Nonequilibrium, thermostats and thermodynamic limit

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Abstract: *The relation between thermostats of "isoenergetic" and "frictionless" kind is studied and their equivalence in the thermodynamic limit is proved in space dimension $d = 1, 2$ and, for special geometries, $d = 3$.*

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Contents

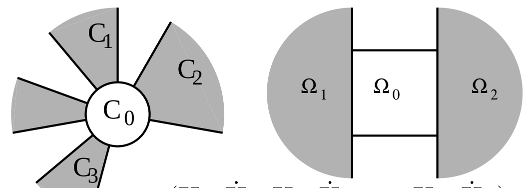
I. INTRODUCTION

In a recent paper [1] equivalence between isokinetic and frictionless thermostats has been discussed heuristically, leaving aside several difficulties on the understanding of the classical dynamics of systems of infinitely many particles. Such an understanding 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 frictionless thermostats, and study the conjectures corresponding to the ones formulated in [1] for isokinetic thermostats, obtaining a complete proof of equivalence in $1, 2, 3$–dimensional systems with various geometries.

In Sec.II the class of models to which our main result applies is described in detail. The main result is informally quoted at the end of the introduction after discussing the physics of the models; a precise statement will be theorem 1 in Sec.IV 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 property holds as a consequence of the theorems 2-10, each of which is interesting on its own right, discussed in the sections following Sec.IV and in the appendices.

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*.

A geometry that will be considered in dimension $d = 2$, to fix the ideas, 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 in the first picture in Fig.1; the second picture illustrates the only gemoetry that we shall consider in dimension $d = 3$:



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

Fig.1: *The $1+\nu$ finite 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 out of the infinitely many 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, contained in Ω_j, $j \ge 0$. The second figure illustrates the special geometry considered for $d = 3$: here two thermostats, symbolized by the shaded regions, Ω_1, Ω_2 occupy half-spaces adjacent to Ω_0.*

Referring, for instance, to the first of Fig.1:
(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 $\mathbf{k}_j$: $\Omega_j = \{\xi \in \mathbb{R}^d, |\xi| > D_0, \xi \cdot \mathbf{k}_j > |\xi| \cos\omega_j\}$, $j = 1, \ldots, \nu$.

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*.

We shall suppose that the forces acting on the particles are due to a repulsive pair interaction of radius r_φ and to external repulsive interactions acting within a distance r_ψ from the boundaries of the containers plus in the not frictionless models some *thermostatting forces* (of Gaussian type), [3]. Furthermore on the test system may act a nonconservative "stirring" force $\boldsymbol{\Phi}$.

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) "approximating" them with evolution equations involving finitely many particles.

There is wide arbitrariness in the choice of the regularization: and the ambiguity should disappear upon regularization removal.

For instance a first regularization, that we call *elastic regularization*, could 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 and will be kept inside Λ by an *elastic reflection* boundary condition at the boundary of Λ. 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.

A second *alternative* regularization, that we shall call *open regularization*, is obtained by letting only the particles initially inside Λ move while their motion is not influenced by the particles external to Λ and they are even allowed to exit the region 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.

In the Λ–regularized evolution the energy in the region $\Omega_j \cap \Lambda$, $j > 0$, will in general change in time. The *isoenergetic thermostat* is defined by adding "frictional" forces $-\alpha_j \dot q_i$ on all particles $(q_i, \dot q_i)$ in $\Omega_j \cap \Lambda$ where α_j is chosen in such a way that the total energy in $\Omega_j \cap \Lambda$ is constant in time, see the next section for details. The thermostatted evolution is then the evolution when such frictional forces are added in each $\Omega_j \cap \Lambda$, $j > 0$.

Isoenergetic models of the kind considered here have been studied also in simulations aiming at checking the thermostats"efficiency", *i.e.* the possibility of a boundary heat exchange sufficient to allow reaching stationarity in systems with many particles, [4].

The *essential physical requirement* that the thermostats should have a well defined temperature and density will be satisfied by an appropriate selection of the initial 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, at least not 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, at least at time 0 and in the thermodynamic limit, the requirement the initial data will be sampled with probability μ_0 where μ_0 is the product of extremal DLR distributions in each Ω_j with distinct temperatures and chemical potentials, see the next section for details.

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

This is proved after theorem 6 in Sec.VII.

The present paper relies heavily on results available in the literature, [5–8], but the results cannot be directly quoted because (minor) modifications of them are needed for our purposes. Therefore this paper is self-contained and the results that could be also found by a careful study of the literature are proved again from scratch: however we have confined such derivations in the Appendices A-F with the exception (for the sake of clarity ot the arguments) of Sec.V,VI; the Appendices G-L give technical details about the new methods, explained in Sec.VII and in the Appendices G-J.

The strong restriction on the thermostats geometry in $d = 3$ is commented in Appendix D after the proof of lemma 2, where it is used.

II. THERMOSTATS

A configuration x is thus 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 ν configurations $(\mathbf{X}_j, \dot{\mathbf{X}}_j)$ with $\mathbf{X}_j \subset \Omega_j$, $\dot{\mathbf{X}}_j \in \mathbb{R}^d)$, $j = 1, \ldots, \nu$:

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

$$x = (\mathbf{X}_0, \dot{\mathbf{X}}_0, \mathbf{X}_1, \dot{\mathbf{X}}_1, \ldots, \mathbf{X}_\nu, \dot{\mathbf{X}}_\nu) \stackrel{def}{=} (\mathbf{X}, \dot{\mathbf{X}}) \qquad (2.1)$$

with $\mathbf{X}_j \subset \Omega_j$, $\dot q_i \in \mathbb{R}^d$*: in every ball* $\Sigma(r')$ *of radius* r' *centered at* O*, fall a finite number of points of* $\mathbf{X}$.

The particles of x located outside Λ will be regarded as immobile or even as non-existing (depending on the choice of elastic or open regularization considered). *It will be convenient to suppose that the regularization region* Λ *is a ball* Λ_n *of radius* $2^n r_\varphi$, $n = n_0, n_0 + 1, \ldots$, with n_0 large so that $2^{n_0} r_\varphi > D_0 + r_\varphi$ so that Λ_n contain the test system and the particles interacting with it.

The particles are supposed to interact with each other, via a potential φ, and with the non artificial walls (*i.e* those of the containers Ω_j), via 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 smooth decreasing potential* $\psi \geq 0$ *of range* $r_\psi \ll r_\varphi$ *and diverging as an inverse power of the distance to the walls* $\cup_j \partial\Omega_j$*, while the (artificial boundary)* $\partial\Lambda$ *will be imagined as a perfectly reflecting elastic barrier in the case of elastic boundary conditions or as a boundary perfectly transparent to the moving particles.*

Hence the potential φ is *superstable* in the sense of [9]: 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 $0<\overline{\varphi}\,{\buildrel def\over=}\,\varphi(\frac{r_\varphi}{2})<\varphi(0)$; the wall potential at distance r from a wall will be supposed given by

$$\psi(r)=\big(\frac{r_\psi}{2r}\big)^\alpha\varphi_0,\qquad r\le\frac{r_\psi}{2}\tag{2.2}$$

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 not necessary: it has the physical interpretation of making easier the interaction between particles in Ω_0 and particles in $\cup_{j>0}\Omega_j$ and, therefore, transfer of energy between test system and thermostats.

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

The Λ–regularized elastic boundary condition equations of motions (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

$$\begin{aligned}m\ddot{\mathbf X}_{0i}=&-\partial_iU_0(\mathbf X_0)-\sum_{j>0}\partial_iU_{0,j}(\mathbf X_0,\mathbf X_j)+\boldsymbol\Phi_i(\mathbf X_0)\\ m\ddot{\mathbf X}_{ji}=&-\partial_iU_j(\mathbf X_j)-\partial_iU_{0,j}(\mathbf X_0,\mathbf X_j)-a\,\alpha_j\dot{\mathbf X}_{ji}\end{aligned}\tag{2.3}$$

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

(2) the potential energies $U_j(\mathbf X_j)$, $j\ge0$ 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:

$$\begin{aligned}U_j(\mathbf X_j)=&\sum_{q\in\mathbf X_j}\psi(q)+\sum_{q,q'\in\mathbf X_j}\varphi(q-q')\\ U_{0,j}(\mathbf X_0,\mathbf X_j)=&\sum_{q\in\mathbf X_0,q'\in\mathbf X_j}\varphi(q-q');\end{aligned}\tag{2.4}$$

(3) the first label in Eq.(2.3), $j=0$ or $j=1,\ldots,\nu$, respectively, refers to the test system or to a thermostat, while the second labels 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 $j=1,\ldots,\nu$,

$$\begin{aligned}\alpha_j\,{\buildrel def\over=}&\,\frac{Q_j}{d\,N_jk_BT_j(x)/m},\qquad\text{with}\\ Q_j\,{\buildrel def\over=}&\,-\dot{\mathbf X}_j\cdot\partial_jU_{0,j}(\mathbf X_0,\mathbf X_j),\end{aligned}\tag{2.5}$$

where $\frac{d}{2}\,N_j\,k_B\,T_j(x)\,{\buildrel def\over=}\,K_{j,\Lambda}(\dot{\mathbf X}_j)\,{\buildrel def\over=}\,\frac{m}{2}\dot{\mathbf X}_j^2$ 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*: the subscript Λ will be omitted unless really necessary. A more general model to which the analysis that follows also applies is in [10].

(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 $t\le t_\Lambda(x)$ where $t_\Lambda(x)$ is the maximum time before which the kinetic energies remain positive (hence the equations of motion remain defined for $t<t_\Lambda(x)$ because the denominators in the α_j stay >0; see Appendix I for technical details).

The equations 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.(2.3) will be considered together with the above and called the Λ–regularized *frictionless equations*.

Remark that Q_j is the work done, per unit time, by the test system on the particles in the j-th thermostat: it will therefore be interpreted as heat ceded to the j–th thermostat.

It will be convenient to consider also the open boundary condition at least in the frictionless thermostats case: the equations of motion are immediately written.

To impose, at least at time 0 and in the thermodynamic limit, the requirement that the thermostats should have a well defined temperature and density the values N_j,E_j, $j>0$, will be such that $\frac{N_j}{|\Omega_j\cap\Lambda|}\xrightarrow[\Lambda\to\infty]{}\delta_j$ and $\frac{E_j}{|\Omega_j\cap\Lambda|}\xrightarrow[\Lambda\to\infty]{}e_j$: 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 thermostats, for $j>0$.

Initial data: *The probability distribution μ_0 for the random choice of initial data will be, if $dx\,{\buildrel def\over=}\,\prod_{j=0}^\nu\frac{d\mathbf X_j\,d\dot{\mathbf X}_j}{N_j!}$, the limit as $\Lambda_0\to\infty$ of the finite volume grand canonical distributions on $\mathcal H$*

$$\begin{aligned}&\mu_{0,\Lambda_0}(dx)=const\;e^{-H_{0,\Lambda_0}(x)}\,dx,\qquad\text{with}\\ &H_{0,\Lambda_0}(x)\,{\buildrel def\over=}\,\sum_{j=0}^\nu\beta_j(K_{j,\Lambda_0}(x)-\lambda_jN_{j,\Lambda_0}+U_{j,\Lambda_0}(x))\\ &\beta_j\,{\buildrel def\over=}\,\frac{1}{k_BT_j}>0,\;\lambda_j\in\mathbb R,\end{aligned}\tag{2.6}$$

Remarks: (a) The values $\beta_0=\frac{1}{k_BT_0}>0,\lambda_0\in\mathbb R$, 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 D_0.
(c) The distribution μ_0 is a Gibbs distribution obtained by taking the "thermodynamic limit" $\Lambda_0 \to \infty$. 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, [11]. 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.
(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) Notice that μ_0 is a product of *independent equilibrium Gibbs distributions* because H_0 does not contain the interaction potentials $U_{0,j}$.
(f) The proofs extend to μ_0's which are product of DLR distributions in each container (which are not necessarily extremal).

III. NOTATIONS AND SIZES

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

$$Z_{\Lambda_0}(\beta,\lambda) = \sum_{N=0}^{\infty}\int \frac{dx_N}{N!}e^{-\beta(-\lambda N + K_j(x_N)+U_j(x_N))} \qquad (3.1)$$

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 thermodynamics, *i.e.*:

$$\begin{aligned}
&\delta_j = -\frac{\partial p(\beta_j,\lambda_j)}{\partial\lambda_j}, \quad k_B T_j = \beta_j^{-1} && (3.2)\\
&e_j = -\frac{\partial \beta_j p(\beta_j,\lambda_j)}{\partial\beta_j} - \lambda_j\delta_j, \qquad u_j = e_j - \frac{d}{2}\delta_j\beta_j^{-1}
\end{aligned}$$

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 μ_0-measure of a volume element in phase space by an amount related to (but different from) the variation of the Liouville volume because, in general,

$$\sigma(x) = \frac{d}{dt}\log\frac{\mu_0(S_t dx)}{\mu_0(dx)}\Big|_{t=0} \not\equiv 0 \qquad (3.3)$$

if $x\to S_t x$ denotes the solution of the equations of motion (for the considered model). The variation $\sigma(x)$, per unit time of a volume element, 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_n–regularized dynamics and for the elastic boundary conditions models,

$$\begin{aligned}
&\sigma(x) = \sum_{j\ge 0}\beta_j Q_j, && a=0 \qquad (3.4)\\
&\sigma(x) = \sum_{j>0}\frac{Q_j}{k_B T_j(x)}\,(1-\frac{1}{d\,N_j}) + \beta_0 Q_0, && a=1
\end{aligned}$$

as it follows by adding the time derivative $\beta_0 Q_0 \stackrel{def}{=} \beta_0(\dot K_0 + \dot U_0)$ to the divergence of Eq.(2.3) (regarded as a first order equation for the q's and $\dot q$'s) using the expression in Eq.(2.5) for α_j.

Remarks: (1) The expressions for $\sigma(x)$ will play a central role in our approach and one can say that the key idea of this work is to control the size of $|\sigma|$ and through it show that "singular" events like all particles come close to a simultaneous stop or accumulate to a high density somewhere or some of them acquire very high speed or approach too closely the walls (hence acquiring huge potential energy) will have zero μ_0-probability. Such events have zero μ_0-probability at time 0 and the variations with time of μ_0 are controlled by $|\sigma|$. Naturally, in view of Eq.(3.4), we shall call such estimates "*entropy bounds.*
(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, [12]. Notice that $\dot K_0 + \dot U_0 \stackrel{def}{=} Q_0$ is also $-\sum_{j>0}\dot{\mathbf{X}}_0\cdot\boldsymbol{\partial}_{\mathbf{X}_0}U_{0,j}(\mathbf{X}_0,\mathbf{X}_j) + \boldsymbol{\Phi}\cdot\dot{\mathbf{X}}_0$.
(3) It is also interesting to consider *isokinetic* thermostats: the multipliers α_j are then so defined that $K_j(x)$ is an exact constant of motion: calling its value $\frac{3}{2}N_j k_B T_j(x)$ the multiplier α_j becomes

$$\alpha_j(x) \stackrel{def}{=} \frac{Q_j - \dot U_j}{d\,N_j k_B T_j(x)/m}, \qquad (3.5)$$

with Q_j defined as in Eq.(2.5). They have been studied heuristically in [1].

The open boundary conditions will only be considered for the Λ_n–regularized frictionless dynamics (Λ_n is defined in the paragraph following Eq.(2.1)) and denoted $x\to\overline{S}_t^{(n,0)}x$: in this case only the particles initially inside Λ_n will move freely allowed to cross $\partial\Lambda_n$ unaffected by the particles initially outside Λ_n which will keep their positions fixed.

The Λ_n–regularized motions with elastic boundary conditions will be denoted $x\to S_t^{(n,a)}x$, $a=0,1$.

Let $S_t^{(a)}x$ or $\overline{S}_t^{(0)}x$ be the infinite volume dynamics $\lim_{n\to\infty} S_t^{(n,a)}x$, $a=0,1$, or $\lim_{n\to\infty}\overline{S}_t^{(n,0)}x$ *provided the limits exist.* We shall often use the notations

$$\begin{aligned} x^{(n,a)}(t) &\stackrel{def}{=} S_t^{(n,a)}x, & \overline{x}^{(n,0)}(t) &\stackrel{def}{=} \overline{S}_t^{(n,0)}x, \\ x^{(0)}(t) &\stackrel{def}{=} S_t^{(0)}x, & \overline{x}^{(0)}(t) &\stackrel{def}{=} \overline{S}_t^{(0)}x. \end{aligned} \tag{3.6}$$

Remarks: (1) In the frictionless case the existence of a solution to the equations of motion poses a problem only if we wish to study the $\Lambda_n \to \infty$ limit, *i.e.* in the case in which the thermostats are infinite: for Λ_n finite $\overline{S}_t^{(n,0)}x$ is well defined. While for the elastic reflections at the artificial regularization boundary $\partial\Lambda_n$ it is shown in [7] that the dynamics is also well defined with μ_0-probability 1.
(2) In the thermostatted case the kinetic energy appearing in the denominator of α_j, see Eq.(2.5), can be supposed to be > 0 with μ_0–probability 1 at $t = 0$. However it can become 0 later at $t_{\Lambda_n}(x)$ (see item (6), p.3, and the example at end of Sec.IV). In the course of the analysis it will be proved that with μ_0–probability 1 it is $t_{\Lambda_n}(x) \xrightarrow[n\to\infty]{} \infty$; therefore $S_t^{(n,1)}x$ is eventually well defined.
(3) It will be shown that the limits $\overline{x}^{(0)}(t)$ and $x^{(0)}(t)$ exist and are identical (as expected). It will become clear why it is necessary to consider first the frictionless thermostats with open boundary conditions.

We shall denote $(S_t^{(n,a)}x)_j$ or $x_j^{(n,a)}(t)$ the positions and velocities of the particles of $S_t^{(n,a)}x$ in Ω_j; a corresponding notation will be used for positions and velocities of $\overline{S}_t^{(n,0)}x$.

If $x_{ji}^{(n,a)}(t)$ denote the pairs of positions and velocities $(q_i^{(n,a)}(t), \dot q_i^{(n,a)}(t))$ 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 *between collisions* with the regularization boundary Λ_n (if any), see Eq.(2.3), as

$$\begin{aligned} q_i(t) =& q_i(0) + \int_0^t \dot q_i(t')\,dt' \\ \dot q_i(t) =& e^{-\int_0^t a\,\alpha_j(t')dt'}\dot q_i(0) \\ &+ \int_0^t e^{-\int_{t''}^t a\,\alpha_j(t')dt'} f_i(x^{(n,a)}(t''))\,dt'' \end{aligned} \tag{3.7}$$

where $mf_i = -\partial_{q_i}\big(U_j(\mathbf{X}_j(t)) + U_{0,j}(\mathbf{X}_0(t), \mathbf{X}_j(t))\big) + \delta_{j0}\Phi_i(\mathbf{X}_0(t))$ and $\mathbf{X}_j(t)$ denotes $\mathbf{X}_j^{(n,a)}(t)$ or $\overline{\mathbf{X}}_j^{(n,0)}(t)$. Here U_j is defined as in Eq.(2.4); $\alpha_0 \equiv 0$.

The open boundary evolution is described by Eq.(3.7) with $a = 0$ and with the appropriate interpretation of f_i.

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.

We shall work with dimensionless quantities: therefore suitable choices of the units will be made. If Θ is prefixed as the maximum time that will be considered, then

$$\begin{aligned} &\varphi_0\,:\,\text{(energy scale)},\ \ r_\varphi\,:\,\text{(length scale)}, \\ &\Theta\,:\,\text{(time scale)},\ \ v_1 = \sqrt{\frac{2\varphi(0)}{m}}\ \ \text{(velocity scale)} \end{aligned} \tag{3.8}$$

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

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 $e(\dot q, q) \stackrel{def}{=} \big(\frac{m\dot q^2}{2} + \psi(q)\big)/\varphi_0$ and, for any region Δ, the following dimensionless quantities:

$$\begin{aligned} &(a)\ N_\Delta(x), N_{j,\Delta}(x) \text{ the number of particles of } x \\ &\qquad\text{located in } \Delta/\Omega_0 \text{ or, respectively, } \Delta\cap\Omega_j \\ &(b)\ e_\Delta(x) \stackrel{def}{=} \max_{q_i\in\Delta/\Omega_0} e(\dot q_i, q_i) \\ &(c)\ U_\Delta(x) = \frac12 \sum_{q_i,q_j\in\Delta/\Omega_0,\, i\ne j} \varphi(q_i - q_j)/\varphi_0 \\ &(d)\ V_\Delta(x) = \max_{q_i\in\Delta/\Omega_0} |\dot q_i|/v_1 \end{aligned} \tag{3.9}$$

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* of the thermostat particles in $\mathcal{B}(\xi, R)$ will be defined as

$$\begin{aligned} W(x;\xi,R) \stackrel{def}{=}& \frac{1}{\varphi(0)} \sum_{q_i\in\mathcal{B}(\xi,R)/\Omega_0} \Big(\frac{m\dot q_i^2}{2} + \psi(q_i) \\ &+ \frac12 \sum_{q_i,q_j\in\mathcal{B}(\xi,R),\, i\ne j} \varphi(q_i - q_j) + \varphi(0)\Big) \end{aligned} \tag{3.10}$$

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

$$\mathcal{E}_\zeta(x) \stackrel{def}{=} \sup_\xi \sup_{R > g_\zeta(\frac{\xi}{r_\varphi})} \frac{W(x;\xi,R)}{R^d} \tag{3.11}$$

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

$$(1)\ \ \mathcal{E}_\zeta(x) < \infty, \qquad (2)\ \frac{K_{j,\Lambda}}{|\Lambda\cap\Omega_j|} > \frac12 \frac{\delta_j\,d}{2\beta_j} \tag{3.12}$$

for all $\Lambda = \mathcal{B}(O, L)$ large enough and for δ_j, T_j, given by Eq.(3.2); here $N_{j,\Lambda}$, $U_{j,\Lambda}$, $K_{j,\Lambda}$ denote the number of particles and their potential or kinetic energy in $\Omega_j \cap \Lambda$.

Remark: Notice that the lower bound in (2) of Eq.(3.12) is *half the value of the average kinetic energy* in the initial data and it will become clear that any prefixed fraction of the average kinetic energy could replace 1/2. Each set $\mathcal{H}_\zeta$ has μ_0-probability 1 for $\zeta \ge 1/d$, see Appendix A.

IV. EQUIVALENCE: ISOENERGETIC VERSUS FRICTIONLESS

Adapting a conjecture, in [1], we are led to expect that the motions considered satisfy the property:

Local dynamics *Given* $\Theta > 0$*, for* $t \in [0, \Theta]$ *and with* μ_0*–probability* 1*:*
(1) The limits $x^{(a)}(t) \stackrel{def}{=} \lim_{n\to\infty} x^{(n,a)}(t)$*,* $\overline{x}^{(0)}(t) \stackrel{def}{=} \lim_{n\to\infty} \overline{x}^{(n,0)}(t)$ *("thermodynamic limits") exist for all* $t \le \Theta$ *and* $a = 0, 1$*.*
(2) For $t \le \Theta$*,* $x^{(n,1)}(t)$ *satisfies the second of Eq.(3.12).*
(3) The functions $t \to x^{(0)}(t)$ *and* $t \to \overline{x}^{(0)}(t)$ *solve uniquely the frictionless equations in a subspace of* $\mathcal{H}$ *to which also* $x^{(1)}(t)$ *belongs (explicit, sufficient, bounds are described in theorem 5).*

Remarks: (a) The limits of $x^{(n,a)}(t), \overline{x}^{(n,0)}(t)$, as $\Lambda_n \to \infty$, 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 $x^{(a)}(t), \overline{x}^{(0)}(t)$ and those of the particles in $x^{(n,a)}(t), \overline{x}^{(n,0)}(t)$ which are in Δ are the same, and for each i the limits of $(q_i^{(n,a)}(t), \dot{q}_i^{(n,a)}(t))$ and $(\overline{q}_i^{(n,a)}(t), \dot{\overline{q}}_i^{(n,a)}(t))$ exist and are continuous, together with their first two derivatives.

(b) Uniqueness in item (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 11, in Appendix F, shows that for $d = 1, 2$ one could suppose such simpler property. However our statement is more general and we have left deliberately undetermined which subspace is meant in item (3) so that the determination of the subspace has to be considered part of the problem of establishing a local dynamics property. The generality becomes relevant in studying the case $d = 3$, where even in equilibrium a proof that the evolution of data in $\mathcal{H}_\zeta$ remains in the same space is lacking. The local dynamics property in $d = 3$ is implied by theorem 9, in Appendix E.

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

Hence for $|q|$ large they are, respectively, bounded proportionally to $[(\log|q|/r_\varphi)^{\frac{1}{d}}]^{\frac{d}{2}}$ and $[(\log|q|/r_\varphi)^{\frac{1}{d}}]^{-\frac{d}{\alpha}}$: 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 11 in Appendix F will show that this property remains true for all times, with μ_0 probability 1.

(d) An implication is that Eq.(3.7) has a meaning at time $t = 0$ with μ_0–probability 1 on the choice of the initial data x, because $\mathcal{E}(x) < \infty$.

(e) 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).

(f) It should also be expected that, with μ_0–probability 1, the limits as $\Lambda \to \infty$ of item (2), Eq.(3.12), 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 (and it is not needed for our purposes).

Assuming the local dynamics property, equivalence, hence the property $\overline{x}^{(0)}(t) \equiv x^{(1)}(t) \equiv x^{(0)}(t)$ for all finite t, can be established as in [1]. This is recalled checking, for instance, $\overline{x}^{(0)}(t) \equiv x^{(1)}(t)$, in the next few lines.

In the thermostatted Λ_n–regularized case it is

$$|\alpha_j(x)| = \frac{|\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)|}{\dot{\mathbf{X}}_j^2} \tag{4.1}$$

The force between pairs located in Ω_0, Ω_j is bounded by $F \stackrel{def}{=} \max|\partial\varphi(q)|$; the numerator of Eq.(4.1) can then be bounded by $FN_0\sqrt{\overline{N}_\Theta}\sqrt{2K_j/m}$ 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 $0 \le t \le \Theta$ (by 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. Hence for $0 \le t \le \Theta$ and large enough n Eq.(3.12) yields:

$$|\alpha_j| \le \frac{\sqrt{m}FN_0\sqrt{\overline{N}_\Theta}}{\sqrt{2K_{j,\Lambda_n}(x^{(1,\Lambda_n)}(t))}} \le \frac{\sqrt{m}FN_0\sqrt{\overline{N}_\Theta}}{\sqrt{|\Omega_j \cap \Lambda_n|\delta_j d/2\beta_j}}. \tag{4.2}$$

Letting $\Lambda_n \to \infty$ it follows that $\alpha_j \xrightarrow[\Lambda_n\to\infty]{} 0$.

Taking the limit $\Lambda_n \to \infty$ of Eq.(3.7) *at fixed i*, this means that, *with* μ_0*–probability* 1, the limit motion as $\Lambda_n \to \infty$ (with β_j, λ_j, $j > 0$, constant) satisfies

$$q_i(t) = q_i + \int_0^t \dot{q}_i(t')dt',\ \dot{q}_i(t) = \dot{q}_i + \int_0^t f_i(t'')dt'' \tag{4.3}$$

i.e. the frictionless equations; 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 frictionless 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 $(k_B\beta_0)^{-1}$ and chemical potential λ_0 as in Eq.(2.6)).

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

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 $x^{(n,1)}(t)$ might be not even well 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_n, an important symmetry of nature: *time reversal*: this certainly explains the favor that they have received in recent years in the simulations.

A corollary will be that neither the frictionless motion nor the dissipative thermostatted motions conserve phase space volume (measured with μ_0), but in both cases the entropy production rate coincides with the phase space volume (measured by μ_0) contraction and, at the thermodynamic limit, is identical in the two cases.

In Appendix G we have discussed the very simple case in which there is no direct mutual interaction between the thermostats particles, *free thermostats*, and the walls are reflecting. Reading this simple case may help understanding the organization of the analysis in the interacting cases.

V. ENERGY BOUND FOR FRICTIONLESS DYNAMICS

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.(3.10). For instance the speed $|\dot q|$ of a particle $q,\dot q$ in x is bounded by $\dot q^2 \le v_1^2 W(x,q,R)$, $R>0$, and its distance ρ from the walls by $\rho \ge \frac{r_\psi}{2} W(x,q,R)^{-\frac{1}{\alpha}}$, $R>0$.

In the geometries described in Fig.1 we shall preliminarily discuss bounds at time 0, *e.g* Eq.(5.3) below, and then we shall use energy conservation to extend the bounds to positive time.

Superstability of the potential φ implies that the number N of points in a region Δ, a cube or a ball, can be bounded in terms of the potential energy U in the same region and of $\varphi_0 = \varphi(0), \overline{\varphi} = \varphi(\frac{r_\varphi}{2}) > 0$ (defined after Eq.(2.1)). The bound derivation is recalled in Appendix A for clarity, and yields the inequality

$$N_\Delta \le C \frac{\sqrt{W}}{\sqrt{|\Delta|}}, \qquad C \stackrel{def}{=} \big(\frac{2\varphi_0}{\overline{\varphi}}\big)^{\frac{1}{2}}, \tag{5.1}$$

Calling $\mathcal{E} \stackrel{def}{=} \mathcal{E}_{1/d}(x)$, Eq.(3.11), consider the sequence of balls $\Lambda_n = \mathcal{B}(O, 2^n)$, of radii $L_n = 2^n r_\varphi$, $n \ge n_0$, see paragraph following Eq.(2.1). Given a configuration x let $N(x;\xi,R)$ the number of particles in the ball of radius $R\, r_\varphi$ centered at ξ and

$$\begin{aligned}
&(1)\ V_n = \text{(max velocity in } \Lambda_n/\Omega_0\,)/v_1\\
&(2)\ \rho_n = \text{ min distance to } \partial(\Omega_j \cap \Lambda_n) \text{ of } q_i \notin \Omega_0\\
&(3)\ \mathcal{N}_n = \max_{q_i \in \Lambda_n/\Omega_0} N(x;q_i,1)
\end{aligned} \tag{5.2}$$

Such quantities can be bounded in terms of the maximum of $W(x,\xi,R)$ over $\xi \in \Lambda_n$ and, by choosing $R = n^{1/d}$, we obtain, see definitions Eq.(3.8),

$$V_n = (n\mathcal{E})^{\frac{1}{2}},\ \rho_n = (n\,\mathcal{E})^{-\frac{1}{\alpha}},\ \mathcal{N}_n \le C(n\mathcal{E})^{\frac{1}{2}} \tag{5.3}$$

under the assumption that the wall potential has range r_ψ and is given by Eq.(2.2); the last inequality is a consequence of the definition of W and of the above mentioned superstability, Eq.(5.1). By controlling the growth in time of the energies W we shall extend the validity of Eq.(5.3) to positive times.

Constants 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): Eq.(5.1) 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 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.

In this and in the next section we shall study only the open regularization $\overline{x}^{(n,0)}(t) \stackrel{def}{=} \overline{S}_t^{(n,0)} x$, $t \le \Theta$, Θ being an arbitrarily fixed positive time. Therefore $\overline{x}^{(n,0)}(\tau)$ will be a finite configuration of particles which are not necessarily in Λ_n (unless $t = 0$).

Call $\rho_n(t), V_n(t), \mathcal{N}_n(t)$ the quantities in Eq.(5.2) evaluated for $\overline{x}^{(n,0)}(t)$ and let $\overline{\rho}_n(t)$, $\overline{V}_n(t), \overline{\mathcal{N}}_n(t)$ be the corresponding quantities defined by taking the maxima and minima in the full Λ_n (*i.e.* not excluding points in Ω_0).

For times $0 \le t \le \Theta$ consider Λ_n*-regularized* motions (see Sec.III) evolving from x with n fixed (see comment (6), p.3). Define

$$R_n(t) \stackrel{def}{=} n^\beta + \int_0^t V_n(s) \frac{v_1\, ds}{r_\varphi}, \tag{5.4}$$

where $R_n(0) = g_{1/d}(2^n) = n^{1/d}$ for $d = 1, 2$ but $R_n(0) = n^{1/2}$ for $d = 3$, and $v_1\, V_n(s)$ is the maximum speed that a moving particle *inside a thermostat* can acquire in the time interval $[0, s]$ under the Λ_n-regularized evolution: formally $v_1 V_n(s) = \max_{q_i \notin \Omega_0, s' \le s} |\dot{q}_i(s')|$.

By the choice of β it is $R_n(0) \ge n^{1/d}$ for $d = 1, 2, 3$: hence it will be possible to claim if $d = 1, 2$ that $W(x(0); \xi, R_n(0)) \le n\, \mathcal{E}(x(0)) < \infty$ with μ_0–probability 1, see Eq.(3.10),(3.11) and Appendix B. If $d = 3$ the somewhat weaker bound $W(x(0); \xi, R_n(0)) \le n^{3/2}\, \mathcal{E}(x(0)) < \infty$ will hold.

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

Then the following *a priori energy bound*, proved in Appendix C, holds:

Theorem 2: *The Λ_n–regularized frictionless dynamics satisfies, for $t \le \Theta$ and if $W(x, R) \stackrel{def}{=} \sup_\xi W(x; \xi, R)$:*

$$W(\overline{x}^{(n,0)}(t), R_n(t)) \le C\, R_n(t)^d \tag{5.5}$$

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

Remarks: (1) hence we obtain also a bound on the force that can be exercised on a particle by the others *including the forces due to the particles in* Ω_0 (as the latter force is bounded proportionally to N_0, hence by a constant):

$$\sum_j |F_{ij}| \le C R_n(t)^{d/2} \tag{5.6}$$

(2) the inequality holds $\forall d$'s. The bounds in Eq.(5.5), (5.6) will be repeatedly used.

By the definition Eq.(3.10) of W it follows that

$$V_n(s) \le C\, R_n(s)^{d/2} \tag{5.7}$$

Therefore for $d = 1, 2$, going back to Eq.(5.4) and solving it, $R_n(t)$ is bounded proportionally to $R_n(0) = n^{1/d}$: hence $R_n(t) \le C n^{1/d}$ for $0 \le t \le \Theta$, $d = 1, 2$ and $W \le Cn$ hence $V_n(t) \le C n^{1/2}$ and the bounds in the first line of Eq.(5.8), in theorem 3 below, are immediate consequences.

Theorem 3: *It is $\rho_n(t) \ge \overline{\rho}_n(t), V_n(t) \le \overline{V}_n(t), \mathcal{N}_n(t) \le \overline{\mathcal{N}}_n(t)$ and up to time $t \le \Theta$ the following inequalities hold for $d = 1, 2$ or $d = 3$ respectively:*

$$\begin{aligned} \overline{V}_n(t) \le & C\, n^{\frac{1}{2}}, \quad \overline{\mathcal{N}}_n(t) \le C n^{\frac{1}{2}}, \quad \overline{\rho}_n(t) \ge c\, n^{-\frac{1}{\alpha}} \\ \overline{V}_n(t) \le & C\, n^{\frac{1}{2}}, \quad \overline{\mathcal{N}}_n(t) \le C n^{\frac{3}{4}}, \quad \overline{\rho}_n(t) \ge c\, n^{-\frac{3}{2\alpha}} \end{aligned} \tag{5.8}$$

The $d = 3$ case is more delicate because the inequality obtained from Eq.(5.4) using Eq.(5.7) gives a blow-up in a finite time.

Following [8] we shall prove in Appendices D,E (theorem 7) that Eq.(5.7) can be improved to $V_n(t) \le C R_n(t)$, hence $V_n(t), R_n(t) \le C n^{1/2}$, which implies the second of Eq.(5.8) for $V_n(t), \mathcal{N}_n(t), \rho_n(t)$. The distinction between $\overline{\rho}_n(t), \overline{V}_n(t), \overline{\mathcal{N}}_n(t)$ and $V_n(t), \mathcal{N}_n(t), \rho_n(t)$ is only really necessary in the $d = 3$ case.

For $d = 1, 2$, the bounds on $V_n(t), \mathcal{N}_n(t), \rho_n(t)$ in the first line Eq.(5.8) have been just discussed as a corollary of theorem 2. For $d = 3$ the bounds in Eq.(5.8) will be proved for $V_n(t), \mathcal{N}_n(t), \rho_n(t)$ first and then they will be shown to imply the bounds in Eq.(5.8) for the $\overline{\rho}_n(t), \overline{V}_n(t), \overline{\mathcal{N}}_n(t)$: see Appendix E, paragraphs after Eq.(E.3)

VI. INFINITE VOLUME. FRICTIONLESS DYNAMICS

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

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

$$\overline{q}_i^{(n,0)}(t) = q_i(0) + t\dot{q}_i(0) + \int_0^t (t - \tau)\, f_i(\overline{x}^{(n,0)}(\tau))\, d\tau \tag{6.1}$$

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).

Existence of the dynamics in the frictionless, open boundary case will be discussed proving

Theorem 4: *If $d \le 3$ and $x \in \mathcal{H}_{1/d}$ the thermodynamic limit evolution $\overline{x}^{(0)}(t)_i = \lim_{n\to\infty} \overline{x}^{(n,0)}(t)_i$ exists.*

Proof: (adapted from the proof of theorem 2.1 in [8, p.32], which applies essentially unaltered). Let

$$\begin{aligned}\delta_i(t,n) &\stackrel{def}{=} |\overline{q}_i^{(n,0)}(t) - \overline{q}_i^{(n+1,0)}(t)|,\\ u_k(t,n) &\stackrel{def}{=} \max_{q_i\in\Lambda_k} \delta_i(t,n),\end{aligned} \tag{6.2}$$

then Eq.(6.1) yields

$$\begin{aligned}\delta_i(t,n) \le \int_0^t \frac{\Theta}{m}\, d\tau\, \big\{ &F'_w \delta_i(\tau,n)\\ &+ F' \sum_j (\delta_j(\tau,n) + \delta_i(\tau,n))\, \big\}\end{aligned} \tag{6.3}$$

where $F'_w = C\frac{\varphi_0}{r_\psi^2}\, n^{\frac{\alpha+2}{\alpha}}$ bounds the maximum gradient of the walls plus the stirring forces (see Eq.(5.8)) for $d = 1,2$ and for $d = 3$ we can take $F'_w = C\frac{\varphi_0}{r_\psi^2}\, n^{\frac{3}{2}\frac{\alpha+2}{\alpha}}$; $F' = \max_q |\partial^2\varphi(q)|$; and the sum is over the number $\overline{\mathcal{N}}_n$ of the particles $\overline{q}_j(\tau)$ that can interact with $\overline{q}_i(\tau)$ at time τ. The latter, by Eq.(5.8), is $\overline{\mathcal{N}}_n \le C n^{1/2}$ $(d = 1,2)$ or $\le C n^{3/4}$ $(d = 3)$ for both $\overline{x}^{(n,0)}(\tau)$ and $\overline{x}^{(n+1,0)}(\tau)$. Let

$$\eta \stackrel{def}{=} (\frac{3}{2} + \frac{3}{\alpha}),\quad 2^{k_1} \stackrel{def}{=} 2^k + r_n \tag{6.4}$$

where $r_n r_\varphi$ is the maximum distance a particle can travel in time $\le \Theta$, bounded by Eq.(5.8) by $C\, r_\varphi\, n^{1/2}$ (for $d = 2$ the η could be taken $\eta = (1 + \frac{2}{\alpha})$). Then

$$\frac{u_k(t,n)}{r_\varphi} \le C\, n^\eta \int_0^t \frac{u_{k_1}(s,n)}{r_\varphi} \frac{ds}{\Theta} \tag{6.5}$$

(C is a function of $\mathcal{E}$ as agreed in Sec.V). Eq.(6.5) can be iterated ℓ times; choosing ℓ so that $2^k + C\,\ell n^{1/2} < 2^n$, *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.(5.8) $u_n(t,n)$ is $\le C\, n^{1/2}$, so that for $n > k$,

$$\frac{u_k(n,t)}{r_\varphi} \le C'\, \frac{(n^\eta)^{\ell+1}}{\ell!} n^{1/2} \le C\, 2^{-2^{n/2}c} \tag{6.6}$$

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

$$\overline{q}_i^{(0)}(t) = \overline{q}_i^{(k,0)}(t) + \sum_{n=k}^{\infty} (\overline{q}_i^{(n+1,0)}(t) - \overline{q}_i^{(n,0)}(t)) \tag{6.7}$$

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

$$\frac{|\dot{\overline{q}}_i^{(n,0)}(t) - \dot{\overline{q}}_i^{(n+1,0)}(t)|}{v_1} \le C\, 2^{-2^{n/2}c} \tag{6.8}$$

follows from Eq.(6.6) and from $\dot{\overline{q}}_i^{(n,0)}(t) - \dot{\overline{q}}_i^{(n+1,0)}(t) = \int_0^t \big(f_i(\overline{q}^{(n,0)}(\tau)) - f_i(\overline{q}^{(n+1,0)}(\tau))\big) d\tau$. Or, for $n > k$ and $|q_i(0)| < r_\varphi 2^k$,

$$|\overline{x}^{(n,0)}(t)_i - \overline{x}^{(n+1,0)}(t)_i| \le C\, e^{-c2^{n/2}} \tag{6.9}$$

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

Hence existence of the thermodynamic limit dynamics in the frictionless case with open boundary conditions is complete and it yields concrete bounds as well. Uniqueness follows from Eq.(6.3): we skip details, [13]. Hence we have obtained:

Theorem 5: *There are $C(\mathcal{E}), c(\mathcal{E})^{-1}$, increasing functions of $\mathcal{E}$, such that the frictionless evolution satisfies the local dynamics property and if $q_i(0) \in \Lambda_k$*

$$\begin{aligned}&|\dot{\overline{q}}^{(n,0)}(t)| \le v_1 C(\mathcal{E})\, k^{\frac{1}{2}},\\ &\text{distance}(\overline{q}_i^{(n,0)}(t), \partial(\cup_j \Omega_j \cap \Lambda)) \ge c(\mathcal{E}) k^{-\frac{3}{2\alpha}} r_\psi\\ &\mathcal{N}_i(t,n) \le C(\mathcal{E})\, k^{3/4}\\ &|\overline{x}_i^{(n,0)}(t) - \overline{x}_i^{(0)}(t)| \le C(\mathcal{E}) r_\varphi e^{-c(\mathcal{E})2^{nd/2}}\end{aligned} \tag{6.10}$$

$\forall\, n > k$. The $\overline{x}^{(0)}(t)$ is the unique solution of the frictionless equations satisfying the first three of Eq.(6.10).

For $d = 1,2$ in the above proof the bounds in the first line of Eq.(5.8) could be used instead of the weaker ones in the second line (which holds also for $d = 3$): in this way the exponents $\frac{3}{2\alpha}$ and $\frac{3}{4}$ can be improved to $\frac{1}{\alpha}$ and $\frac{1}{2}$ respectively.

It would also be possible to show the stronger result that $\overline{x}^{(0)}(t) \in \mathcal{H}_{1/d}$ for $d = 1,2$ and $\overline{x}^{(0)}(t) \in \mathcal{H}_{3/2}$ for $d = 3$: but, for the proof of theorem 1, theorems 2-5 are sufficient, hence the proof of the stronger property is relegated to theorem 11 in Appendix F.

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).

VII. ENTROPY BOUND. THERMOSTATTED DYNAMICS

In this section the regularized motion, thermostatted and with *elastic boundary conditions*, will be compared to the thermodynamic limit of the frictionless dynamics with *open boundary conditions* whose existence and main properties have been established in Sec.VI.

A direct comparison of the two evolutions along the lines of Sec.VI does not seem possible because the quantity α_j is not small enough compared to the "Lyapunov exponent" n^η in Eq.(6.5): the extra α_j introduces a small inhomogeneous term in attempting a derivation of the analogue of Eq.(6.5). The extra term is of order 2^{-nd} which is amplified at rate Cn^η, $\eta > 1$ by Eq.(6.4), to a quantity $O(2^{-nd}e^{C\Theta n^\eta})$ diverging with n.

The strategy will be to introduce a stopping time $T_n(x)$ in the Λ_n–regularized dynamics defined by the time in which either the total kinetic energy in any thermostat or a local energy reaches a conveniently fixed threshold. The threshold will be defined so that within $T_n(x)$ the α_j are small and the frictionless and thermostatted dynamics are very close at least well inside Λ_n. We shall then conclude that the number of particles M and their maximal speed Vv_1 in a region $\mathcal{D}$ of width r_φ adjacent to Ω_0 are, in the thermostatted dynamics, bounded in terms of the respective values in the frictionless motion with the same initial conditions (finite as shown in Theorem 3 for $\mathcal{E}(x) \le E$). See Eq.(7.3), (7.4) below.

Thus *before the stopping time* $T_n(x)$ the entropy production in the thermostatted motion is simply controlled (by Eq.(3.4) it is $\le C\,M\,V$), showing that the measure μ_0 is "quasi invariant". This will imply that with large μ_0 probability the thermostatted motion cannot have a too short stopping time and, actually, that the stopping time cannot be reached before Θ. The precise statements can be found in the proof of theorem 6.

Restricting attention to the set $\mathcal{X}_E \subset \mathcal{H}_{1/d}$ of initial data $\mathcal{X}_E \stackrel{def}{=} \big\{x \,|\, \mathcal{E}(x) \le E;\ \big\}$ the constants $C, C', \ldots,$ $c, c', \ldots$ will be functions of E as stated in Sec.V.

Let $\rho_{\Omega_0}(\xi)$ be the distance of $\xi \notin \Omega_0$ from the boundary $\partial\Omega_0$ and let

$$\Lambda_* \stackrel{def}{=} \{\xi : \rho_{\Omega_0}(\xi) \le r_\varphi\},\ \Lambda_{**} \stackrel{def}{=} \{\xi : \rho_{\Omega_0}(\xi) \le 2r_\varphi\} \tag{7.1}$$

By the result in Sec.VI there are M and V (which depend on E) so that for all $x \in \mathcal{X}_E$, with the notations Eq.(3.9), for n large enough:

$$\begin{aligned}&\max_{t\le\Theta} N_{\Lambda_{**}}(\overline{S}_t^{(n,0)}x) < M\\ &\max_{t\le\Theta} V_{\Lambda_{**}}(\overline{S}_t^{(n,0)}x) < V-1\end{aligned} \tag{7.2}$$

Fix, once and for all, $\kappa > 0$ smaller than the minimum of the kinetic energy densities of the initial x in the ν thermostats (x-independent with μ_0–probability 1, by the "no phase transition" assumption, *i.e.* by ergodicity, see comment (c) p.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.(3.9)

$$\|x\|_n \stackrel{def}{=} \max_{\xi\in\Lambda_n} \frac{\max(N_{C_\xi}(x), \varepsilon_{C_\xi}(x))}{g_{1/2}(\xi/r_\varphi)}, \tag{7.3}$$

where $\varepsilon_{C_\xi}(x) \stackrel{def}{=} \sqrt{e_{C_\xi}(x)}$. Fixed γ once and for all, arbitrarily with $\frac12 < \gamma < 1$, define the stopping times

$$\begin{aligned}T_n(x) \stackrel{def}{=} \max\big\{t :\ t \le \Theta : \forall\,\tau < t,\\ \frac{K_{j,n}(S_\tau^{(n,1)}x)}{\varphi_0} > \kappa 2^{nd}, \quad \|S_t^{(n,1)}x\|_n < (\log n)^\gamma\big\}.\end{aligned} \tag{7.4}$$

Theorem 6: *If $d \le 3$, $\exists\, C, C', c > 0$ depending only on E such that for all n large enough:*
(1) For all $x \in \mathcal{X}_E$, $t \le T_n(x)$ and all $q_i(0) \in \Lambda_{(\log n)^\gamma}$

$$\begin{aligned}|q_i^{(n,a)}(t) - \overline{q}_i^{(n,0)}(t)| \le C\, r_\varphi\, e^{-(\log n)^\gamma\, c},\\ |\dot q_i^{(n,a)}(t) - \dot{\overline{q}}_i^{(n,0)}(t)| \le C\, v_1\, e^{-(\log n)^\gamma\, c}.\end{aligned} \tag{7.5}$$

furthermore with the notations Eq.(3.9), for n large enough and for all $t \le T_n(x)$:

$$N_{\Lambda_*}(S_t^{(n,1)}x) \le M,\ V_{\Lambda_*}(S_t^{(n,1)}x) \le V \tag{7.6}$$

(2) the μ_0-probability of the set $\mathcal{B} \stackrel{def}{=} \{x \,|\, x \in \mathcal{X}_E$ and $T_n(x) \le \Theta\}$ is

$$\mu_0(\mathcal{B}) \le C\, e^{-c(\log n)^{2\gamma} + C'MV}. \tag{7.7}$$

Assuming theorem 6 it is immediate to see that it implies the assumptions of theorem 1 (locality of the dynamics) because $\gamma > 1/2$ in Eq.(7.7) will imply (by Borel–Cantelli's lemma) that, with μ_0–probability 1, eventually for large n, $T_n(x) > \Theta$ and therefore, by Eq.(7.5), the thermodynamic limits of $x^{(n,a)}(t), \overline{x}^{(n,0)}(t)$ will coincide for $t \le \Theta$. Hence *theorem 6 implies theorem 1.*

Remarks: (1) The proof of theorem 6 contains a standard part, namely proving Eq.(7.5) and its corollary Eq.(7.6) *for* $t \le T_n(x)$: it follows from the existing literature, see [5, 8] and the proof in Section VI, and for completeness it is discussed, providing the details, in appendix K.
(2) The proof of Eq.(7.7), *i.e.* the proof that the Eq.(7.6) is not an empty statement, *is the technically original contribution of this paper.* It is based on an "entropy estimate" and the strategy of its use is discussed below, deferring to the Appendix J the actual computations to obtain the estimate.
(3) The proof below refers only to the case $a = 1$: the same argument applies for the (easier case of) frictionless motions with elastic boundary conditions, $a = 0$.

Proof: The stopping time $T_n(x)$ is the time when the trajectory $S_t^{(n,1)}x$, $x \in \mathcal{X}_E$, crosses the (piecewise smooth) surface Σ' of points y where either the kinetic energy in some $\Omega_j \cap \Lambda_n$ has the value $\kappa 2^{nd}$ or $\|S_t^{(n,1)}y\|_n$ crosses from below the value $(\log n)^\gamma$. Denote by Σ the subset of Σ' of all points $S_{T_n(x)}^{(n,1)}x$, $x \in \mathcal{X}_E$, $T_n(x) \le \Theta$. Thus $\Sigma = \cup_{\tau \le \Theta} S_\tau^{(n,1)} \Sigma_\tau$ where

$$\Sigma_\tau \stackrel{def}{=} \big\{x \in \mathcal{X}_E \,|\, T_n(x) = \tau\big\} \qquad (7.8)$$

and $\mathcal{B}$ is the disjoint union of Σ_τ over $\tau \le \Theta$.

The surfaces Σ, Σ' and Σ_τ, $\tau < \Theta$, are symbolically described in Fig.2.

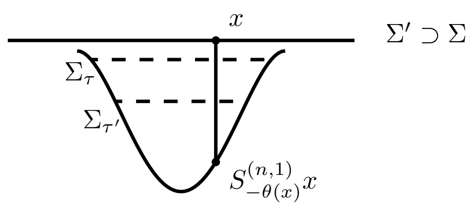


Fig.2: *The horizontal "line" represents Σ', Σ is the subset of Σ' under the "curve" $S_{-\theta(x)}^{(n,1)}x$; $\theta(x) \le \Theta$ is such that $S_{-\theta(x)}^{(n,1)}x \in \mathcal{X}_E$ while $S_{-t}^{(n,1)}x \notin \mathcal{X}_E$ for all $t \in (\theta(x), \Theta]$; the vertical line represents the trajectory of the point $S_{-\theta(x)}^{(n,1)}x$, the incomplete ("dashed") lines the "levels" $\Sigma_\tau, \Sigma_{\tau'}$, their missing parts are made of points not in $\mathcal{X}_E$ but with an "ancestor" in $\mathcal{X}_E$.*

This is the setup described in Appendix H, with Σ a "base" and $\theta(x) = \max_{\tau \le \Theta} \big\{\tau \,|\, S_{-\tau}^{(n,1)}x \in \Sigma_\tau\big\}$ a "ceiling function", so that (see Appendix H and, for early applications of this key estimate, see [5, 6, 14]):

$$\mu_0(\mathcal{B}) \le \int_\Sigma \nu_{0,\Sigma}(dy) \int_0^{\theta(y)} dt\; w(y)\; e^{\widehat{\sigma}(y,t)} \qquad (7.9)$$

where (1) $\nu_{0,\Sigma'}$ denotes the surface area measure (measuring the volume with μ_0) on Σ',
(2) $w = |v_x \cdot n_x|$ with v_x the $\dot{x}^{(n,1)}$ evaluated at x (by the equations of motion) and n_x is the normal to Σ at x,
(3) $\widehat{\sigma}(y,t) \stackrel{def}{=} \int_{-t}^0 |\sigma(y^{(n,1)}(t'))|\, dt'$ bounds the phase space contraction, *i.e.* the entropy production.

Effectively this means that the distribution μ_0 can be treated as an invariant one for the purpose of estimating probabilities in $\mathcal{B}$ via Eq.(7.9), because phase space contraction $\sigma = \sigma(x)$ is given by Eq.(3.3) and Q_0, see comment (2) following Eq.(3.3), can be estimated in the same way as Q_j, by $C'MV$ (ı.e by a bound on the speed times the number of particles in Λ_* times the number of particles in Ω_0). It follows that the integral $\int_0^{T_n(x)} |\sigma(x^{(n,a)}(t))|\, dt$ is also uniformly bounded (in $\mathcal{B}$) by CMV. Therefore a volume element in $\mathcal{B}$ contracts at most by e^{-CMV} on the trajectory of μ_0-almost all points $x \in \mathcal{B}$, up to the stopping time $T_n(x)$, and it follows

$$\mu_0(\mathcal{B}) \le e^{CMV} \int_{\Sigma'} |w(y)| \nu_{0,\Sigma'}(dy) \qquad (7.10)$$

which we call, naturally, *entropy bound*.

The derivation of the Eq.(7.7) becomes, by Eq.(7.10), an "equilibrium estimate", as it does not involve times $t > 0$ and is a standard consequence of the superstability property of the potential φ: the detailed calculations are in Appendix J.

Remark: The analysis in this section is valid for all dimensions except for the use of the properties of $\overline{x}^{(0)}(t)$, theorem 6, which have been derived only for $d \le 3$.

VIII. CONCLUSIONS

Equivalence between different thermostats is widely studied in the literature and the basic ideas, extended here, were laid down in [15]. A clear understanding of the problem was already set up in comparing isokinetic, isoenergetic and Nosé-Hoover bulk thermostats in [15], where a history of the earlier results is presented as well, see also [1, 16, 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].

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 difficult, see [21], and new ideas may be needed.

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 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.

It should be noted that the key bounds Eq.(5.8) hold for the open boundary conditions motions $\overline{x}^{(n,0)}(t)$ (as needed for our purposes) and have *not* been proved for $x^{(n,a)}(t)$. A careful analysis of our argument shows that the bounds hold only for particles initially in Λ_k, $k < n$, in the cases of reflecting boundary conditions, but not for $k = n$: the results of Sec.VII show that the maximal speed $V_n(t)$ is bounded by $C\, n^{1/2} (\log n)^\gamma$ in the Λ_n-regularized thermostatted or frictionless dynamics rather than by $Cn^{1/2}$, which is the bound obtained for the frictionless dynamics with open boundary conditions.

The main problem left open is what can be said about the limit $t \to \infty$, *i.e* the study of the stationary state reached at infinite time. A conjecture has been proposed, [22], that can be interpreted as saying that if $d = 1, 2$ the limit will be "trivial": *i.e* it will be an *equilibrium Gibbs distribution* at some intermediate temperature if $\boldsymbol{\Phi} = 0$. But, again interpreting the conjecture in [22], for $d = 3$ the stationary distribution(s) will be nontrivial and asymptotically they will be Gibbs distributions at the initial temperatures and densities of the thermostats.

APPENDIX A: SUPERSTABILITY. SETS OF FULL MEASURES

In our simple case ($\varphi \ge 0$, decreasing and $r_\varphi < \infty$) the superstability bound is reduced to Schwartz' inequality. In fact, by the dimensionless energy definition in Eq.(3.10), $W \ge (\frac{U}{\varphi_0} + N) \ge \frac{\overline{\varphi}}{2\varphi_0} \sum_p N_p^2$ with the sum running over labels p of disjoint boxes of diameter $\frac{r_\varphi}{2}$ covering a cube or a ball 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 $\sqrt{\overline{\varphi}/2\varphi_0} N \le \sqrt{W\,\ell}$, hence Eq.(5.1).

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

$$\mu_0\Big(\{W(x, 0, R) \ge c R^d\}\Big) \le e^{-\gamma(c) R^d} \tag{A.1}$$

(which more generally holds for superstable but not necesssarily positive φ, [9]).

If $g : \mathbb{Z}^d \to \mathbb{R}_+$, $g(i) \ge 1$, $c \ge c_0$, the probability

$$\mu_0\Big(\cap_{i \in \mathbb{Z}^d, r \in \mathbb{Z}, r \ge g(i)} \{W(x; i, r) \le c\, r^d\}\Big) \tag{A.2}$$

is $\ge 1 - \sum_{i \in \mathbb{Z}^d, r \in \mathbb{Z}, r \ge g(i)} e^{-\gamma(c) r^d}$ 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.

APPENDIX B: CHOICE OF $R_n(t)$

The proof of the inequalities Eq.(5.5) yields $\forall t \le \Theta$ that $W(\overline{S}_t^{(n,0)} x, R) \le c W(x, R + \int_0^t V_n(\tau) d\tau/\Theta)$ provided R is such that $\frac{R + \int_0^t V_n d\tau/\Theta}{R} \le 2$, which is implied by $R \ge R_0 + \int_0^t V_n(s) ds/\Theta,\ R_0 \ge 0$. The maximal speed $v_1 V_n(t)$ at time t is bounded by $V_n(t) \le \sqrt{W(\overline{S}_t^{(n,0)} x, R)}$. The choice $R_0 = R_n(0) = n^{1/d}$ 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.

APPENDIX C: THEOREMS 2 ($d \le 3$) AND 3 ($d \le 2$)

Consider the ball $\mathcal{B}(\xi, R_n(t, s))$ around $\xi \in \mathbb{R}^d$ of radius

$$R_n(t, s) \overset{def}{=} R_n(t) + \int_s^t \frac{v_1 V_n(s)}{r_\varphi} ds \ge 1. \tag{C.1}$$

The ball radius shrinks as s increases between 0 and t at speed $v_1 V_n(s)$: therefore no particle can enter it.

The quantity $R_n(t, s)$ can be used to obtain a bound on the size of $W(\overline{x}^{(n,0)}(t); \xi, R_n(t))$ in terms of the initial data $x(0) = x$ and of

$$W(x, R) \overset{def}{=} \sup_\xi W(x; \xi, R). \tag{C.2}$$

Remark that $W(\overline{x}^{(n,0)}(\tau), R)$ is finite if the just defined meaning of $\overline{x}^{(n,0)}(\tau)$ is kept in mind (so that $\overline{x}^{(n,0)}(\tau)$ contains finitely many particles).

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 $2(r_\varphi R)^{-1}$. Let also

$$\begin{aligned}\widetilde{W}(x; \xi, R) &\overset{def}{=} \frac{1}{\varphi_0} \sum_{q \notin \Omega_0} \chi_\xi(q, R) \\ &\cdot \Big(\frac{m\dot{q}^2}{2} + \psi(q) + \frac{1}{2} \sum_{q' \notin \Omega_0,\, q' \ne q} \varphi(q - q') + \varphi_0\Big), \\ \widetilde{W}(x; R) &\overset{def}{=} \sup_\xi \widetilde{W}(x; \xi, R).\end{aligned} \tag{C.3}$$

Denoting B an estimate of how many balls of radius 1 are needed in $\mathbb{R}^d$ to cover a ball of radius 3 (a multiple of the radius large enough for later use in Eq.(C.7)) 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.(C.2), so that:

$$\begin{aligned}W(\overline{x}^{(n,0)}(\tau); \xi, R) &\le \widetilde{W}(\overline{x}^{(n,0)}(\tau); \xi, R) \\ &\le W(\overline{x}^{(n,0)}(\tau); \xi, 2R), \\ \widetilde{W}(x; \xi, R) &\le B\, W(x, R)\end{aligned} \tag{C.4}$$

Although W has a direct physical interpretation $\widetilde{W}$ turns out to be mathematically more convenient and equivalent, for our purposes, because of Eq.(C.4).

The proof of theorem 2 is taken, from the version in [8, p.34] of an idea in [5, p.72]: it is repeated for completeness because quite a few minor modifications are needed here. It could be extended, essentially unaltered to the other boundary conditions, see [23, Sec.6-A], but we shall not need it here.

Consider $\widetilde{W}(\overline{x}_{\Lambda_n}(s); \xi, R_n(t,s))$, for $0 \le s \le t \le \Theta$:

$$\frac{d}{ds}\widetilde{W}(\overline{x}_{\Lambda_n}(s); \xi, R_n(t,s)) \le \sum_{q\notin\Omega_0} \frac{\chi_\xi(q(s), R_n(t,s))}{\varphi_0} \cdot \frac{d}{ds}\Big(\frac{m\dot q(s)^2}{2} + \psi(q(s)) + \frac12 \sum_{q'\notin\Omega_0} \varphi(q(s)-q'(s))\Big) \tag{C.5}$$

because the s–derivative of $\chi_\xi(q(s), R_n(t,s))$ is ≤ 0 since no particle can enter the shrinking ball $\mathcal{B}(\xi, R_n(t,s))$ as s grows: *i.e.* $\chi_\xi(q(s), R_n(t,s))$ cannot increase with s. The sums are restricted to the q's of $\overline{x}_{\Lambda_n}(s)$.

In the frictionless case a computation of the derivative in Eq.(C.5) 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

$$\frac{d}{ds}\widetilde{W}(\overline{x}_{\Lambda_n}(s); \xi, R_n(t,s)) \le \sum_{q\notin\Omega_0} \frac{\dot q(s) F(x(s))}{\varphi_0}\chi_{\xi,q,t,s} - \sum_{q,q'\notin\Omega_0} \big(\chi_{\xi,q,t,s} - \chi_{\xi,q',t,s}\big)\frac{\dot q(s)\partial_q\varphi(q(s)-q'(s))}{2\varphi_0} \tag{C.6}$$

where $F(x(s))$ denotes the force that the particles in Ω_0 exercise on the thermostats particles and the dot indicates a s–derivative; keep in mind that positions and velocities of particles outside Λ_n are not considered, in the Λ_n–regularized dynamics at open boundary conditions.

Since the non zero terms have $|q(s) - q'(s)| < r_\varphi$, the gradient of χ is $\le 2\,(r_\varphi R_n(t,s))^{-1}$ and $|\dot q|, |\dot q'| \le v_1 V_n(s) = r_\varphi |\dot R_n(t,s)|$ it follows, since $F = \max(N_0|\partial\varphi|)$ is an upper bound on the force that particles in Ω_0 can exercise on a particle in the thermostats,

$$\begin{aligned}\frac{d}{ds}\widetilde{W}(\overline{x}_{\Lambda_n}(s); \xi, R_n(t,s)) &\le \frac{Fv_1}{\varphi_0}\widetilde{W}(\overline{x}_{\Lambda_n}(s); \xi, R_n(t,s)) \\ &+ \frac{Fr_\varphi}{\varphi_0}\frac{|\dot R_n(t,s)|}{R_n(t,s)} B\,\widetilde{W}(\overline{x}_{\Lambda_n}(s); \xi, 2R_n(t,s)+1) \\ &\le B^2\,\frac{Fv_1}{\varphi_0}\Big(\frac{r_\varphi}{v_1}\frac{|\dot R_n(t,s)|}{R_n(t,s)} + 1\Big)\widetilde{W}(\overline{x}_{\Lambda_n}(s); R_n(t,s))\end{aligned} \tag{C.7}$$

where $\widetilde{W}(x;R)$ is defined in analogy with Eq.(C.2), and the first term in the *r.h.s.* is obtained by bounding the corresponding term in Eq.(C.6) as $\sum_q(|\dot q|\sqrt{\chi})\sqrt{\chi}$ followed by Schwartz' inequality.

By Eq.(C.7),(C.4), $R_n(t,s)/R(t,0) \le 2$, $\widetilde{W}(\overline{x}_{\Lambda_n}(s),\xi, R_n(t,s)) \le \widetilde{W}(\overline{x}_{\Lambda_n}(s), R_n(t,s))$ we get the inequality

$$W(\overline{x}_{\Lambda_n}(s), R_n(t,s)) \le C\,W(\overline{x}_{\Lambda_n}(0), R_n(t,0)) \tag{C.8}$$

with $C \stackrel{def}{=} \exp\big((\frac{Fr_\varphi}{\varphi_0}\log 2 + \frac{3Fv_1}{\varphi_0})\,\Theta\, B\big)$.

This concludes the proof of theorem 2.

To prove theorem 3 for $d = 2$ the inequalities Eq.(5.8) for $\rho_n(t), V_n(t), \mathcal{N}_n(t)$ follow from $R_n(t) \le Cn^{1/d}$ and from Eq.(5.5),(5.7). It remains to check them for $\overline{\rho}_n(t), \overline{V}_n(t), \overline{\mathcal{N}}_n(t)$, *i.e.* it remains to consider the particles moving inside Ω_0.

The inequalities certainly extend to the initial time $t = 0$ and to any t for $\overline{\mathcal{N}}_n(t)$ because the number of particles in Ω_0 is fixed and bounded in terms of $\mathcal{E}$. The variation $E(t) - E(0)$ of the energy contained inside the region Ω_0 equals the work $\mathcal{L}_{ext}$ done by the particles outside Ω_0 plus the work $\mathcal{L}_\Phi$ of the stirring forces in the time t. By the bounds Eq.(5.6),(5.7) this implies, for $t \le \Theta$:

$$\sum_{q\in\Omega_0}\big(\frac{m}{2}\dot q(t)^2 + \psi(q(t))\big) \le E(0) + (\frac{N_0^2}{2} + N_0 n^{1/2})C + \int_0^t (N_0\|\Phi\| \max_{q\in\Omega_0}|\dot q(\tau)| + N_0 n^{1/2}\,C\,V_n(\tau))d\tau \tag{C.9}$$

Therefore if $v(t) = \max_{q\in\Omega_0, t'\le t}|\dot q(t')|$ it follows that $v(t)^2 \le C'n + C''v(t)$ which implies $v(t) \le v_1 C n^{1/2}$; hence $\psi(q(t) \le Cn$ and the Eq.(5.8) are checked for $d = 2$.

Theorem 3 will be complete after the proof of the second line of Eq.(5.8) which follows from the speed bounds in Appendix E.

APPENDIX D: WORK BOUNDS. THERMOSTATS IN $d = 3$

In this and and in the next appendix we study the 3*-d dynamics* $\overline{S}^{(n,0)}_t x \equiv \overline{x}^{(n,0)}(t) \equiv (\overline{q}^{(n,0)}_h(t), \dot{\overline{q}}^{(n,0)}_h(t))$*, frictionless and with open boundary conditions.* We follow the method of [8].

Time intervals will be often subdivided into subintervals of equal length δ: in general, however, the number may be not an integer. We shall intend, without mention, that the last of the intervals might be shorter. This is used, without mention, only in cases in which the bounds considered remain valid also for the "left over" interval.

Let $\varepsilon(\dot q, q) \stackrel{def}{=} \sqrt{\frac{1}{\varphi_0}(\frac{m}{2}\dot q^2 + \psi(q))}$, abridged as $\varepsilon_j(t) \stackrel{def}{=} \varepsilon(\dot{\overline{q}}_j(t), \overline{q}_j(t))$ when $q, \dot q$ are time dependent. Remark that the speed of a particle is $\le v_1\varepsilon(q,\dot q)$ and its energy in the field of the walls forces is $\frac{mv_1^2}{2}\varepsilon(\dot q, q)^2$.

A particle $q_i \notin \Omega_0$ will be called *fast* in a time interval $J \subset [0,t]$ if $\varepsilon_{min} \stackrel{def}{=} \min_{\tau\in J}|\varepsilon_j(\tau)| \ge R_n(t)$.

The main property on which the analysis rests is an estimate by $CR_n(t)^{2-\gamma}$ of the work $\mathcal{L} \stackrel{def}{=} \int_J \sum_j \dot q_j F_{ij}$ that the i-th particle, assumed "fast", performs over the neighbors in the "short" time interval $J = [s-\theta, s]$, with $\theta \stackrel{def}{=} \frac{r_\varphi}{v_1}R_n(t)^{-\gamma}$ with $s \le t$ and $1 > \gamma > 0$, [8]. And the precise property that we shall need is expressed by the lemma:

Lemma 1: *Consider the dynamics $\overline{S}_t^{(n,0)}$ in the geometry of Fig.1 and in a time interval $J\subset[0,\Theta]$ of size $\theta=\frac{r_\varphi}{v_1}R_n(t)^{-\gamma}$. Then the work $\mathcal{L}\stackrel{def}{=}\int_J\sum_j\dot q_jF_{ij}$ that the i-th particle, assumed "fast" and in Ω_j, $j>0$, performs over the neighbors in the time interval J is bounded by $|\mathcal{L}|\le CR_n(t)^{2-\gamma}$ if $\gamma\in(\frac12,\frac23]$ and $J\subset[0,t]$.*

This will be proved considering *the special geometry in Fig.1*, following [8].

All things considered it will turn out that if $d=3$ the parameter γ can be arbitrarily fixed in the interval $(\frac12,\frac23]$.

Remark: The restriction on the geometry is severe: it is used only to prove lemma 5 below. It is very likely, however, that lemma 5 holds for *all thermostats considered in Sec.I, and* that *our equivalence holds in the general cases as well.*

Notice that all particles q_j interacting with a given particle at a given time τ are contained inside a ball of radius $2r_\varphi R_n(\tau)$.

Identifying particles with their labels and imagining the following maxima to be taken over $\tau\in J$, divide the particles $(q_j,\dot q_j)$ into three groups, [8], as "slow", "intermediate", "quick":

(a) $\mathcal{A}_0=$ *slow* $=\{j|\max|\varepsilon_j(\tau)|\le R_n(t)^\gamma\}$,

(b) $\mathcal{A}_k=$ *intermediate* $=\{j|2^{k-1}R_n(t)^\gamma<\max|\varepsilon_j(\tau)|\le 2^kR_n(t)^\gamma\}$, for $k=1,\ldots,k_m-1$, with k_m being determined by the condition $2^{k_m}R_n(t)^\gamma=R_n(t)$,

(c) $\overline{A}=$ *quick* $=\{j|\max|\varepsilon_j(\tau)|>\frac12R_n(t)\}$,

Correspondingly the work $\mathcal{L}=\mathcal{L}_0+\sum_k\mathcal{L}_k+\overline{\mathcal{L}}$: the three contributions will be estimated separately.

This corresponds to proposition 4.3 in [8]. The time interval $J=[s-\theta,s]$ $(s\ge\theta)$ is assumed, for simplicity, to be of length $\theta=R_n(t)^{-\gamma}r_\varphi/v_1$. The estimates, however, hold also for shorter intervals.

C-1 Work $\mathcal{L}_0$ of fast particles on slow particles

Divide the time interval J into H consecutive intervals $\Delta_h=[s_h,s_{h+1}]$ of size equal to $\frac{r_\varphi}{2v_1R_n(t)}$ and let $H=2R_n^{1-\gamma}$ be their number. The work $\mathcal{L}_0$ is bounded by

$$\begin{aligned}|\mathcal{L}_0|\le&\|\partial\varphi\|v_1R_n(t)^\gamma\int_JN(\tau)d\tau\\ \le&CR_n(t)^\gamma\sum_{h=1}^H|\Delta_h|\max_{\tau\in\Delta_h}N(\tau)\end{aligned}\tag{D.1}$$

where: $N(\tau)$ is the number of slow particles in the ball of radius r_φ and center $\overline{q}_i^{(n,0)}(\tau)$. The time intervals of size $\theta=R_n(t)^{-\gamma}r_\varphi/v_1$ are so short that a slow particle cannot travel a distance greater than the range r_φ away from $q_j(s-\theta)$.

A slow particle contributes to $N(\tau)$ if $|\overline{q}_j^{(n,0)}(\tau)-\overline{q}_i^{(n,0)}(\tau)|\le r_\varphi$, hence $|\overline{q}_j^{(n,0)}(s-\theta)-\overline{q}_i^{(n,0)}(\tau)|\le 2r_\varphi$ because $|\overline{q}_j^{(n,0)}(s-\theta)-\overline{q}_j^{(n,0)}(\tau)|\le r_\varphi$.

If $N_h\stackrel{def}{=}\max_{\tau\in\Delta_h}N(\tau)$ then:

$$|\mathcal{L}_0|\le CR_n(t)^{-(1-\gamma)/2}(\sum_kN_h^2)^{1/2}\tag{D.2}$$

having used $\sum_{h=1}^HN_h\le\sqrt{H}\sqrt{\sum_hN_h^2}$ and $H=2R_n^{1-\gamma}$.

Notice that N_h^2 is bounded by $W(\overline{x}(s-\theta)),\overline{q}_i^{(n,0)}(\tau),2)$ where τ is the time when the maximum defining N_h is reached.

Hence, if $\mathcal{T}_h$ denotes the tube spanned by the ball of radius $2r_\varphi$ and center at $\overline{q}_i^{(n,0)}(t)$ for $t\in\Delta_h$, N_h^2 is bounded by $W(\mathcal{T}_h)$ provided $W(\Gamma)$ is defined as in Eq.(3.10) with $\mathcal{B}(\xi,R)$ replaced by Γ.

Lemma 2: *Each $\mathcal{T}_h$ can be intersected by at most C other $\mathcal{T}_{h'}$.*

Remark: Thus $\mathcal{T}_h$ is a set contained in a ball of radius $r_\varphi R_n(t)$ (which is, by definition, the maximum distance *any* particle can travel) and each point is in at most C different $\mathcal{T}_h$'s. This implies $\sum_hW(\mathcal{T}_h)\le CW(\mathcal{T})\le C\,\mathcal{E}\,R_n(t)^d$, if $\mathcal{T}\stackrel{def}{=}\cup_h\mathcal{T}_h$. Concluding: $(\sum_hN_h^2)^{1/2}\le CW(\mathcal{T})^{1/2}$ so that by Eq.(D.2) it is $|\mathcal{L}_0|\le C\varphi_0R_n^{-\frac{1-\gamma}{2}}R_n^{d/2}$, $d=3$, because $\mathcal{T}$ is contained in the ball of radius $R_n(t)\,r_\varphi$ centered at $\overline{q}_i^{(n,0)}(s-\theta)$, or

$$|\mathcal{L}_0|\le C\varphi_0R_n(t)^2R_n^{-(1-\frac{\gamma}{2})}\le C\varphi_0R_n(t)^{2-\gamma}\tag{D.3}$$

by Eq.(5.5), provided $1-\frac{\gamma}{2}\ge\gamma$. This is possible for $d=3$ if $\gamma\le\frac23$.

Proof: To check lemma 2 let $\tau\to\lambda_0(\tau)$ be the path that the fast particle would follow under its own inertia and the walls forces, which act in a small strip $\mathcal{D}$ of width $r_\psi<r_\varphi$ near the containers walls, in a time interval of size $\theta=R_n(t)^{-\gamma}r_\varphi/v_1$.

Given a point $\xi\in\Omega_j$ the particle following $\lambda_0(\tau)$ might spend up to two intervals of time $J_1,J_2\subset J$ inside the ball of radius r_φ centered on ξ (possibly one before the collision with the wall and one after bouncing). However the actual path $\tau\to\lambda(\tau)$ differs from λ_0.

Suppose that initially the fast particle is outside $\mathcal{D}$: until outside $\mathcal{D}$ it proceeds, in time $\le\theta$, over a distance

$$\begin{aligned}\ell(\tau)\ge&|\dot q_i(s_h)|(\tau-s_h)-\int_{s_h}^\tau(\tau-s)\frac{|F_i(s)|}{m}\,ds\\ \ge&|\tau-s_h|\,(v_{\min}-Cv_1R_n(t)^{-\gamma+d/2}),\end{aligned}\tag{D.4}$$

by Eq.(5.6), undergoing a deflection by an angle which is at most $CR_n(t)^{-\gamma+d/2}/R_n(t)$ and will have velocity $\ge\frac{v_1}{2}R_n(t)$, for n large.

At the entrance into the region $\mathcal{D}$ at a time t_1 the difference between $\lambda(t_1)$ and $\lambda_0(t_1)$ will be $\le|t_1-$

$s_h| C\, v_1 R_n(t)^{-\gamma+d/2}$ and there are two possibilities for n large. The component of the velocity along the normal to the wall is $\ge \frac{1}{\sqrt{2}} v_1 \frac{R_n(t)}{2}$ or its tangential component is $\ge \frac{1}{\sqrt{2}} v_1 \frac{R_n(t)}{2}$.

In the first case the time spent by λ_0 inside $\mathcal{D}$ will be $\le \frac{4\sqrt{2} r_\psi}{v_1} R_n(t)^{-1}$ and then at a time t_2 the particle will be again out of $\mathcal{D}$ with a position $|\lambda(t_2) - \lambda_0(t_2)| \le (t_2 - s_h)\, C\, v_1\, R_n(t)^{-\gamma+d/2}$ and speed normal to the wall $> c\, R_n(t)$. The motion will then proceed a distance bounded as in Eq.(D.4) (with a larger C).

In the second case the tangential velocity is large and the particle will move away from the entrance point into $\mathcal{D}$ keeping its velocity component parallel to the wall within $\le C R_n(t)^{-\gamma+d/2}/R_n(t)$ dashing away from any fixed ball of radius r_φ, without coming close to any point within $2r_\varphi$ more than twice.

Next we can consider the case of a fast particle initially in $\mathcal{D}$: if the velocity component normal to the wall is $\ge \frac{1}{2\sqrt{2}} v_1 R_n(t)$ the particle will get out of $\mathcal{D}$ in a short time $< C \frac{r_\psi}{v_1} R_n(t)^{-1}$; if the tangential component is large the particle will move away from initial position in $\mathcal{D}$, keeping its velocity component parallel to the wall and undergoing a deflection $\le C R_n(t)^{-\gamma+d/2}/R_n(t)$.

Remark: Lemma 2 is likely to hold under the sole assumption that the fast particle path λ_0 moves away from the origin at radial speed bounded below proportionally to the initial value of ε_i. Hence it holds probably in full generality for the thermostats considered in Sec.I.

C-2 Work $\mathcal{L}_k$ of fast particles on intermediate speed particles

If $N(\tau)$ is the number of intermediate speed particles within an interaction radius of $\overline{q}_i(\tau)$, $\mathcal{L}_k$ is bounded by

$$|\mathcal{L}_k| \le ||\partial\varphi|| v_1 2^k R_n(t)^\gamma \int_{s-\theta}^{s} N(\tau)\, d\tau \tag{D.5}$$

analogously to Eq.(D.1).

The relative speed of the particles q_i and q_j, by the definition of $\mathcal{A}_k$, can be bounded below by $|\varepsilon_i(\tau) - \varepsilon_j(\tau)| \ge R_n(t) - 2^{k_m - 1} R_n(t)^\gamma \ge \frac{1}{2} R_n(t)$ for n large as long as the fast particle is outside $\mathcal{D}$.

The contribution of the j-th particle to $\mathcal{L}_k$ lasts, therefore, a time bounded by $C R_n(t)^{-1}$ except for the time, also of the order of $R_n(t)^{-1}$, spent by the fast particle within the wall with tangential speed smaller than a fraction of $R_n(t)$, say $3R_n(t)/4$. If at $\tau_j \in J$ the $\varepsilon_j(\tau)$ is maximum, then

$$\begin{aligned} &|\mathcal{L}_k| \le |\mathcal{A}_k|\, C\, R_n(t)^{-1}\, 2^k\, R_n(t)^\gamma, \qquad \text{and}\\ &|\mathcal{A}_k| 2^{2(k-1)} R_n^{2\gamma} \le \sum_{j\in\mathcal{A}_k} \varepsilon_j(\tau_j)^2 \\ &\le \sum_{j\in\mathcal{A}_k} \Big(\varepsilon_j(s-\theta)^2 + C \int_{s-\theta}^{s} d\tau |\dot{q}_j(\tau)| N_j(\tau) \Big) \end{aligned} \tag{D.6}$$

where $N_j(\tau)$ is the number of particles of $\overline{x}^{(n,0)}(\tau)$ which interact with $q_j(\tau)$. We multiply both both sides of (D.6) by 2^{-k}, bound $|\dot{q}_j(\tau)| 2^{-k} \le v_1 R_n(t)^\gamma$ and

$$\sum_k \sum_{j\in\mathcal{A}_k} N_j(\tau) \le C R_n(t)^d, \qquad d = 3 \tag{D.7}$$

which can be proved as follows: let $\mathcal{B}', \mathcal{B}$ be the balls with some center $q_i(s-\theta)$ and radius $2R_n(t)$ and $3R_n(t)$, respectively. Then

$$\begin{aligned} &\sum_k \sum_{j\in\mathcal{A}_k} N_j(\tau) \le \sum_{j:\, q_j(\tau)\in\mathcal{B}'} \ \sum_{\ell\,:|q_\ell(\tau)-q_j(\tau)|\le r_\varphi} 1 \\ &\le \sum\nolimits^{*} N_{C_i} N_{C_j} \end{aligned} \tag{D.8}$$

where the C_i's are elements of a covering of $\mathcal{B}$ by disjoint cubes of diameter $r_\varphi/2$ and N_{C_i} are the numbers of particles in the C_i's; and the $\sum^*$ denotes sum over $C_i, C_j \subset \mathcal{B}$ with $dist(C_i, C_j) \le r_\varphi$. The inequality continues as

$$\begin{aligned} &\sum\nolimits^{*} \frac{1}{2}(N_{C_i}^2 + N_{C_j}^2) \le C \sum_{C_i\subset\mathcal{B}} N_{C_i}^2 \\ &\le W(x(\tau), q_i(s-\theta), R_n(t)) \le C R_n(t)^d \end{aligned} \tag{D.9}$$

(by Eq.(5.5)) which proves Eq.(D.7). Since $\sum_k 2^{-k} \sum_j \varepsilon_j(\tau)^2 \le C R_n(t)^3$, by Eq.(5.5), we get from Eq. (D.6)), using Eq.(D.7):

$$\begin{aligned} &\sum_k |\mathcal{A}_k| 2^{k-2} R_n^{2\gamma} \le \sum_k 2^{-k} \sum_{j\in\mathcal{A}_k} \varepsilon_j(s-\theta)^2 \\ &+ C' R_n(t)^\gamma R_n(t)^3 R_n(t)^{-\gamma} \le C'' R_n(t)^3. \end{aligned} \tag{D.10}$$

Therefore $\sum_k |\mathcal{A}_k| 2^k \le \overline{C}(R_n^{3-2\gamma}) \le C R_n(t)^{3-\gamma} \theta/\Theta$ and $\sum_k \mathcal{L}_k$ is bounded, via Eq(D.6), proportionally to

$$R_n(t)^\gamma R_n(t)^{-1} R_n(t)^{3-\gamma} \frac{\theta}{\Theta} = C R_n(t)^{2-\gamma} \tag{D.11}$$

C-3 Work $\overline{\mathcal{L}}$ of a fast particle on quick particles

The work (of the inner forces) on the quick particles can be bounded by first remarking that their $\varepsilon_j(\tau)^2$ at a time $\tau \in J$ is bounded below by $\frac{1}{4} R_n(t)^2$ minus $C R_n(t)^{\frac{d}{2}-\gamma} \varepsilon_j$ (upper bound on the work done by the other particles in time $\frac{r_\varphi}{v_1} R_n(t)^{-\gamma}$). Therefore it follows that $\varepsilon_j(\tau) \ge c\, R_n(t)$ for n large enough, since $\gamma > \frac{1}{2}$.

So that $|\overline{\mathcal{A}}| \big(c\, R_n(t)\big)^2 \le \sum_j |\dot{q}_j(\tau)|^2 \le C v_1^2 R_n(t)^3$, by Eq(5.5).

It follows that $|\overline{\mathcal{A}}| \le C\mathcal{E} R_n(t)$. Therefore by the energy estimate (see Eq.(5.5)) an application of Schwartz' inequality bounds $|\overline{\mathcal{L}}|$ above by

$$\le C'|\overline{\mathcal{A}}|^{\frac12}\int_{s-\theta}^{s} d\tau(\sum_{j\in\overline{\mathcal{A}}}\varepsilon_j(\tau)^2)^{1/2}\le CR_n(t)^{\frac12}R_n(t)^{\frac32}\theta \tag{D.12}$$

by Eq.(5.5), *i.e.* $|\overline{\mathcal{L}}|\le CR_n(t)^{2-\gamma}$.

APPENDIX E: SPEED BOUNDS IN $d=3$

We can now infer an estimate for maximal speed, $v_1V_n(t)$, and maximal distance, $R_n(t)r_\varphi$, that a thermostat particle can travel in the Λ_n-regularized motion.

Theorem 7: *Given $x\in\mathcal{H}_{1/d}$, $d=3$, there is a constant G depending only on $\mathcal{E}=\mathcal{E}(x)$ and Θ such that for any particle of x initially in Λ_n it is $\varepsilon(t)<G\,R_n(t)$ for all $t\le\Theta$. Therefore, by Eq.(5.4), $V_n(t)\le CR_n(t)$ and $R_n(t)\le CR_n(0)\equiv C\,n^{1/2}$ for $t\le\Theta$.*

Proof. Suppose that there are $t^*\le t\le\Theta$ and $q_i(0)\in\Lambda_n$ so that $\varepsilon(t^*)=GR_n(t)$. We claim that the above cannot hold if $G^2>\frac43C''$, where C'' is a constant defined below, in the course of the proof.

Remark that the claim implies theorem 7 with $G=(4C'')/3)^{1/2}$. And the claim is proved as follows. Let C_1 be such that $\varepsilon_i(0)\le C_1R_n(0)$ for all x with $\mathcal{E}(x)\le E$. Then by choosing C'' large enough it will be $G\ge 2C_1$. Since $\varepsilon_i(t^*)=GR_n(t)>C_1R_n(t)\ge\varepsilon_i(0)$ there exists $t_1<t^*$ and $\varepsilon_i(\tau)\ge C_1R_n(t)$ for all $\tau\in[t_1,t^*]$. We shall next prove that $t^*-t_1\ge CR_n^{-1/2}$ so that $[t_1,t^*]$ splits into the union of H intervals of length $\theta=\frac{r_\varphi}{v_1}R_n(t)^{-\gamma}$ with H large. In fact $\frac{d\varepsilon_i(\tau)^2}{d\tau}\le C\varepsilon_i(\tau)\frac{1}{2m}|F_i(x(\tau))|$, hence $\frac{d\varepsilon_i(\tau)}{d\tau}\le C\,\frac{1}{2m}|F_i(x(\tau))|$, and by Eq.(5.6) (for non integer H see the comment at the beginning of Appendix D):

$$GR_n(t)\le C_1R_n(t)+C(t^*-t_1)R_n(t)^{d/2} \tag{E.1}$$

which yields $t^*-t_1\ge cR_n^{-\frac12}\gg R_n^{-\gamma}\Theta$ if $\gamma>\frac12$, $d=3$.

The variation $(\varepsilon_i(t^*)^2-\varepsilon_i(t_1)^2)$ equals the work of the pair interaction forces over the i-th particle. It is therefore the variation of the pair-potentials energy of the particle q_i in the configurations $\overline{x}^{(n.0)}(t_1),\overline{x}^{(n.0)}(t^*)$ *not taking into account* the N_0 particles in Ω_0, plus the work that the particles in Ω_0 perform on the particle q_i, plus the work that particle i performs on the neighbors. The three terms are bounded by

(a) $||\partial\varphi||$ times the number of particles interacting with i at the two times, hence by $CR_n(t)^{d/2}$ and by Eq.(5.6),(5.5) (valid also if $d=3$, see Sec.V),

(b) the work performed on the particle q_i by the N_0 particles in Ω_0 is bounded by $CN_0R_n(t)^{d/2}$ by Eq.(5.5),

(c) $|\sum_{h=1}^{H}\int_{t_1+(h-1)\theta}^{t_1+h\,\theta}\sum_j\dot q_j(\tau)F_{ij}(x(\tau))d\tau|$

so that, by the work estimates and by $H\theta\le\Theta$, it follows

$$G^2R_n(t)^2\le C_1^2R_n(t)^2+C''\,R_n(t)^2 \tag{E.2}$$

for n (hence $R_n(t)$) large enough if C'' is the largest of all constants met so far. Since $G\ge 2C_1$, Eq.(E.2) implies $G^2\le\frac43C''$ and the proof of theorem 7 is complete.

Going back to the definition of $R_n(t)$ in Eq.(5.4) it follows that $\exists\,C>0$, depending only on $\mathcal{E}$, such that for $t\le\Theta$,

$$\begin{aligned}&W(\overline{x}^{(n,0)}(t),R_n(t))\le CR_n(t)^d,\\ &R_n(t)\le C\,n^{1/2},\qquad V_n(t)\le Cn^{1/2},\end{aligned} \tag{E.3}$$

which means that the maximum speed and the maximum distance a particle *not in* Ω_0 can travel in the Λ_n-regularized dynamics grows as a power of n, at most.

It remains to consider the particles in Ω_0 to derive the bounds Eq.(5.8) with $V_n(t),\mathcal{N}_n(t),\rho_n(t)$ replaced by $\overline{V}_n(t),\overline{\mathcal{N}}_n(t),\overline{\rho}_n(t)$, *i.e* by the quantities in which the particles in Ω_0 are also taken into account. However the proof of the corresponding statement for $d=1,2$ (see paragraphs preceding and following Eq.(C.9) in Appendix C) applies unaltered as it only depends on bounds on $V_n(t)$ proportional to $n^{1/2}$.

It can be remarked that the Eq.(E.3) summarizes results that in the cases $d=1,2$ were the contents of theorems 3,4 in [23]. However the bound on $R_n(t)$ is substantially worse than the corresponding in dimensions $1,2$ because it only allows us to bound the maximum number of particles that can fall inside a ball of radius r_φ by $Cn^{d/4}$ rather than by $Cn^{1/2}$ as in Eq.(5.8).

A key implication of the above results is a proof of Theorem 4 in $d=3$:

Theorem 8: *If $x\in\mathcal{H}_{1/d}$ the thermodynamic limit evolution $\overline{x}^{(0)}(t)_i=\lim_{n\to\infty}(\overline{S}_t^{(n,0)}x)_i$ exists.*

Proof: Remark that in Sec.VI no use has been made of entropy bounds. The only difference is that with the new bound in Eq.(E.3) η in Eq.(6.4) is one unit larger.

By the final remark to Sec.VII the analysis leads to

Theorem 9: *With μ_0–probability 1 in $x\in\mathcal{H}_{1/d}$, $d=3$: the frictionless motions have the local dynamics property and, as $n\to\infty$, the limits of $\overline{S}_t^{(n,0)}x,S_t^{(n,1)}x$ exist and coincide, and furthermore the Eq.(2.3) with $\Lambda=\mathbb{R}^d$ for $\overline{x}^{(0)}(t)$ have a unique solution for data in $\mathcal{H}_{1/3}$ and with values in $\mathcal{H}_{3/2}$.*

This is proved but for the uniqueness statement: as in $d=1,2$ the proof is by iteration of the integral equations for two solutions with the initial data in $\mathcal{H}_\zeta$ and with values in $\mathcal{H}_{9\zeta/2}$: we skip the details, see [13].

The analysis in Sec.VII can also be followed word by word to check the expected result

Theorem 10: *The limits* $\lim_{n\to\infty} S_t^{(n,0)}x$ *exist and coincide with* $\lim_{n\to\infty} \overline{S}_t^{(n,0)}x$.

The check is left to the reader.

APPENDIX F: FRICTIONLESS MOTION IS A FLOW IF $d = 2$

The following theorem is obtained by a straightforward adaptation of theorem 2.2 in [13].

Theorem 11: *Let* $E > 0$ *and* $d = 1, 2$. *Then, given any* Θ *there is* E' *(depending on* Θ, E*) so that for all* x *such that* $\mathcal{E}(x) \le E$

$$\mathcal{E}(\overline{S}_t^{(0)}x) \le E', \qquad \textit{for all } t \le \Theta \tag{F.1}$$

so that the evolution $x \to \overline{S}_t^{(0)}x$ *is a flow in* $\mathcal{H}_{1/d}$. *For* $d = 3$ *data in* $\mathcal{H}_{1/3}$ *evolve into data in* $\mathcal{H}_{3/2}$. *Hence the same holds for* $S_t^{(a)}x$ *for* $a = 0, 1$ *by theorem 7.*

Proof. The proof is based on the bounds Eq.(6.8),(6.9) derived in the proofs of the theorems 6,7 (for $d = 1, 2$) and 10 (for $d = 3$).

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

$$\widetilde{W}\big(\overline{x}_t^{(0)}, \xi, \rho\big), \quad \text{for} \quad \rho \ge (\log_+(|\xi|/r_\varphi))^{1/d} \tag{F.2}$$

with $\widetilde{W}$ defined as in Eq.(C.3). 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 $\forall t \le \Theta$

$$\begin{aligned}\widetilde{W}\big(\overline{x}_t^{(0)}, \xi, \rho\big) &\le \widetilde{W}\big(\overline{x}_t^{(n_\xi,0)}, \xi, \rho\big)\\ &+ |\widetilde{W}\big(\overline{x}_t^{(0)}, \xi, \rho\big) - \widetilde{W}\big(\overline{x}_t^{(n_\xi,0)}, \xi, \rho\big)|\end{aligned} \tag{F.3}$$

The particles which at any time $t \le \Theta$ contribute to Eq.(F.3) are in $\Lambda_{n_\xi} - 1$. Via theorem 6, maximal speed, distance to the walls and number of interacting particles are bounded by $C' 2^{n_\xi/2}$; hence:

$$|\widetilde{W}\big(\overline{x}_t^{(0)}, \xi, \rho\big) - \widetilde{W}\big(\overline{x}_t^{(n_\xi,0)}, \xi, \rho\big)| \le C' e^{-c 2^{n_\xi/4}} \tag{F.4}$$

Consider first the case of ρ large, say $\rho > \rho_{n_\xi}$. Then $\widetilde{W}\big(\overline{x}_t^{(0)}; \xi, \rho\big)$ can be estimated by remarking that the argument leading to Eq.(5.5) remains unchanged if $R(t) = \rho + \int_0^t V_{n_\xi}(\tau) d\tau/\Theta$ 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

$$\widetilde{W}(\overline{x}_t^{(0)}; \xi, \rho + \rho_{n_\xi}) \le C\widetilde{W}(x, \rho + 2\rho_{n_\xi}) \tag{F.5}$$

as in Eq.(5.5) (see also Eq.(C.3)).

Suppose $\rho_0 - \rho_{n_\xi} > g_\zeta(\xi/r_\varphi)$, hence $\rho_0 > C n_\xi^\zeta$, then $\widetilde{W}(\overline{x}_t^{(0)}; \xi, \rho_0) \le C'\widetilde{W}(x, \rho_0 + \rho_{n_\xi}) \le C''(\rho_0 + \rho_{n_\xi})^d \le C\rho_0^d$ and $\mathcal{N}' \le C\rho_0^{d-1} n_\xi^{1/2} \le C\rho_0^{d-1+1/(2\zeta)}$. Hence $\widetilde{W}\big(\overline{x}_t^{(0)}, \xi, \rho\big) \le C\,(\rho_0^d + \rho_0^{d-1+1/(2\zeta)}) \le C\rho_0^d$ if $\zeta = 1/d$ for $d = 2$ and $\zeta = 1/2$ if $d = 3$; likewise one finds $\zeta = 1$ if $d = 1$.

The values of $(n_\xi - 1)^\zeta \le \rho_0 \le C n_\xi^\zeta$ 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 $\widetilde{W}(\overline{x}_t^{(0)}; \xi, \rho)$ is bounded by $\widetilde{W}(x; \xi, \rho + C n_\xi^\zeta) \le C' \rho^d$.

Conclusion: there is $C > 0$, depending only on $\mathcal{E}$ and for all $\rho > g_\zeta(\xi/r_\varphi)$, $t \le \Theta$ it is $W(x_t^{(0)}; \xi, \rho) \le C\,\rho^d$ if $\zeta = 1/d$ for $d = 1, 2$ and $\zeta = 1/2$ if $d = 3$.

APPENDIX G: FREE THERMOSTATS

The need for interaction between particles in order to have a physically sound thermostat model has been stressed in [24, 25] and provides a measure of the importance of the problems met above.

The discussion in Sec.IV is heuristic unless the local dynamics assumption is 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 interaction between particles in the same Ω_j, $j > 0$, and, furthermore, replacing the wall potentials by an elastic collision rule (*i.e.* supposing elastic collisions with the walls and $U_j(\mathbf{X}_j) \equiv 0$, $j > 0$) the analysis can be further pursued and completed. This will be referred as the "*free thermostats*" model.

In the frictionless case this is the classical version of the frictionless 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 $n \ge n_0$ (see the paragraph following Eq.(2.1)). If $\overline{N}$ bounds the number of particles in the ball $\mathcal{B}(O, 2^{n_0})$ up to an arbitrarily prefixed time Θ, the first inequality Eq.(4.2) and the supposed isoenergetic evolution (which in this case is *also* isokinetic) imply

$$|\alpha_j| \le N_0 F \sqrt{\frac{\overline{N}}{2K_j/m}} \le \frac{N_0 F}{\sqrt{d\, k_B T_j/m}} \stackrel{def}{=} \ell. \tag{G.1}$$

It follows that, for $\zeta \ge 1/d$, the speed of the particles initially in the shell Λ_n/Λ_{n-1} with radii $2^n r_\varphi, 2^{n+1} r_\varphi$ will remain within the initial speed up to, at most, a factor $\lambda^{\pm 1} = e^{\pm \ell \Theta}$. The initial speed of the latter particles is bounded by, see Eq.(3.11),

$$V_n = v_1 \sqrt{\mathcal{E}_\zeta(x)}\, n^{\frac{1}{2}\zeta d} \tag{G.2}$$

Hence, if $n(\Theta)$ is the smallest value of n for which the inequality $2^n r_\varphi - V_n\,\lambda\,\Theta < D_0 + r_\varphi$ *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

$$V_\Theta = (\overline{V} + F\, N_0\, \overline{N}\,\Theta)\,\lambda \tag{G.3}$$

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

$$|\alpha_j \dot{q}_i| \le \frac{N_0 \overline{N} V_\Theta^2 F}{\omega_{j,n} 2^{dn} r_\varphi^d \delta\, k_B T/m} \xrightarrow[n\to\infty]{} 0 \tag{G.4}$$

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 12: *Free isoenergetic and frictionless 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.(G.1) are constant.

It would be possible to consider non rigid walls, modeled by a soft potential ψ diverging near them. We do not do so because it will be a trivial consequence of the analysis in this paper. The example of this section has been chosen because it pedagogically illustrates well the simplest among the ideas of the coming analysis.

APPENDIX H: 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, *i.e* 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.

Let ds_x be the surface element on Σ and $\nu(ds_x)$ its area computed by measuring the volume with μ. Then the following *Sinai's lemma*, [5, 6, 14], holds:

Lemma 3: *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*

$$\begin{aligned}\int_E f(y)\mu(dy) &\le e^\lambda \int_\Sigma \int_0^{\theta(x)} f(S_{-\tau}x)\,|v_x\cdot n_x|\,\nu(ds_x)d\tau,\\ &\ge e^{-\lambda} \int_\Sigma \int_0^{\theta(x)} f(S_{-\tau}x)\,|v_x\cdot n_x|\,\nu(ds_x)d\tau \end{aligned}\tag{H.1}$$

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. Then the set of points into which the parallelepiped Δ with base ds_x and height $d\tau$ evolves 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 $\int_\Sigma \int_0^{\theta(x)} f(S_{-t}x)\rho(x)\nu(ds_x)d\tau$ if $\rho(x)\nu(ds_x)d\tau$ is the measure of Δ: the latter is $|v_x\cdot n_x|\nu(ds_x)d\tau$. Notice that $\rho(x) = |r(x)\, v_x \cdot n_x|$ if $\mu(dx) = r(x)dx$.

APPENDIX I: REGULARIZED THERMOSTATTED DYNAMICS

Consider N particles in $\cup_j \Omega_j \cap \Lambda$ with a configuration of immobile particles outside Λ. The analysis in [7] can be followed and the solution of the equations of motion can be defined on the set Γ^+ consisting of the configurations x in which 1 of the particles is at ξ on the boundary $\partial\Lambda$, where elastic collisions take place, with normal speed $\dot{q}\cdot n(\xi) > 0$. The time evolution makes sense until the time $\tau_+(x)$ of next collision; it can then be continued after the elastic collision because, apart from a set of zero volume, the normal speed of the collision can be assumed $\ne 0$, until the time $t_\Lambda(x) > 0$, *if any*, in which the total kinetic energy in one of the containers Ω_j, $j \ge 0$, vanishes.

Consider the subset $\Gamma(\Theta) \subset \Gamma^+$ of the points with $\tau(x) < \Theta$. If $\Delta \subset \Gamma(\Theta)$ and if ν is the measure $\nu_{0,\Sigma'}$, see Eq.(7.9) and appendix D, is a small set it will be $\nu(T\Delta) \ge \lambda^{-1}\nu(\Delta)$ where $\lambda(x)$ is an upper bound on the entropy production in any interval within $[0, \tau(x)]$.

There cannot be infinitely many collisions, except on a set of 0 ν–measure, as long as $\lambda(T^n x) < L < \infty$. If T denotes the return map the only way an accumulation of collision times with $\sum_{k=0}^{\infty}\tau(T^k x) = \theta < \Theta$ could occur is if also $K(S_t^{(n,1)}x) \xrightarrow[t\to\theta]{} 0$ and $\sup_{t',t''\le\Theta}\int_{t'}^{t''}\sigma(S_t^{(n,1)}x)dt = +\infty$: hence the limit $\lim_{t\to\theta} K(S_t^{(n,1)}x) = 0$. The reason is that if λ remains finite then Poincaré's recurrence argument will apply implying, as in [7], that $\sum_{k=0}^{\infty}\tau(T^k x) = +\infty$ outside a set of ν–measure 0.

This means that the thermostatted time evolution is well defined until the first time $t_\Lambda(x)$ when $K(S_{t_\Lambda}^{(n,1)}x) = 0$. Since the thermostat force $\frac{Q_j}{K_j}\dot q_i$ is bounded even if $K_j \to 0$ the time evolution will be defined in the closed interval $[0, t_\Lambda(x)]$: *the evolution proceeds, well defined, until the first time $t_\Lambda(x)$ (included, if any) when some of the $K_{\Lambda,j}$ vanishes*, see remark (6) p.3.

APPENDIX J: ENTROPY BOUNDS: CHECK OF EQ.(7.7)

Writing k_ξ for the smallest integer $\ge (\log n)^\gamma g_\gamma(\xi/r_\varphi)$ (here g_γ is chosen instead of the natural $g_{1/2}$ in order to simplify the formulae: recall that by defiinition $\gamma > 1/2$), then $\mu_{0,\Sigma'}$ almost surely, Σ' splits into an union over $\xi \in \Lambda_n \cap r_\varphi\mathbb{Z}^d$ of the union of $\mathcal{S}_\xi^1 \cup \mathcal{S}_\xi^2 \cup \mathcal{S}^3$, where

$$\begin{aligned}\mathcal{S}_\xi^1 =&\{y\in\Sigma' : |y\cap C_\xi| = k_\xi, |y\cap\partial C_\xi| = 1\}\\ \mathcal{S}_\xi^2 =&\{y\in\Sigma' : y\cap C_\xi \ni (q,\dot q), \varepsilon(q,\dot q) = \widetilde\varepsilon_\xi\}\\ \mathcal{S}^3 =&\{y\in\Sigma' : K_{j,n}(y = \frac12\kappa 2^{nd}\}\end{aligned}\tag{J.1}$$

if $\widetilde\varepsilon_\xi \stackrel{def}{=} \big((\log n)^\gamma g_\gamma(\xi/r_\varphi)\big)$.

Consider first the case of $\mathcal{S}^3$. Let $D\subset\mathcal{S}^3$ be the set of the x which satisfy $K_{j,\Lambda_n}(x) = \frac{\varphi_0}{2}\kappa 2^{dn}$ for a given $j>0$ while $K_{j',\Lambda_n}(x) > \frac12\kappa 2^{dn}$ for $j'>0$, $j'\ne j$.

Recall the DLR-equations, [26], and consider the classical superstability estimate on the existence of $c>0$ such that $p_n = e^{-c2^{2dn}}$ bounds the probability of finding more than $\rho 2^{dn}$ particles in $\Lambda_n\cap\Omega_j$ if ρ is large enough (*e.g.* $\rho > \max_j \delta_j$). Then the probability $\mu_0(D)$ can be bounded by p_n (summable in n) plus, see Appendix H,

$$\begin{aligned}&e^{CMV}\int\overline\mu_0(dq')\sum_{\ell=1}^{\rho 2^{nd}}\Theta\int\frac{e^{-\beta_j(U_{\Lambda_n,j}(q,q')-\lambda_j\,\ell)}}{Z_{\Lambda_n,j}(q')}\frac{dq}{\ell!}\\ &\cdot\, e^{-\beta_j P^2}\,\widehat P\,P^{\ell\,d-1}\,\frac{\omega(\ell\,d)}{(\pi/\beta)^{\ell d/2}}\end{aligned}\tag{J.2}$$

where $\overline\mu_0$ is the distribution of the positions in μ_0, $q = (q_1,\ldots,q_l)\in(\Omega_j\cap\Lambda_n)^l$, $P^2 = \frac12\kappa 2^{dn}$, $U_{\Lambda_n,j}(q,q')$ is the sum of $\varphi(q-q')$ over pairs of points $q_i, q'_\ell \in \Omega_j\cap\Lambda_n$ and pairs $q_i\in\Lambda_n\cap\Omega_j, q'_\ell\notin\Lambda_n\cap\Omega_j$, and

(1) $Z_{\Lambda_n,j}(q')$ is the partition function for the region $\Lambda_n\cap\Omega_j$ (defined as in Eq.(3.1) with the integral over the q's extended to $\Lambda_n\cap\Omega_j$ and with the energies $U_{\Lambda_n}(q,q')$);

(2) The volume element $P^{ld-1}dP$ has been changed to $P^{ld-1}\dot P d\tau \stackrel{def}{=} P^{ld-2}\widehat P d\tau$ where $\widehat P$ is a *short hand* for

$$\sum_{q,q';\,q\in\Lambda_n\cap\Omega_j}|\partial_q\varphi(q-q')| + \sum_{q\in\Lambda_n\cap\Omega_j}|\partial_q\psi(q)|\tag{J.3}$$

so that $P\widehat P$ is a bound on the time derivative $2P\dot P$ of the total kinetic energy P^2 contained in Λ_n evaluated on the points of D: hence $2P\widehat P$ is bounded by $\le CP^2\widehat P$).

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

(4) The e^{CMV} takes into account the entropy estimate *i.e.* the bound, CMV, of the non-invariance of μ_0.

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 $P^{\ell\,d-1}$ is replaced by $\frac{((1-\varepsilon)P)^{\ell\,d-1}}{(1-\varepsilon)^{d\rho 2^{nd}-1}}$ the average over ε becomes an upper bound. Changing ε to $P\varepsilon$ (*i.e.* hence $d\varepsilon$ to $(\frac{2}{\kappa 2^{dn}})^{\frac12}dP\varepsilon$) the bound becomes the μ_0-average $\frac{2e^{\overline\varepsilon\rho 2^{nd}}}{\overline\varepsilon\kappa 2^{dn}}\langle\widehat P\,\chi_{\kappa,\overline\varepsilon}\rangle_{\mu_0}$ bounded by

$$\frac{2^{\frac12}e^{\overline\varepsilon C2^{nd}}}{\overline\varepsilon\kappa^{1/2}2^{dn/2}}\langle\widehat P^2\rangle_{\mu_0}^{1/2}\,\cdot\,\langle\chi_{\kappa,\overline\varepsilon}\rangle_{\mu_0}^{1/2}\le C\,e^{-c\,2^{nd/2}}\tag{J.4}$$

where $\chi_{\kappa,\varepsilon}$ is the characteristic function of the set $\big\{(1-\overline\varepsilon)^2\frac{\kappa}{2}2^{dn} < K_j < \frac{\kappa}{2}2^{dn}\big\}$. 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 $C,c>0$ and is summable in n (and of course on $j>0$).

Similarly, the surface areas $\nu_{0,\Sigma'}(\mathcal{S}_\xi^1)$ and $\nu_{0,\Sigma'}(\mathcal{S}_\xi^2)$ on $\mathcal{S}^1,\mathcal{S}^2$ induced by μ_0 are bounded by

$$\nu_{0,\Sigma'}(\mathcal{S}_\xi^i)\le Ce^{CMV}\sqrt{n}e^{-c[(\log n)^\lambda g_\lambda(\xi/r_\varphi)]^2},\tag{J.5}$$

(for suitable C,c, functions of E). Summing (as $\gamma>1/2$) over $\xi\in\Omega_j\cap\Lambda_n$ as discussed below and adding Eq.(J.2) the Eq.(7.7) will follow.

Consider the case of $\mathcal{S}_\xi^1$. By Eq.(J.1) 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 $x\in\mathcal{X}_E$ within a time $T_n(x) < \Theta$: hence Eq.(5.8) applies. By Eq.(5.8)

$$\begin{aligned}&\int_{\mathcal{S}^1_\xi}\mu_{0,\Sigma'}(dy)\int_0^{\theta(y)}dt\,w(y)\\&\le\Theta v_1 C n^\eta\int\mu(dx)\frac{J_1}{Z_{C_\xi}(x)}\end{aligned}\tag{J.6}$$

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

$$J_1=\int_{\partial C_\xi}dq_1\int_{C_\xi^{k_\xi-1}}\frac{dq_2\dots dq_{k_\xi}}{(k_\xi-1)!}\int_{\mathbb{R}^{dk_\xi}}d\dot q e^{-\beta_j H(q,\dot q|x)}\tag{J.7}$$

The estimate of the *r.h.s.* of Eq.(A.1), as remarked, is an "equilibrium estimate". By superstability, [9], and since $\varphi\ge0$, the configurational energy $U(q|x)\ge bk_\xi^2-b'k_\xi$, so that J_1 is bounded by:

$$B\,e^{-\beta_j(bk_\xi^2-b'k_\xi)}\frac{|C_\xi|^{k_\xi-1}|\partial C_\xi|}{(k_\xi-1)!}(\frac{2\pi}{\beta_j m})^{\frac d2 k_\xi}\tag{J.8}$$

while $\int\mu(dx)\frac{1}{Z_{C_\xi}(x)}\le1$ because $Z_{C_\xi}(x)\ge1$: and the bound can be summed over k_ξ. Thus the contribution from $\mathcal{S}^1_\xi$ to Eq.(7.7) is bounded by

$$C'e^{CMV}n^\eta\,e^{-b[(\log n)^\gamma g_\gamma(\xi/r_\varphi)]^2}\tag{J.9}$$

with C,b suitable positive constants. Since $\gamma>1/2$, this is summable over ξ and yields the part of the Eq.(7.7) coming from the integration over $\mathcal{S}^1$.

Let, next, $y\in\mathcal{S}^2_\xi$ and let $(q,\dot q)$ as in (J.1). The function w is, if $E(q,\dot q)\equiv\varepsilon(q,\dot q)^2$,

$$w=\frac{|dE(q,\dot q)/dt|}{|\mathrm{grad}E(q,\dot q)|}\tag{J.10}$$

and $|dE(q,\dot q)/dt|\le C\,|\dot q|n^\eta$ because dE/dt is the work on the particle $(q,\dot q)$ done by the pair interactions (excluding the wall forces). It is 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, $|\mathrm{grad}E(q,\dot q)|=\sqrt{|\partial\psi(q)|^2+m^2|\dot q|^2}\ge m|\dot q|$ hence $w\le Cn^{1/2}$ again by Eq.(5.8) and the remark preceding Eq.(J.6).

Then, analogously to (J.6), the integral under consideration is bounded by $Ce^{C'MV}\sqrt n$ (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:

$$\begin{aligned}&\sum_k\int_{C_\xi^{k-1}\times\mathbb{R}^{k-1}}\frac{dq_2\dots dq_k d\dot q_2\dots d\dot q_k}{(k-1)!}e^{-\beta_j H(q,\dot q|x)+\beta_j\lambda_j k}\\&\quad\cdot e^{-\beta_j\tilde E_\xi}\,\mathrm{area}(\{E(q,\dot q)=\tilde E_\xi\})\end{aligned}\tag{J.11}$$

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 (J.1)). Then J_2 is bounded by

$$\sum_k\frac{B}{(k-1)!}\Big(e^{\beta_j\lambda_j}|C_\xi|\big(\frac{2\pi}{\beta_j m}\big)^{\frac d2}\Big)^{(k-1)}|C_\xi|(\tilde E_\xi)^{(d-1)/2}e^{-\beta_j\tilde E_\xi}\tag{J.12}$$

so that, suitably redefining C,C' (functions of E), the contribution from $\mathcal{S}^2_\xi$ is bounded by

$$C'e^{CMV}\sqrt n e^{-\frac12\beta_j[(\log n)^\gamma g_\gamma(\xi/r_\varphi)]^2}\tag{J.13}$$

and Eq.(7.7) follows from Eq.(J.2), from (J.9) and from Eq.(J.13).

APPENDIX K: DETAILS THE DERIVATION OF EQ.(7.5),(7.6)

To prove item (1) and Eq.(7.6), thus completing the proof of theorem 7, we shall compare the evolutions $x^{(n,1)}(t)$ with $\overline{x}^{(n,0)}(t)$, at same initial datum $x\in\mathcal{X}_E$ and $t\le T_n(x)$, the latter being the stopping time defined in Eq.(7.4). We start by proving that there is $C>0$ so that for all n large enough the following holds.

Lemma 4: *For $t\le T_n(x)$, see Eq.(7.4), and $k\ge(\log n)^\gamma$, then*

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

for $q_i(0)\in\Lambda_k$.

The necessity of this lemma is due to the fact that we cannot control the positions and speed at time t in terms of the norms $\|x\|_n$ at time 0: since the particles move we must follow them (a "Lagrangian" viewpoint).

A corollary of the above will be:

Lemma 5: *Let $\mathcal{N}$ and ρ be the maximal number of particles which at any given time $\le T_n(x)$ interact with a particle q_i initially in Λ_{k+1} and, respectively, the minimal distance of a particle from the walls. Then*

$$\mathcal{N}\le C\,(k\log n)^{d\gamma},\quad\rho\ge\,c\,(k\log n)^{-2(d\gamma+1)/\alpha}\tag{K.2}$$

for all integers $k\in((\log n)^\gamma,2(\log n)^\gamma)$.

The proof of the lemmas is in Appendix L. The interval allowed to k could be much larger, as it appears from the proof.

We have now all the ingredients to bound $\delta_i(t,n)\overset{def}{=}|q_i^{(n,1)}(t)-\overline{q}_i^{(n,0)}(t)|$. Let f_i be the acceleration of the particle i due to the other particles and to the walls.

In the equations of motion for the evolution, Eq.(3.7), for $q_i^{(n,1)}(t)$ the elastic collisions with $\partial\Lambda_n$ (implicit in Eq.(3.7)) can be disregarded if the particle initially in q_i does not experience a collision with $\partial\Lambda_n$. For n large such a collision cannot take place if $q_i(0)\in\Lambda_{k+1}$, $k<2(\log n)^\gamma$ and $t\le T_n(x)$, by Eq.(K.1).

Then, for $2(\log n)^\gamma>k>(\log n)^\gamma$, by Eq.(K.2) and if $q_i\in\Lambda_{k+1}$, it follows that $|f_i|\le C\,(k\log n)^\eta$, with η a suitable constant ($\eta\stackrel{def}{=}d\,\gamma+2(d\,\gamma+1)(1+\frac1\alpha)$), so that subtracting the Eq.(3.7) and Eq.(6.1) 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)

$$\begin{aligned}\delta_i(t,n)\le{}& C\,(k\log n)^\eta 2^{-nd}\\ &+\Theta\int_0^t|f_i(q^{(n,1)}(\tau))-f_i(\overline{q}^{(n,0)}(\tau))|\,d\tau,\end{aligned}\tag{K.3}$$

because, recalling the definition of α_j and the third condition on the stopping time in Eq.(7.2), the denominator of $|\alpha_j|$ is bounded proportionally to 2^{nd}.

Remarking, by lemma 4 for $q_i^{(n,1)}(t)$, that

$$\max_{t\le T_n(x)}|q_i^{(n,1)}(t)-q_i|\le C\,r_\varphi(k\log n)^\gamma,\tag{K.4}$$

and, by theorem 5 for $\overline{q}_i^{(n,0)}(t)$), also $\overline{q}_i^{(n,0)}(t)$ satisfies an identical relation, let $\ell>0$ be an integer, k_ℓ such that

$$2^{k_\ell}=2^k+\ell\,C\,(k\log n)^\gamma.\tag{K.5}$$

and let $u_{k_\ell}(t,n)$ the max of $\delta_i(t,n)$ over $|q_i|\le r_\varphi 2^{k_\ell}$. Then by Eq.(K.3) and Eq.(K.2),

$$\frac{u_{k_\ell}(t,n)}{r_\varphi}\le C\,(k\log n)^\eta\,\big(2^{-nd}+\int_0^t\frac{u_{k_{\ell+1}}(s,n)ds}{r_\varphi\Theta}\big),\tag{K.6}$$

for $\ell\le\ell^*=2^k/((k\log n)^\gamma C)$, the latter being the largest ℓ such that $2^{k_\ell}\le 2^{k+1}$. By Eq.(K.6),(6.10), and Eq.(K.2)

$$\begin{aligned}\frac{u_k(t,n)}{r_\varphi}\le{}& e^{C\,(k\,\log n)^\eta}C(k\log n)^\eta 2^{-dn}\\ &+\frac{(C\,(k\,\log n)^\eta)^{\ell^*}}{\ell^*!}\,C\,(2^k+k(\log n)^\gamma+k^{1/2}),\end{aligned}\tag{K.7}$$

for $(\log n)^\gamma<k<2(\log n)^\gamma$.

Thus $u_k(t,n)$ is bounded by the r.h.s. of the first of Eq.(7.5); analogous argument shows that also the velocity differences are bounded as in Eq.(7.5) which is thus proved for all $t\le T_n(x)$.

Therefore given $q_i(0)$ with $|q_i(0)|/r_\varphi\le 2^{k_0}$ it is, for $n>e^{k_0^{1/\gamma}}$ large enough and i fixed, $|q_i^{(n,1)}(t)-\overline{q}_i^{(n,0)}(t)|/r_\varphi<u_{(\log n)^\gamma}(t,n)\le C\,2^{-c\,(\log n)^\gamma}$, *i.e.* for n large $q_i^{(n,1)}(t)$ is closer than r_φ to $\overline{q}_i^{(n,0)}(t)$.

It remains to check Eq.(7.6): for n large the number of particles in $x_i^{(n,1)}(t)$ which are in Λ_* is smaller than the number of particles of $\overline{x}_i^{(n,0)}(t)$ in Λ_{**} which in turn is bounded by M up to time Θ, by theorem 6. An analogous argument for the velocities allows to conclude Eq.(7.6).

Applying again Eq.(7.5) the proof of theorem 7 is complete apart from the uniqueness statement: the latter can be proved (as usual by iteration of the equations in integral form) but we skip the details, see [8, 13]. The uniqueness is within the solutions of the equations of motion in the infinite volume and with data subect to the condition of being in $\mathcal{H}_{1/d}$.

APPENDIX L: PROOF OF LEMMAS 4,5

With the notations of Appendix K and $\gamma>\frac12$:

Proof (lemma 4): If $t\le T_n(x)$ then

$$|\dot q_i^{(n,1)}(t)|\le v_1\big((\log n)\log_+\frac{|q_i^{(n,1)}(t)|+\sqrt2 r_\varphi}{r_\varphi}\big)^\gamma,\tag{L.1}$$

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.(L.1) with $=$ replacing $\le$ and initial datum $|q_i^{(n,1)}(0)|\le 2^k r_\varphi$. And $r(t)$ can be taken $r(t)\stackrel{def}{=}2^k+2v_1\big((\log n)\log_+2^k\big)^\gamma\frac{t}{r_\varphi}$, for $t\le\Theta$, provided

$$\big((\log n)(\log_+r(\Theta)+\sqrt2)\big)^\gamma\le 2\big((\log n)\log_+2^k\big)^\gamma\tag{L.2}$$

which, since $\frac{(k\log n)^\gamma}{2^k}$ vanishes as n diverges (because $k\ge(\log n)^\gamma$), is verified for all n large enough. 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 $t\le T_n(x)$, and the lemma is proved.

Proof (lemma 5): By lemma 1 the following properties hold for all n large enough and all $t\le T_n(x)$:

(i) for all $q_i\in\Lambda_{k+2}$,

$$\max_{t\le T_n(x)}|q_i^{(n,1)}(t)-q_i|\le C\,r_\varphi(k\log n)^\gamma,\tag{L.3}$$

which implies the first of Eq.(K.2).

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

By Eq.(L.3) we see that if $q_i\in\Lambda_{k+1}$ then $q_i^{(n,1)}(t)\in\Lambda_{k+2}$ so that, by the definition of the set $\mathcal{B}$, recalling that $\gamma>1/2$, the lemma follows because the work of the pair forces on q_i is bounded $\mathcal{N}\le C(k\log n)^{d\gamma}$ times the speed bound $C(k\log n)^\gamma$, by Eq.(K.1) and the second of (K.2).

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