\frac{|\dot R_n(t,s)|}{R_n(t,s)}+1)\widetilde W_n(x(s);R_n(t,s))\end{aligned} \tag{6.3}$$

where $\widetilde W_n(x;R)$ is defined in analogy with Eq.(5.6). Eq.(6.3), $R_n(t,s)/R(t,0)\le2$ and $W_n(x(s),\xi,R_n(t,s))\le W_n(x(s),R_n(t,s))$ imply the inequality

$$W_n(x(s),R_n(t,s))\le e^\Gamma\,W_n(x(0),R_n(t,0)), \tag{6.4}$$

with $\Gamma\stackrel{def}{=}(\frac{Fr_\varphi}{\varphi_0}\log2+\frac{3Fv_1}{\varphi_0})\,\Theta\,B$.

B. Thermostatted systems

In the thermostatted dynamics case, Eq.(6.2),(6.3) have to be modified by adding to the r.h.s the work, per unit time, done by the thermostatic forces (measured in units of φ_0) which is, see Eq.(1.5),

$$\frac{\sum_i^* \dot q_i(s) F_i(x(s))}{\varphi_0 \sum_i \dot q_i(s)^2} \sum_{q_i\in\mathcal{B}(\xi,R_n(t,s))} \chi_\xi(q_i,R_n(t,s))\,\dot q_i(s)^2 \tag{6.5}$$

here the $*$ means restriction of the sum to the particles $q_i(t)$ in Ω_j and within distance r_φ from the boundary of Ω_0, which is a ball of radius D_0. Then Eq.(6.5) is bounded by

$$N_0\,\frac{Fv_1}{\varphi_0}\,\widetilde W_n(x(s),R_n(t,s)) \tag{6.6}$$

because the bounds of the various terms in Eq.(6.5) can be obtained as:

(a) the $\sum_i \dot q_i(s)F_i(q(s))$ by (Schwarz' inequality) $\le N_0 F(\sum_i^* \dot q_i^2)^{\frac12}(\sum_i^* 1)^{\frac12}$ with $F=\max|\partial\varphi|$. Leaving aside the factor FN_0 the rest is bounded above proportionally to $\widetilde W_n(x(s),R_n(t,s))$.
(b) the kinetic energy in the last sum in Eq.(6.5) is also bounded by the total kinetic energy and is compensated by the denominator.
(c) N_0 is bounded in terms of $\mathcal{E}$ (and constant in time).

Therefore, given n, the new inequality which replaces Eq.(6.3) in the thermostatted case gives a bound of the s-derivative $\dot{\widetilde W}_n \stackrel{def}{=} \frac{d}{ds}\widetilde W_n(x(s);\xi,R_n(t,s))$ in terms of, see Eq.(5.6),(5.8), $\widetilde W_n \stackrel{def}{=} \sup_\xi \widetilde W_n(x(s);\xi,R_n(t,s))$, namely

$$\dot{\widetilde W}_n \le C\,\Big(\frac{\dot R_n(t,s)}{R_n(t,s)}+(N_0+1)\,\frac{\overline F v_1}{\varphi_0}\Big)\,\widetilde W_n\,, \tag{6.7}$$

The second addend in Eq.(6.7) is bounded, by (c) above. The differential inequality Eq.(6.7) implies, for suitable C',C^2, functions of $\mathcal{E}$:

$$W_n(x(t),R_n(t)) \le C' W_n(x(0),R_n(t)) \le C^2 R_n(t)^d \tag{6.8}$$

for $t\le \min\{t_{\Lambda_n}(x),\Theta\}$ (see p.2, item (6)). Hence the bound on the speed, for instance for $d=2$, $\frac{V_n(t)}{v_1}\le C R_n^{d/2}$ with $R_n=R_n(\Theta)$.

C. The bound

Therefore the following *energy bound* holds:

Theorem 3: *For a suitable constant C the following energy bound holds for the Λ_n–regularized Hamiltonian or thermostatted dynamics and for $t\le\Theta$ or $t\le\min\{t_{\Lambda_n}(x),\Theta\}$, respectively,*

$$W_n(x^{(n,0)}(t),R_n(t)) \le C^2\,R_n(t)^d \tag{6.9}$$

and n large enough and $C>0$ (depending only on $\mathcal{E}$).

Remark: the inequality holds for all d's and in the Hamiltonian case the constant C can be taken $\mathcal{E}$–independent, see Eq.(6.4).

By the definition Eq.(2.9) of W it follows that

$$V_n(s)\le v_1\,C\,R_n(s)^{\frac d2} \tag{6.10}$$

and going back to Eq.(5.5), and solving it, $R_n(t)$ is bounded proportionally to $R_n(0)=n^{1/d}$.

Calling $\rho_n(t),V_n(t),\mathcal{N}_n(t)$ the quantities in Eq.(5.2) for $S_t^{(n,1)}x$ the following bounds can be formulated simultaneously for the thermostatted and Hamiltonian cases and extend to positive times the estimates in Eq.(5.3).

Theorem 4: *If $d\le2$ the maximal velocity $V_n(t)$ and the maximal displacement $R_n(t)\,r_\varphi$, in the Λ_n–regularized motion up to time $t\le\min\{\Theta,t_{\Lambda_n}(x)\}$ in the thermostatted case or $t\le\Theta$ in the Hamiltonian case satisfy:*

$$\begin{aligned} R_n(t) &\le C\,n^{\frac1d}, & V_n(t) &\le v_1 C\,n^{1/2}\\ \rho_n(t) &\le C^{-1}n^{-\frac1\alpha}, & \mathcal{N}_n(t) &\le C n^{\frac12}\end{aligned} \tag{6.11}$$

with $C>0$ (a suitable function of $\mathcal{E}$).

The use of Eq.(6.10) to solve Eq.(5.4), which then implies Eq.(6.11), will force the restriction on the dimension to be $d\le2$.

VII. ENTROPY BOUND AND PHASE SPACE CONTRACTION

The kinetic energy density $K_{j,n}(x)/|\Omega_j\cap\Lambda_n|$, *i.e.* the kinetic energy contained in the j-th thermostat at time t in the Λ_n–regularized thermostatted or Hamiltonian dynamics divided by its volume, will initially have a value as close as wished to $\delta_j\frac d2 k_BT_j$ for n large enough. So that $\frac{K_{j,n}}{\varphi_0}\stackrel{def}{\simeq}\kappa_j\,2^{dn}$ if n is large enough: because this is an event which has probability 1 with respect to μ_0.

Therefore if the infinite volume μ_0–average value of $\frac{K_{j,n}(x)}{\varphi_0}$ is denoted $\kappa_j 2^{n\,d}$ then there is $n(x)$ such that

$$\frac{K_{j,n}(x)}{\varphi_0} > \frac12\kappa\,2^{n\,d},\qquad \forall\ n\ge n(x). \tag{7.1}$$

where $\kappa=\min_{j>0}\kappa_j$. The notation $x(t),x(s),\ldots$ will be temporarily used below for simplicity instead of $x^{(n,a)}(t),x^{(n,a)}(s),\ldots$. The equations of motion are now Eq.(1.3), or (2.6), with $a=1$.

With μ_0–probability 1 it is $\mathcal{E}(x),n(x)<\infty$. Let $\Xi_{E,h}$ be the set of configurations for which $\mathcal{E}(x)\le E, n(x)=h$.

Let $\nu_h(x)$ be the smallest $n \ge h$ such that the event $\min_{j>0} \frac{K_{j,n}(x(t))}{\varphi_0} = \frac12 \kappa\, 2^{n\,d}$ is realized for $t = t_{n,h}(x) < \Theta$ but not earlier.

Remark: the definition of $\Xi_{E,h}$ implies that the time $t_{\Lambda_n}(x)$ (see comment (6), p.2) is, for $x \in \Xi_{E,h}$, certainly $> t_{n,h}(x)$.

Let $\Xi_{E,h,n}$ be the set of the $x \in \Xi_{E,h}$, $\nu_h(x) = n$. It will be shown that $\sum_{n\ge h} \mu_0(\Xi_{E,h,n}) < \infty$: hence with μ_0–probability 1 a point x will be out of $\Xi_{E,h,n}$ for all n large enough and Eq.(7.1) will hold for all $t \le \Theta$ with μ_0–probability 1.

For $x \in \Xi_{E,h,n}$, consider Q_j as in Eq.(1.5). *Notice that Q_j has the physical interpretation of the heat ceded per unit time to the j-th thermostat by the system.*

If N_0 is the number of particles in Ω_0, $\mathcal{N}_n(t)$, $\underline{V_n}(t)$ are as in Eq.(6.11), F is the maximum of $|\partial\varphi|$, and $\overline{N}$ is the maximum number of particles within r_φ of the boundary of Ω_0, then $|Q_j| \le N_0 \overline{N} F V_n(t) \le C n^{\frac12+\frac12}$ because $V_n(t)$ is bounded by Eq.(6.11) proportionally to $n^{1/2}$, $\overline{N}$ is bounded proportionally to the (finite) number of balls of radius r_φ needed to cover the ball of radius $D_0 + r_\varphi$ times the $\mathcal{N}_n(t)$ in Eq.(6.11) (*i.e* also proportionally to $n^{\frac12}$): the estimates hold for $t \le \Theta$ in the Hamiltonian case and for $t \le t_{h,n}(x) \le \Theta$ in the thermostatted case..

The phase space contraction $\sigma = \sigma(x)$, see Eq.(2.3), is

$$\sigma = \sum_{j>0} dN_j \frac{Q_j}{2K_{j,n}(x,t)} \Big(1 - \frac{1}{dN_j}\Big) + \beta_0 Q_0 \tag{7.2}$$

in the thermostatted case, if $Q_0 \stackrel{def}{=} -\sum_{q\in\Omega_0} \sum_{j>0} \dot{\mathbf{X}}_0 \cdot \partial_{\mathbf{X_0}} U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \dot{\mathbf{X}}_0 \cdot \boldsymbol{\Phi}$; in the Hamiltonian case, it is:

$$\sigma(x) = \sum_{j\ge0} \beta_j Q_j \tag{7.3}$$

It has to be kept in mind that there is contraction of phase space even in the fully Hamiltonian case when Liouville's theorem holds (already for the regularized dynamics): this is no contradiction because the phase space volume is measured with the volume defined by μ_0.

Since Q_0 can be estimated in the same way as Q_j, above, it follows that the integral $|\int_0^{t_{h,n}(x)} \sigma(x^{(n,a)}(t))|$ is, *in either cases*, also uniformly bounded (in $\Xi_{E,h}$) by

$$\overline{\sigma}\Theta n, \qquad \forall\, n \ge h \tag{7.4}$$

where $\overline{\sigma}$ is a suitable non decreasing function of E. This is a first *entropy estimate*; it is rather far from optimal and it will appear, Sec.IX, that it will be essential to impove it.

Therefore a volume element in $\Xi_{E,h,n}$ contracts at most by $e^{-\overline{\sigma}\Theta n}$ on the trajectory of μ_0-almost all points $x \in \Xi_{E,h,n}$ up to the stopping time $t_{h,n}(x)$.

Effectively this means that the distribution μ_0 can be treated as an invariant one for the purpose of estimating the probability that the kinetic energy, in $\Omega_j \cap \Lambda_n$ of the initial data $x \in \Xi_{E,h,n}$, in the time $t_{h,n}(x)$ grinds down to $\frac{\kappa}{2} 2^{dn}$ (*i.e.* to half (say) of the value $\kappa 2^{nd}$ to which it is intially very close, if n is large). The estimate can be carried out via the technique introduced by Sinai, [12], which has been applied in [11, 13]; for completeness see the following appendix D.

Let $D = D_n$ be the set of the $x \in \Xi_{E,h,n}$ which satisfy $K_{j,\Lambda_n}(x) = \frac12 \kappa 2^{dn}$ for a given $j > 0$ while $K_{j',\Lambda_n}(x) = \frac12 \kappa 2^{dn}$ for $j' > 0, j' \ne j$.

Recalling the DLR-equations, [14], and the classical superstability estimate on the existence of $b > 0$ such that $p_n \le e^{-b 2^{dn}}$ bounds the probability of finding more than $\rho 2^{dn}$ particles in $\Lambda_n \cap \Omega_j$ if ρ is large enough (e.g. $\rho > \max_j \delta_j$), the probability $\mu_0(\Xi_{E,h,n})$ can be bounded by p_n (summable in n) plus

$$\begin{aligned} & e^{\overline{\sigma}\Theta n} \int \mu_0(dq' d\dot q') \sum_{l=1}^{\rho 2^{nd}} \Theta \frac{e^{-(\beta_j U_{\Lambda_n,j}(q,q') - \lambda_j\, l)}}{Z_{\Lambda_n,j}(q')} \frac{dq}{l!} \\ & \cdot\, e^{-\beta_j P^2} P^{l\,d-1} \widehat{P}\, \omega(l\,d) \end{aligned} \tag{7.5}$$

where $q = (q_1, \ldots, q_l) \in (\Omega_j \cap \Lambda_n)^l$, $P^2 = \frac12 \kappa 2^{dn}$, $U_{\Lambda_n,j}(q,q')$ is the sum of $\varphi(q - q')$ over the pairs of points $q_i, q'_\ell \in \Omega_j \cap \Lambda_n$ plus the sum over the pairs with $q_i \in \Lambda_n \cap \Omega_j, q'_\ell \notin \Lambda_n \cap \Omega_j$, and

(1) $Z_{\Lambda_n,j}(q')$ is the partition function for the region $\Lambda_n \cap \Omega_j$ (defined as in Eq.(2.1) with the integral over the q's extended to $\Lambda_n \cap \Omega_j$ and with the energies $U_{\Lambda_n}(x,z)$);

(2) The volume element $P^{ld-1} dP$ has been changed to $P^{ld-1} \dot P d\tau = P^{ld-2} \widehat{P} d\tau$ where $\widehat{P}$ is a *short hand* for $\sum_{q,q';\, q\in\Lambda_n} |\partial_q \varphi(q - q')| + \sum_{q\in\Lambda_n} |\partial_q \psi(q)|$ so that $P\widehat{P}$ is a bound on the time derivative of the total kinetic energy P^2 contained in Λ_n evaluated on the points of D_n (the latter is $2P\dot P = |\sum_{i,j;q_i\in\Lambda_n} \partial\varphi(q_i - q_j)(\dot q_i - \dot q_j) + \sum_{q\in\Lambda_n} \partial_q \psi(q) \dot q|$ hence $\le P^2 \widehat{P}$).

(3) $\omega(l\,d)$ is the surface of the unit ball in $\mathbb{R}^{l\,d}$.

(4) The factor $e^{\overline{\sigma}\Theta n}$ takes into account the entropy estimate, *i.e.* the estimate Eq.(7.4) of the non-invariance of μ_0.

The integral over τ in Eq.(7.5) gives a factor Θ and the integral can be trivially imagined averaged over an auxiliary parameter $\varepsilon \in [0, \overline{\varepsilon}]$ with $\overline{\varepsilon} > 0$ arbitrary (but to be suitably chosen shortly) on which it does not depend at first. Then if P is replaced by $(1-\varepsilon)P$ in the exponential while $P^{l\,d-1}$ is replaced by $\frac{((1-\varepsilon)P)^{l\,d-1}}{(1-\varepsilon)^{\rho 2^{nd}-1}}$ the average over ε becomes an upper bound. Changing ε to $P\varepsilon$ (*i.e.* hence $d\varepsilon$ to $\frac{dP\varepsilon}{P} = \frac{2dP\varepsilon}{\kappa 2^{dn}}$) the bound becomes the μ_0-average

$$\begin{aligned}&\frac{2e^{\overline{\varepsilon}\rho 2^{nd}}}{\overline{\varepsilon}\kappa 2^{dn}}\langle\widehat{P}\,\chi_{\kappa,\overline{\varepsilon}}\rangle_{\mu_0}\equiv\frac{2e^{\overline{\varepsilon}\rho 2^{nd}}}{\overline{\varepsilon}\kappa 2^{dn}}\langle\widehat{P}^2\rangle_{\mu_0}^{\frac12}\cdot\langle\chi_{\kappa,\overline{\varepsilon}}\rangle_{\mu_0}^{\frac12}\\&\le B\,e^{-b\,2^{nd/2}}\end{aligned}\tag{7.6}$$

where $\chi_{\varepsilon,\kappa}$ is the characteristic function of the set $\{(1-\overline{\varepsilon})^2\frac{\kappa}{2}2^{dn}<K_j<\frac{\kappa}{2}2^{dn}\}$. The inequality is obtained by a bound on the first average, via a superstability estimate, proportional to 2^{2dn} and by the remark that the second average is over a range in which K shows a large deviation from its average (by a factor 2) hence it is bounded above by $e^{-b2^{nd}}$ with b depending on κ but independent on $\overline{\varepsilon}$ for n large. Therefore fixing $\overline{\varepsilon}$ small enough (as a function of κ) the bound holds with suitable $B,b>0$ and is summable in n (and of course on $j>0$).

Hence, fixed h, with μ_0–probability 1 it is $K_{j,n}\ge\frac12\kappa 2^{n\,d}$ (by Borel-Cantelli's theorem) for all n large enough and $j>0$. As mentioned after Eq.(7.1) this means that for all $t\le\Theta$ it is $K_{j,n}\ge\frac12\kappa 2^{n\,d}$ for all n large enough, with μ_0 probability 1. Therefore the bounds in Eq.(6.11) can be assumed, with μ_0–probability 1 also for the *thermostatted and Hamiltonian dynamics* and for all n large enough.

Theorem 5: *With μ_0–probability 1 the phase space contraction $\sigma(x)$ admits a bound $\overline{\sigma}(x)<\overline{\sigma}n$ for all times $t\le\Theta$ for the Λ_n–regularized thermostatted or Hamiltonian dynamics. Furthermore the kinetic energy $K_{j,n}(x^{(n,a)}(t))$, $a=0,1$, in the j–th thermostat remains $\ge\kappa 2^{nd}$ for all $n>n(x)$ for suitable $\kappa,n(x)>0$. The constants $\overline{\sigma}(x),n(x)$ depend on x only through $\mathcal{E}(x)$.*

This proves item (2) of the local dynamics property.

VIII. INFINITE VOLUME HAMILTONIAN DYNAMICS

It remains to check that also the $n\to\infty$ limit of the dynamics exists in the sense of the local dynamics assumption (*i.e.* the existence of the limit $x(t)\equiv x^{(0)}(t)\stackrel{def}{=}\lim_{n\to\infty}x^{(n,0)}(t)$ and a suitable form of its uniqueness).

The equation of motion, for a particle in the j-th container (say), can be written both in the Hamiltonian and in the thermostatted cases as

$$\begin{aligned}q_i^{(n,a)}(t)=q_i(0)+\int_0^t&\big(e^{-\int_0^\tau a\alpha_j(x^{(n,a)}(s))ds}\dot q_i(0)\\&+(t-\tau)\,e^{-\int_\tau^t a\alpha_j(x^{(n,a)}(s))ds}f_i(x^{(n,a)}(\tau))\big)\,d\tau\end{aligned}\tag{8.1}$$

where the label j on the coordinates (indicating the container) is omitted and f_i is the force acting on the selected particle divided by its mass (for $j=0$ it includes the stirring force). The Hamiltonian case is simply obtained setting $a=0$ while the thermostatted case corresponds to $a=1$.

The existence of the dynamics in the Hamiltonian case, $a=0$, will be discussed first, proving

Theorem 6: *If $x\in\mathcal{H}_{1/d}$ the thermodynamic limit evolution $x^{(0)}(t)_i=\lim_{n\to\infty}x^{(n,0)}(t)_i$ exists.*

The following proof reproduces the proof of theorem 2.1 in [10, p.32] for $d=2$, which applies essentially unaltered. Define

$$\begin{aligned}\delta_i(t,n)&\stackrel{def}{=}|q_i^{(n,0)}(t)-q_i^{(n+1,0)}(t)|,\\u_k(t,n)&\stackrel{def}{=}\max_{q_i\in\Lambda_k}\delta_i(t,n),\end{aligned}\tag{8.2}$$

then, for $a=0$, Eq.(8.1) yields

$$\begin{aligned}\delta_i(t,n)\le\int_0^t\frac{\Theta}{m}d\tau\,\{&F'_w\delta_i(\tau,n)\\&+F'\sum_j(\delta_j(\tau,n)+\delta_i(\tau,n))\,\}\end{aligned}\tag{8.3}$$

where the sum is over the number $\mathcal{N}_n$ of the particles $q_j(\tau)$ that can interact with $q_i(\tau)$ at time τ; $F'=\max|\partial^2\varphi|$ is the maximal gradient of the interparticle force; $F'_w=C\alpha(\alpha+1)\frac{\varphi_0}{r_\psi^2}n^{\frac{\alpha+2}{\alpha}}$ bounds the maximum gradient of the walls plus the stirring forces, the bound follows from Eq.(6.11). The number $\mathcal{N}_n$ is bounded by theorem 4, Eq.(6.11), by $\mathcal{N}_n\le Cn^{1/2}$ for both $x^{(n,0)}(\tau)$ and $x^{(n+1,0)}(\tau)$. Let

$$\eta\stackrel{def}{=}(1+\frac{2}{\alpha}),\quad 2^{k_1}\stackrel{def}{=}2^k+r_n\tag{8.4}$$

where r_n is the maximum distance a particle can travel in time $\le\Theta$, bounded by Eq.(6.11) by $C\,r_\varphi\,n^{1/2}$. Then

$$\frac{u_k(t,n)}{r_\varphi}\le C\,n^\eta\int_0^t\frac{u_{k_1}(s,n)}{r_\varphi}\frac{ds}{\Theta}\tag{8.5}$$

(C is a function of $\mathcal{E}$ as agreed in Sec.V). Eq.(8.5) can be iterated ℓ times if $2^k+C\,\ell n^{1/2}<2^n$, *i.e.* $\ell=\frac{2^n-2^k}{2Cn^{1/2}}$ which is $\ell>c\,2^{n/2}\,\delta_{k<n}$ for n large.

By Eq.(6.11) $u_k(t,n)$ is $\le C\,n^{1/2}$ so that for $n>k$,

$$\frac{u_k(n,t)}{r_\varphi}\le C'\,\frac{(n^\eta)^{\ell+1}}{\ell!}n^{1/2}\le C\,2^{-2^{n/2}c}\tag{8.6}$$

for suitable $C',C,c>0$ (n–independent functions of $\mathcal{E}$). Hence the evolutions locally (*i.e.* inside the ball Λ_k) become closer and closer as the regularization is removed (*i.e.* as $n\to\infty$) and very fast so.

If $q_i(0)\in\Lambda_k$, for $n>k$ it is

$$q_i^{(0)}(t)=q_i^{(k,0)}(t)+\sum_{n=k}^\infty(q_i^{(n+1,0)}(t)-q^{(n,0)}(t))\tag{8.7}$$

showing the existence of the dynamics in the thermodynamic limit because also the inequality, for $n > k$,

$$\frac{|\dot q^{(n,0)}(t) - \dot q^{(n+1,0)}(t)|}{v_1} \le C\, 2^{-2^{n/2}c} \tag{8.8}$$

follows from Eq.(8.6) and from $\dot q^{(n,0)}(t) - \dot q^{(n+1,0)}(t) = \int_0^t \big(f_i(q^{(n,0)}(\tau))d\tau - f_i(q^{(n+1,0)}(\tau))\big)d\tau$. Or, for $n > k$,

$$|x_i^{(n,0)}(t) - x_i^{(0)}(t)| \le C\, e^{-c2^{nd/2}} \tag{8.9}$$

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

Hence the proof of the existence of the dynamics in the Hamiltonian case and in the thermodynamics limit is complete and it yields concrete bounds as well, *i.e*

Theorem 7: *There are $C(\mathcal{E}), c(\mathcal{E})^{-1}$, increasing functions of $\mathcal{E}$, such that the Hamiltonian evolution satisfies the local dynamics property and if $q_i(0) \in \Lambda_k$*

$$\begin{aligned}
&|\dot q_i^{(n,0)}(t)| \le v_1 C(\mathcal{E})\, k^{\frac12},\\
&\text{distance}(q_i^{(n,0)}(t), \partial(\cup_j \Omega_j \cap \Lambda)) \ge c(\mathcal{E}) k^{-\frac{1}{\alpha}} r_\psi\\
&\mathcal{N}_i(t,n) \le C(\mathcal{E})\, k^{1/2}\\
&|x_i^{(n,0)}(t) - x_i^{(0)}(t)| \le C(\mathcal{E}) r_\varphi e^{-c(\mathcal{E})2^{nd/2}}
\end{aligned} \tag{8.10}$$

for all $n > k$. The $x^{(0)}(t)$ is the unique solution of the Hamilton equations satisfying the first three of Eq.(8.10).

The uniqueness follows from Eq.(8.3) and we skip the details, [15].

It would also be possible to show the stronger result that $x^{(0)}(t) \in \mathcal{H}_{1/d}$: but for the proof of theorem 1 the theorems 5,6,7 are sufficient, hence the proof of the stronger property is relegated to theorem 9 in the appendix.

The corresponding proof for the thermostatted evolution will be somewhat more delicate: and *it will be weaker* as it will not hold under the only assumption that $\mathcal{E}(x) < \infty$ but it will be necessary to restrict further the initial data to a subset of the phase space (which however will still have μ_0–probability 1).

Remark: An immediate consequence is that the *entropy production $\sigma(x)$*, see Eq.(7.3), is estimated by a constant $s(\mathcal{E})$ in the Λ_n–dynamics for n large: *i.e* a much better estimate than the growth bounded by a power of n, see Eq.(7.4), implied by Eq.(6.11).

IX. INFINITE VOLUME THERMOSTATTED DYNAMICS

Eq.(8.1) will be used to compare the Hamiltonian and the thermostatted evolutions in Ω_j with the same initial data assuming that the initial data satisfy theorem 5, Sec.VII. We shall see that the problem will reduce to obtain a better estimate of the entropy production, *i.e.* better than proportional to n, as in Eq.(7.4).

Fixing once and for all $\kappa > 0$ to be smaller than the minimum of the kinetic energy densities of the initial x in the various thermostats (which is x-independent with μ_0–probability 1), the problem can be solved by restricting attention to a suitable subset of the set $\mathcal{X}_E \subset \mathcal{H}_{1/d}$:

$$\mathcal{X}_E \stackrel{def}{=} \big\{x \,|\, \mathcal{E}(x) \le E;\ \min_{\substack{t\le\Theta\\ j>0}} \frac{K_{j,n}(S_t^{(n,1)}x)}{\varphi_0} \ge \kappa 2^{nd}\big\} \tag{9.1}$$

In this section (and in the corresponding appendix E) the constants $C, C', \ldots, c, c', \ldots$ will be functions of E as stated in Sec.V.

Consider the bands of points ξ at distance $\rho_{\Omega_0}(\xi)$ from the boundary $\partial\Omega_0$ of Ω_0 within r_φ or $2r_\varphi$

$$\begin{aligned}
&\Lambda_* \stackrel{def}{=} \{q : \rho_{\Omega_0}(q) \le r_\phi\},\\
&\Lambda_{**} \stackrel{def}{=} \{q : \rho_{\Omega_0}(q) \le 2r_\phi\}
\end{aligned} \tag{9.2}$$

By the result in Sec.VIII there are M and V (which depend on E) so that for all $x \in \mathcal{X}_E$ and with the notations Eq.(2.8), for n large enough:

$$\begin{aligned}
&\max_{t\le\Theta} N_{\Lambda_{**}}(S_t^{(n,0)}x) < M\\
&\max_{t\le\Theta} V_{\Lambda_{**}}(S_t^{(n,0)}x) < V - 1
\end{aligned} \tag{9.3}$$

Define for x the stopping times

$$\begin{aligned}
T_{M,V;n}(x) \stackrel{def}{=} \max\big\{&t \le \min\{t_{\Lambda_n}(x), \Theta\} : \forall\tau \le t,\\
&N_{\Lambda_*}(S_\tau^{(n,1)}x) \le M,\ V_{\Lambda_*}(S_\tau^{(n,1)}x) \le V\big\}
\end{aligned} \tag{9.4}$$

Let C_ξ the cube with side r_φ centered at a point ξ in the lattice $r_\varphi\mathbb{Z}^d$, and using the definitions in Eq.(2.8), let

$$\|x\|_n \stackrel{def}{=} \max_{\xi\in\Lambda_n} \frac{\max(N_{C_\xi}(x), \sqrt{E_{C_\xi}(x)})}{g_\lambda(\xi/r_\varphi)}. \tag{9.5}$$

with $\frac12 < \lambda < 1$. Split $\mathcal{X}_E = \mathcal{A} \cup \mathcal{B}$ where

$$\begin{aligned}
&\mathcal{A} \stackrel{def}{=} \{x \in \mathcal{X}_E : \max_{t\le T_{M,V;n}(x)} \|S_t^{(n,1)}x\|_n \le (\log n)^\lambda\}\\
&\mathcal{B} \stackrel{def}{=} \{x \in \mathcal{X}_E : \max_{t\le T_{M,V;n}(x)} \|S_t^{(n,1)}x\|_n > (\log n)^\lambda\}.
\end{aligned} \tag{9.6}$$

Fixed, once and for all, $\gamma > 0$ arbitrarily

Theorem 8: *In $d = 1,2$ there are positive constants C, C', c depending only on E such that for all n large enough:*

(1) if $x \in \mathcal{A}$ then $T_{M,V;n}(x) = \Theta$, $S_t^{(n,0)}x$ and $S_t^{(n,1)}x$ are close in the sense that for $q_i(0) \in \Lambda_{(\log n)^\gamma}$

$$\begin{aligned}|q_i^{(n,1)}(t) - q_i^{(n,0)}(t)| &\le C\, r_\varphi\, e^{-(\log n)^\gamma\, c},\\ |\dot q_i^{(n,1)}(t) - \dot q_i^{(n,0)}(t)| &\le C\, v_1\, e^{-(\log n)^\gamma\, c}.\end{aligned} \tag{9.7}$$

(2) the set $\mathcal{B}$ has μ_0–probability bounded by

$$\mu_0(\mathcal{B}) \le C\, e^{-c(\log n)^{2\lambda} + C' M^2 V}. \tag{9.8}$$

Remark: Since $\lambda > 1/2$ Eq.(9.8) will imply (by Borel–Cantelli's lemma) that, with μ_0–probability 1, eventually x is in $\mathcal{A}$ and therefore, as soon as Eq.(9.7) will have been proved, the thermodynamic limits of $q^{(n,a)}(t)$ will coincide for $t \le \Theta$, $a = 0, 1$: concluding the proof of theorem 1 as well.

A. Check of Eq.(9.8)

We begin by defining the surface, see it symbolic description in Fig.2 below:

$$\begin{aligned}\Sigma_\tau \stackrel{def}{=} \big\{ & x \in \Xi_E \,|\, \|S_\tau^{(n,1)} x\|_n \ge (\log n)^\lambda,\\ & \forall\, t < \tau,\ \|S_t^{(n,1)} x\|_n < (\log n)^\lambda\\ & T_{M,V;\,n}(x) \ge \tau \big\}\end{aligned} \tag{9.9}$$

Recalling the definition of the existence time $t_{\Lambda_n}(x)$ in Sec.I, p.2, item (6), we remark that for $x \in \Xi_E$, $t_{\Lambda_n}(x) \ge \Theta$ so that $S_\tau^{(n,1)} x$, $\tau \le \Theta$ is well defined.

Moreover $S_\tau^{(n,1)} \Sigma_\tau$ is contained in the *surface* Σ' (piecewise smooth) of points x for which $S_t^{(n,1)} x$ is well defined for $t < 0$ near 0 and $\|S_t^{(n,1)} x\|$ crosses from below the value $(\log n)^\lambda$ at time $t = 0$.

With the above geometric considerations (see Fig.2) the set $\Sigma \stackrel{def}{=} \cup_{\tau \le \Theta} S_{-\tau}^{(n,1)} x \in \Sigma_\tau \subset \Sigma'$ and for $x \in \Sigma$ we define $\theta(x) = \max_{\tau \le \Theta} \{\tau \,|\, S_{-\tau}^{(n,1)} x \in \Sigma_\tau\}$.

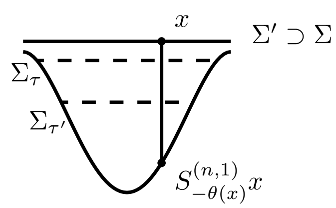

Fig.2: *The horizontal "line" represents Σ'; the "curve" represents the points $S_{-\theta(x)}^{(n,1)} x$, i.e the set of points in $\mathcal{X}_E$ which in time $\theta(x)$ reach Σ' and determine on it a subset Σ; the incomplete ("dashed") lines represent the "levels" $\Sigma_\tau, \Sigma_{\tau'}$; the missing parts are made of points which are not in $\mathcal{X}_E$ but have an "ancestor" in $\mathcal{X}_E$; the vertical line represents the trajectory of the point $S_{-\theta(x)} x$.*

The Σ_τ are represented in Fig.2 as dashed lines to remind that it might be that the trajectories that reach the surface Σ' will have a value of $\mathcal{E}(S_{-t}^{(n,1)} x) > E$ or a kinetic energy $< \kappa 2^{nd}/\varphi_0$, see Eq.(9.1), at some $t \in (0, \theta(x))$.

Remark: We can also say that Σ is the subset of the surface Σ' consisting of the points of Σ' that are reached by trajectories of points $y \in \Xi_E$ within a time interval $\le T_{M,V;\,n}(y)$.

In the notations of Appendix D, Σ is the base and $\theta(x)$ the ceiling function. We then have

$$\mu_0(\mathcal{B}) \le \int_{\Sigma'} \mu_{0,\Sigma'}(dy) \int_0^{\theta(y)} dt\, w(y)\, e^{\widehat{\sigma}(y,t)} \tag{9.10}$$

where $\mu_{0,\Sigma'}$ denotes the projection of μ_0 on Σ', $w = |v_x \cdot n_x|$ and $\widehat{\sigma}(y,t) \stackrel{def}{=} \int_{-t}^0 \sigma(y^{(n,1)}(t'))dt'$ is the phase space contraction. By the definition of Σ_τ it then follows that $T_{M,V;\,n}(x) \ge \theta(x)$, $\forall x \in \Sigma$ and $|\widehat{\sigma}(y,t)| \le C M^2 V$.

Writing k_ξ for the smallest integer $\ge (\log n)^\lambda g_\lambda(\xi/r_\phi)$, $\mu_{0,\Sigma'}$ almost surely, Σ' splits into an union over $\xi \in \Lambda_n \cap r_\varphi \mathbb{Z}^d$ of the union of $\mathcal{S}_\xi^1 \cup \mathcal{S}_\xi^2$, where

$$\begin{aligned}\mathcal{S}_\xi^1 =& \{y \in \Sigma' : |y \cap C_\xi| = k_\xi, |y \cap \partial C_\xi| = 1\}\\ \mathcal{S}_\xi^2 =& \{y \in \Sigma' : y \cap C_\xi \ni (q, \dot q), E(q, \dot q) = \widetilde{E}_\xi\}\end{aligned} \tag{9.11}$$

if $\widetilde{E}_\xi \stackrel{def}{=} \big((\log n)^\lambda g_\lambda(\xi/r_\phi)\big)^2$.

Both $\mu_{0,\Sigma'}(\mathcal{S}_\xi^1)$ and $\mu_{0,\Sigma'}(\mathcal{S}_\xi^2)$ are bounded by

$$\mu_{0,\Sigma'}(\mathcal{S}_\xi^i) \le C e^{C M^2 V} \sqrt{n} e^{-c[(\log n)^\lambda g_\lambda(\xi/r_\varphi)]^2}, \tag{9.12}$$

(for suitable C, c, functions of E). The proof of Eq.(9.12) does not involve dynamics but only classical equilibrium estimates, *the details are expounded in Appendix* E. Summing (as $\lambda > 1$) over $\xi \in \Omega_j \cap \Lambda_n$ the Eq.(9.8) follows.

B. Two remarks

To prove item (1) and Eq.(9.7), thus completing the proof of theorem 8, we shall compare the evolutions $x^{(n,a)}(t)$ with $a = 0, 1$, same initial datum $x \in \mathcal{A}$ and $t \le T_{M,V;\,n}(x)$, the latter being the stopping time defined in Eq.(9.4). We start by proving that there is $C > 0$ so that for all n large enough the following holds.

Lemma 1: *Let $\gamma > 0$. For $x \in \mathcal{A}$ and $h \ge (\log n)^\gamma$, then*

$$\begin{aligned}|\dot q_i^{(n,1)}(t)| &\le C\, v_1\, \big(h\, \log n\big)^\lambda,\\ |q_i^{(n,1)}(t)| &\le r_\varphi\, (2^h + C\, \big(h\, \log n\big)^\lambda).\end{aligned} \tag{9.13}$$

for $q_i(0) \in \Lambda_h$ and $t \le \Theta$.

Proof: if $x \in \mathcal{A}$ and $t \le T_{M,V;\,n}(x)$ then

$$|\dot q_i^{(n,1)}(t)| \le v_1 \big((\log n) \log_+ \frac{|q_i^{(n,1)}(t)| + \sqrt{2} r_\varphi}{r_\varphi}\big)^\lambda, \tag{9.14}$$

implying: $|q_i^{(n,1)}(t)| \le r(t) r_\varphi$ if $r(t)\, r_\varphi$ is an upper bound to a solution of Eq.(9.14) with = replacing $\le$ and initial datum $|q_i^{(n,1)}(0)| \le 2^h r_\varphi$. And $r(t)$ can be taken $r(t) \stackrel{def}{=} 2^h + 2v_1\big((\log n)\log_+ 2^h\big)^\lambda \frac{t}{r_\varphi}$, for $t \le \Theta$, provided

$$\big((\log n)\log_+ r(\Theta) + \sqrt{2}\big)^\lambda \le 2\big((\log n)\log_+ 2^h\big)^\lambda \quad (9.15)$$

which is verified for all n large enough, because $\frac{(h\log n)^\lambda}{2^h}$ vanishes as n diverges (keeping in mind that $h \ge (\log n)^\gamma$). Thus $|q_i^{(n,1)}(t)| \le r_\varphi\, r(t)$, hence $|\dot q_i^{(n,1)}(t)| \le r_\varphi\, C\, \dot r(t)$ for all $t \le T_{M,V;\,n}(x)$, *i.e.* when Eq.(9.14) holds: and the lemma is proved. Fix $\gamma > 0$.

Lemma 2: *Let $\mathcal{N}$ and ρ be the maximal number of particles which at any given time $\le \Theta$ interact with a particle initially in Λ_{k+1} and, respectively, the minimal distance of any such particle from the walls in either dynamics and for $t \le T_{M,V;\,n}(x)$. Then*

$$\mathcal{N} \le C\,(k\log n)^\lambda, \quad \rho \ge c\,(k\log n)^{-2\lambda/\alpha} \quad (9.16)$$

for all integers $k > (\log n)^\gamma$.

Proof: As a consequence of lemma 1 and of theorem 7 the following properties hold for all n large enough and all $t \le T_{M,V;\,n}(x)$, both for the Hamiltonian and the thermostatted evolutions.

(i) for all $q_i \in \Lambda_{k+2}$ and $a = 0, 1$,

$$\max_{t \le T_{M,V;\,n}(x)} |q_i^{(n,a)}(t) - q_i| \le C\, r_\varphi (k\log n)^\lambda, \quad (9.17)$$

(ii) particles $\in \Lambda_k$ do not interact with those $\notin \Lambda_{k+2}$;

By Eq.(9.17) we see that if $q_i \in \Lambda_{k+1}$ then $q_i^{(n,a)}(t) \in \Lambda_{k+2}$ so that, by the definition of the set $\mathcal{A}$ and by Eq.(9.6) (or by theorem 7 in the Hamiltonian case, recalling that $\lambda > 1/2$), Eq.(9.16) follows.

C. Check of Eq.(9.7) and comparison of Hamiltonian versus thermostatted motions

We have now all the ingredients to bound $\delta_i(t,n) \stackrel{def}{=} |q_i^{(n,1)}(t) - q_i^{(n,0)}(t)|$. Let f_i be the acceleration of the particle i due to the other particles and to the walls. By Eq.(9.16) if $q_i \in \Lambda_{k+1}$, $|f_i| \le C\,(k\log n)^{\eta'}$, $\eta' \stackrel{def}{=} 2d\,\lambda\,(1 + \frac{1}{\alpha})$ so that, subtracting the Eq.(8.1) for the two evolutions, it follows that for any $q_i \in \Lambda_{k+1}$ (possibly close to the origin hence very far from the boundary of Λ_k if n is large, because $k > (\log n)^\gamma$)

$$\delta_i(t,n) \le C\,(k\log n)^{\eta'} 2^{-nd} + \Theta \int_0^t |f_i(q^{(n,1)}(\tau)) - f_i(q^{(n,0)}(\tau))|\, d\tau. \quad (9.18)$$

because, recalling Eq.(9.1), $|\alpha_j|$ is bounded proportionally to 2^{-nd}.

Let ℓ be a non-negative integer, k_ℓ such that

$$2^{k_\ell} = 2^k + \ell\, C\,(k\log n)^\lambda \quad (9.19)$$

(see Eq.(9.17)) and $u_{k_\ell}(t,n)$ the max of $\delta_i(t,n)$ over $|q_i| \le 2^{k_\ell}$. Then by Eq.(9.18) and Eq.(9.16) and writing $\eta'' \stackrel{def}{=} 2\,d\,\lambda(1 + \frac{2}{\alpha})$,

$$\frac{u_{k_\ell}(t,n)}{r_\varphi} \le C\,(k\log n)^{\eta'} 2^{-nd} + C(k\log n)^{\eta''} \int_0^t \frac{u_{k_{\ell+1}}(s)}{r_\varphi}\frac{ds}{\Theta}. \quad (9.20)$$

for $\ell \le \ell^* = 2^k/((k\log n)^\lambda C)$, the latter being the largest ℓ such that $2^{k_\ell} \le 2^{k+1}$. By Eq.(9.20) and Eq.(9.16)

$$u_k(t,n) \le e^{C\,(k\,\log n)^{\eta''}} C(k\log n)^{\eta'} 2^{-dn} + \frac{(C\,(k\,\log n)^{\eta''})^{\ell^*}}{\ell^*!}\, C\,(k\log n)^\lambda. \quad (9.21)$$

Thus $u_k(t,n)$ is bounded by the r.h.s. of the first of Eq.(9.7); analogous argument shows that also the velocity differences are bounded as in Eq.(9.7) which is thus proved for all $t \le T_{M,V;\,n}(x)$. On the other hand such a result proves that $q_i^{(n,1)}(t)$ is closer than r_φ to $q_i^{(n,0)}(t)$. Hence, remarking that we know "everything" about the Hamiltonian motion we can use such knowledge by applying Eq.(9.7) to particles which are initially within a distance $r_\varphi 2^{k_0}$ of the origin, with k_0 fixed arbitrarily,

Therefore the number of particles in $q_i^{(n,1)}(t)$ which are in Λ_* is smaller than the number of particles of $q_i^{(n,0)}(t)$ in Λ_{**} which is bounded by M. An analogous argument for the velocities allows to conclude that Eq.(9.3) hold in Λ_{**} also for the thermostatted motion ($a = 1$, being valid for the Hamiltonian motion in the smaller Λ_*, given the closenes of the positions and speeds), $T_{M,V;\,n} \equiv \Theta$ with μ_0–probability 1. Applying again Eq.(9.7) the proof of theorem 8 is complete: with $\gamma = 2$ (but any $\gamma > 0$ would also lead to a corresponding result).

X. CONCLUDING REMARKS

Equivalence between different thermostats is widely studied in the literature and the basic ideas, extended here, were laid down in [16]. A clear understanding of the problem was already set up in comparing isokinetic, isoenergetic and Nosé-Hoover bulk thermostats in [16], where a history of the earlier results is presented as well, see also [1, 17].

There are, since a long time, studies of systems with free thermostats, starting with [2]. Such thermostats are somewhat pathological and may not always lead to the stationary states that would be expected: as exemplified in the case of simple spin chains, [18, 19]. More recently similar or identical thermostat models built with free systems have been considered starting with [20].

The case of dimension 3 is very similar: it is not difficult to prove, that the key bounds (6.9) hold; however a naive application of the ideas developed in [10] to prove that $R_n(t)$ satisfies Eq.(6.11) is not possible.

Isokinetic thermostats should be treated in a very similar way, [1]: the extra difficulty is that the entropy production in a finite time interval receives a contribution also from the time derivative of the total energy of the reservoirs, [1], and further work seems needed.

More general cases, like Lennard-Jones interparticle potentials are more difficult, see [21]. Finally here the interaction potential has been assumed smooth: singularities like hard core could be also considered at a heuristic level. It seems that in presence of hard cores plus smooth repulsive potentials all estimates of Sec.V,VI are still valid but the existence of the limiting motion as $\Lambda\to\infty$ remains a difficult point because of the discontinuities in the velocities due to collisions.

XI. APPENDICES

A. Appendix: Sets of full measures

There are c_0 and R_0 and a strictly positive, non decreasing function $\gamma(c)$, $c\ge c_0$, so that $\forall c\ge c_0, \forall R\ge R_0$,

$$\mu_0\Big(W(x,0,R)\ge CR^d\Big)\le e^{-\gamma(c)R^d} \tag{11.1}$$

If $g:\mathbb{Z}^d\to\mathbb{R}_+$, $g(i)\ge1$, $c\ge c_0$, the probability

$$\mu_0\Big(\cap_{i\in\mathbb{Z}^d,r\ge g(i)}W(x;i,r)\le c\,r^d\Big) \tag{11.2}$$

is $\ge 1-\sum_{i\in\mathbb{Z}^d,r\ge g(i)}e^{-\gamma(c)r^d}$ with the sum being bounded proportionally to the sum $\sum_{i\in\mathbb{Z}^d}e^{-\gamma(c)[g(i)]^d}$ which converges if $g(i)\ge c'(\log_+|i|)^{1/d}$, with c' large enough.

B. Appendix: Choice of $R_n(t)$

The proof of the inequalities Eq.(6.4),(6.9) yields $\forall t\le\Theta$ that $W(S^{(n)}_t x,R)\le cW(x,R+\int_0^t V_n)$ provided R is such that $\frac{R+\int_0^t V_n}{R}\le 2$, which is implied by $R\ge R_0+\int_0^t V_n(s)ds$, $R_0\ge0$. The maximal speed $V(t)$ at time t is bounded by $V(t)\le v_1\sqrt{2W_n(S^{(n)}_t x,R)}$. Choosing $R_0=R_n(0)=n^{\frac1d}$ we get $V_n(t)\le C'v_1R_n(t)^{d/2}\le Cv_1n^{\frac12}$: such choice is the weakest that still insures that the set of initial data has $W(x,0,R)/R^d$ finite with μ_0–probability 1, see appendix A.

C. Appendix: The Hamiltonian motion is a flow in $\mathcal{H}_\zeta$, $\zeta\ge\frac1d$

The following theorem is obtatined by a straightforward adaptation to the case $d=1,2$ of theorem 2.2 in [15].

Theorem 9: *Let $d=1,2$, $\zeta\ge1/d$, $E>0$. Then, given any Θ there is E' (depending on ζ,Θ,E) so that for all x such that $\mathcal{E}_\zeta(x)\le E$*

$$\mathcal{E}_\zeta(S^{(0)}_t x)\le E',\qquad \textit{for all } t\le\Theta \tag{11.3}$$

so that the evolution $x\to S^{(0)}_t x$ is a flow in all spaces $\mathcal{H}_\zeta$, $\zeta\ge1/d$.

So far, for the sake of definiteness, $\zeta=1/d$ has been assumed: therefore in the following proof the quantity ζ has to be intended equal to $1/d$; however ζ is left undetermined because the proof would still hold for arbitrary $\zeta\ge1/d$, if larger values were consistently assigned to it since the beginning of this paper, under the *essential restriction* $d\le2$.

Proof. Let $x^{(n,0)}_t\stackrel{def}{=}S^{(n,0)}_t x$ and consider

$$\widetilde W\big(x^{(0)}_t,\xi,\rho\big),\quad\text{for}\quad \rho\ge(\log_+(|\xi|/r_\varphi))^\zeta \tag{11.4}$$

with $\widetilde W$ defined as in Eq.(5.7) with no restriction in the sums over q,q'. Let $n_\xi-1$ be the smallest integer such that $\Lambda_{n_\xi-1}$ contains the ball of center ξ and radius $\rho\,r_\varphi$. Then $\forall t\le\Theta$

$$\begin{aligned}\widetilde W\big(x^{(0)}_t,\xi,\rho\big)\le{}&\widetilde W_{n_\xi}\big(x^{(n_\xi,0)}_t,\xi,\rho\big)\\&+|\widetilde W\big(x^{(0)}_t,\xi,\rho\big)-\widetilde W_{n_\xi}\big(x^{(n_\xi,0)}_t,\xi,\rho\big)|\end{aligned} \tag{11.5}$$

The motions $x^{(n_\xi,0)}_t$ and $x^{(0)}_t$ are very close for all points which initially are in $\Lambda_{n_\xi-1}$: by Eq.(8.6)–(8.8) the difference of positions and velocities are bounded by $C\exp -c\,2^{n_\xi/2}$.

Setting $\chi_\xi(q)$ equal to the smoothed characteristic function $\chi_\xi(q,\rho)$ introduced in Eq.(5.7), $\chi_\xi(q^{(n,0)}_i(t))$ and $\chi_\xi(q^{(0)}_i(t))$ force their arguments to be within Λ_{k_1} if $2^{k_1}=2^{n_\xi-1}+\rho\ll2^{n_\xi}$. Hence the inequality

$$\begin{aligned}&|\widetilde W\big(x^{(0)}_t,\xi,\rho\big)-\widetilde W_{n_\xi}\big(x^{(n_\xi,0)}_t,\xi,\rho\big)|\\&\le C'e^{-cn_\xi}\sum\chi_\xi(q^{(n_\xi,0)}_i(t))\{|\dot q^{(n_\xi,0)}_i(t)|+\mathcal{N}_i(t)\}\\&\le C\,e^{-cn_\xi}\sup_{\xi'\in\Lambda_{n_\xi}}\widetilde W\big(x^{(n_\xi,0)}_t,\xi',\rho+\rho_{n_\xi}\big)\end{aligned} \tag{11.6}$$

where $\mathcal{N}_i$ = number of points in $x^{(n_\xi,0)}_t$ which interact with $q^{(n_\xi,0)}_i(t)$ and $\rho_{n_\xi}\stackrel{def}{=}\int_0^\Theta V_{n_\xi}(\tau)d\tau$: recall that

$V_{n_\xi}(t) = C\, v_1\, n_\xi^{\zeta d/2}$, see Eq.(6.10) (using the better estimate Eq.(6.11), $V_n \le C\, v_1\, n^{\frac12}$, valid for all ζ, would lead to the same end result because $\zeta d \ge 1$). Actually e^{-cn_ξ} could be replaced by $\exp -(c\, 2^{n_\xi/2})$ as in Eq.(8.6)–(8.8).

Consider first the case of ρ large, say $\rho > \rho_{n_\xi} = O(n_\xi^\zeta)$. Then $\widetilde W\big(x_t^{(0)};\xi,\rho\big)$ can be estimated by remarking that the argument leading to Eq.(6.9) remains unchanged if $R(t) = \rho + \int_0^t V_{n_\xi}(\tau)d\tau$ and $R(t,s) = R(t) + \int_s^t V_{n_\xi}(\tau)d\tau$ are used instead of the corresponding $R_{n_\xi}(t), R_{n_\xi}(t,s)$ (as long as $\rho \ge 0$). Then

$$\widetilde W(x_t^{(0)};\xi,\rho+\rho_{n_\xi}) \le C\widetilde W(x,\rho+2\rho_{n_\xi}) \tag{11.7}$$

as in the first of Eq.(6.8).

Suppose $\rho_0 - \rho_{n_\xi} > g_\zeta(\xi/r_\varphi)$, *i.e.* if $\rho_0 > Cn_\xi^\zeta$, then $\widetilde W(x_t^{(0)};\xi,\rho_0)) \le C'\widetilde W(x,\rho_0+\rho_{n_\xi})) \le C''(\rho_0+\rho_{n_\xi}))^d \le C\rho_0^d$: hence only the values of $(n_\xi-1)^\zeta \le \rho_0 \le Cn_\xi^\zeta$ are still to be examined.

In this case, however, the bound $\widetilde W(x_t^{(0)};\xi,\rho+\rho_{n_\xi}) \le C\widetilde W(x,\rho+2\rho_{n_\xi})$ involves quantities ρ,ρ_{n_ξ} with ratios bounded above and below by a constant, hence $\widetilde W(x_t^{(0)};\xi,\rho)$ is bounded by $\widetilde W(x;\xi,\rho+Cn^\zeta) \le C'\rho^d$.

Conclusion: there is $C > 0$, depending only on $\mathcal{E}_\zeta$ and for all $\rho > g_\zeta(\xi/r_\varphi)$, $t \le \Theta$ it is $W(x_t^{(0)};\xi,\rho) \le C\,\rho^d$.

D. Appendix: Quasi invariance

A probability distribution μ on a piecewise regular manifold M is *quasi invariant* for a flow $x \to S_t x$ generated by a differential equation $\dot x = v_x$ if $e^{-\lambda(t)} \le \mu(S_{-t}dx)/\mu(dx) \le e^{\lambda(t)}$ and $\lambda(t) < \infty$.

Suppose given $\Theta > 0$, a piecewise smooth surface $\Sigma \subset M$ with unit normal vector n_x and a "stopping time" $x \to \theta(x) \le \Theta$ defined on Σ consider all points $x \in \Sigma$ which are reached *for the first time* in positive time $t \le \theta(x)$ from data $y \notin \Sigma$. Call E, the set of such points, the *tube with base* Σ *and ceiling* $\theta(x)$.

The probability distribution μ is *quasi invariant* with respect to Σ and to the stopping time $x \to \theta(x)$ if it is absolutely continuous with respect to the volume measure, its density $r(x)$ is continuous and $e^{-\lambda} \le \mu(S_{-t}dx)/\mu(dx) \le e^\lambda$ for some $\lambda > 0$ and for all $0 \le t \le \theta(x)$: this is referred to by saying that μ is quasi invariant with respect to the stopping time $\theta(x)$ on Σ: symbolically μ is $(\Sigma,\theta(x))$–λ-quasi invariant.

Then the following *Sinai's lemma*, [11–13], holds:

Lemma: *If μ is $(\Sigma,\theta(x))$–λ-quasi invariant the integral of any non negative function f over the tube with base Σ and ceiling $\theta(x)$ can be bounded by*

$$\int_E f(y)\mu(dy) \le e^\lambda \int_\Sigma\int_0^{\theta(x)} r(x)\,f(S_{-\tau}x)\,v_x\cdot n_x\,ds_x d\tau,$$

$$\ge e^{-\lambda} \int_\Sigma\int_0^{\theta(x)} r(x)\,f(S_{-\tau}x)\,v_x\cdot n_x\,ds_x d\tau \tag{11.8}$$

The lemma can been used to reduce dynamical estimates to equilibrium estimates.

Proof: Let the trajectory of a point y which reaches Σ within the stopping time at $x \in \Sigma$ be parameterized by the time τ and let ds_x be the surface element on Σ. Then the set of points into which the parallelepiped Δ with base ds_x and height $d\tau$ becomes a parallelepiped $S_{-t}\Delta$ with base $S_t ds_x$ and the same height $d\tau$. Therefore the measure of $\mu(S_t\Delta)$ is $e^{-\lambda} \le \frac{\mu(S_t\Delta)}{\mu(\Delta)} \le e^\lambda$ hence the integral of any positive function $f(y)$ over the set E can be bounded above and below by the integral of $\int_\Sigma\int_0^{\theta(x)} f(S_t x)\rho(x)ds_x d\tau$ if $\rho(x)ds_x d\tau$ is the measure of Δ: the latter is $r(x)v_x\cdot n_x ds_x d\tau$. Therefore $\rho(x) = r(x)\,v_x\cdot n_x$.

E. Appendix: Proof of Eq.(9.12)

The factor $e^{-C'M^2V}$ arises because of the entropy bound (*i.e.* from the phase space contraction estimate within the stopping time). Therefore it is sufficient to find a bound to the integral in Eq.(9.10) *without the factor* $e^{\widehat\sigma(y,t)}$.

Consider first the case of $\mathcal{S}_\xi^1$. By Eq.(9.11) if $y \in \mathcal{S}_\xi^1$ then $|y\cap C_\xi| = k_\xi$ and there is $(q,\dot q) \in y$ with $q \in \partial C_\xi$.

Remark that y is the configuration reached starting from an initial data $x \in \Xi_E$ within a time $< T_{M,V;n}(x) < t_{\Lambda_n}(x)$: hence Eq.(6.11) applies. By Eq.(6.11) $w(y) \le |\dot q| \le v_1\,C\,\sqrt n$ so that

$$\begin{aligned}&\int_{\mathcal{S}_\xi^1}\mu_{0,\Sigma'}(dy)\int_0^{\theta(y)} dt\,w(y)\\ &\le \Theta v_1 C\sqrt n\int\mu(dx)\frac{J_1}{Z_{C_\xi}(x)}\end{aligned} \tag{11.9}$$

where $\mu(dx)$ is the μ_0-distribution of configurations x outside C_ξ and

$$J_1 = \int_{\partial C_\xi} dq_1 \int_{C_\xi^{k_\xi-1}} \frac{dq_2\ldots dq_{k_\xi}}{(k_\xi-1)!}\int_{\mathbb{R}^{dk_\xi}} d\dot q e^{-\beta_j H(q,\dot q|x)} \tag{11.10}$$

The estimate of the *r.h.s.* of Eq.(11.9), as remarked, is an "equilibrium estimate". By superstability, [3], the configurational energy $U(q|x) \ge bk_\xi^2 - b'k_\xi$, so that J_1 is bounded by:

$$B\,e^{-\beta_j(bk_\xi^2-b'k_\xi)}\frac{|C_\xi|^{k_\xi-1}|\partial C_\xi|}{(k_\xi-1)!}(\frac{2\pi}{\beta_j m})^{\frac d2 k_\xi} \tag{11.11}$$

while $\int \mu(dx) \frac{1}{Z_{C_\xi}(x)} \le 1$ because $Z_{C_\xi}(x) \ge 1$: and the bound can be summed over k_ξ. Thus the contribution from $\mathcal{S}_1$ to Eq.(11.9) is bounded by

$$C' e^{CM^2 V} \sqrt{n}\, e^{-b[(\log n)^\lambda g_\lambda(\xi/r_\varphi)]^2} \tag{11.12}$$

with C, b suitable positive constants. Since $\lambda > 1/2$, this is summable over ξ and yields the part of the Eq.(9.8) coming from the integration over $\mathcal{S}^1_\xi$.

Let, next, $y \in \mathcal{S}^2_\xi$ and let $(q, \dot q)$ as in (9.11). The function w is

$$w = \frac{|dE(q,\dot q)/dt|}{|\mathrm{grad} E(q,\dot q)|} \tag{11.13}$$

$|dE(q,\dot q)/dt| \le C\, |\dot q| n^{1/2}$ because dE/dt is the work on the particle $(q, \dot q)$ done by the pair interactions (excluding the wall forces). It is then bounded proportionally to the number of particles which can interact with $(q, \dot q)$, which, by theorem 4, is bounded proportionally to $n^{1/2}$ (as the total configuration is in Σ'). On the other hand, $|\mathrm{grad} E(q,\dot q)| = \sqrt{|\partial\psi(q)|^2 + m|\dot q|^2} \ge \sqrt{m}|\dot q|$ hence $w \le C n^{1/2}$ again by Eq.(6.11) and the remark preceding Eq.(11.9).

Then, analogously to (11.9), the integral under consideration is bounded by $C e^{C' M^2 V} \sqrt{n}$ (C, C' are suitable constants functions of E) times an equilibrium integral $\int \mu(dx) \frac{J_2}{Z_{C_\xi}(x)}$ with J_2 defined by:

$$\sum_k \int_{C_\xi^{k-1} \times \mathbb{R}^{k-1}} \frac{dq_2 \dots dq_k d\dot q_2 \dots d\dot q_k}{(k-1)!} e^{-\beta_j K(\dot q_2, .., \dot q_k)} \cdot e^{-\beta_j \tilde E_\xi}\, \mathrm{area}(\{E(q,\dot q) = \tilde E_\xi\}) \tag{11.14}$$

where the area$(\{E(q,\dot q) = \tilde E_\xi\})$ is the area of the surface $\{(q,\dot q) : E(q,\dot q) = \tilde E_\xi\}$ in $\mathbb{R}^{2d}$ (the $\widetilde E_\xi$ is defined in (9.11)). Then J_2 is bounded by

$$\sum_k \frac{B}{(k-1)!} \Big(|C_\xi| \big(\frac{2\pi}{\beta_j m}\big)^{\frac{d}{2}} \Big)^{(k-1)} |C_\xi| (\tilde E_\xi)^{(d-1)/2} e^{-\beta_j \tilde E_\xi} \tag{11.15}$$

so that, suitably redefining C, C' (functions of E), the contribution from $\mathcal{S}_2$ is bounded by

$$C' e^{CM^2 V} \sqrt{n} e^{-\frac{\beta_j}{2}[(\log n)^\lambda g_\lambda(\xi/r_\varphi)]^2} \tag{11.16}$$

and Eq.(9.8) follows from Eq.(11.12) and (11.16).

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