Thermodynamic limit for isokinetic thermostats

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Abstract: *Thermostats models in space dimension $d = 1, 2, 3$ for nonequilibrium statistical mechanics are considered and it is shown that, in the thermodynamic limit, the motions of frictionless thermostats and isokinetic thermostats coincide.*

I. THERMOSTATS

A *test system* of particles in a container Ω_0 and ν systems of particles in containers $\Omega_1, \ldots, \Omega_\nu$ interact and define a model of a system in interaction with ν thermostats if the particles in $\Omega_1, \ldots, \Omega_\nu$ can be considered at fixed temperatures $T_1, \ldots, T_\nu$.

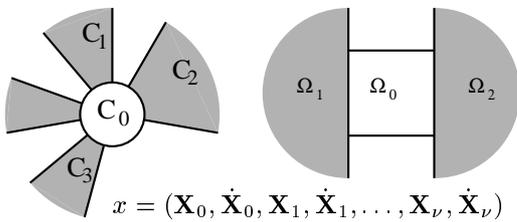A representation of the system is in Fig.1:

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

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, $j \geq 0$ and considered in the $d = 1, 2$ cases. The second figure illustrates the special geometry considered for $d = 3$ (as well as for $d = 1, 2$): here two thermostats, symbolized by the shaded regions, Ω_1, Ω_2 occupy half-spaces adjacent to Ω_0.*

A formal description of the model can be found in [1, 2]. The temperatures in the thermostats will be identified with their average kinetic energy per particle.

To implement the physical requirement that the thermostats have well defined temperatures and densities the initial data will be imagined to be randomly chosen with a suitable distribution. If Λ is a ball centered at the origin the space $\mathcal{H}(\Lambda)$ will be the space of the finite configurations $(\mathbf{X}, \dot{\mathbf{X}})$ with $\mathbf{X} \subset \cup_{j \geq 0} \Omega_j \cap \Lambda$.

Initial data: *The probability distribution for the random choice of initial data will be, if $dx \overset{def}{=} \prod_{j=0}^{\nu} \frac{d\mathbf{X}_j \, d\dot{\mathbf{X}}_j}{N_j!}$, the distribution on $\mathcal{H}(\Lambda)$*

$$\mu_\Lambda(dx) = \frac{e^{-H_0(x)}}{Z(\Lambda)} \prod_{j > 0} \delta\left(K_{j,\Lambda}(x) - \frac{d}{2\beta_j} N_j\right) dx \quad (1.1)$$

with $H_0(x) = \sum_{j=0}^{\nu} \beta_j (K_j(\dot{\mathbf{X}}_j) + U_j(\mathbf{X}_j))$, and $N_j = \delta_j |\Lambda \cap \Omega_j|$ with $\beta_j \overset{def}{=} \frac{1}{k_B T_j} > 0, \delta_j > 0, j > 0$; the values

$\beta_0 = \frac{1}{k_B T_0} > 0, \delta_0 > 0$ *will also be fixed (but bear no particular physical meaning because the test system is kept finite).*

Here $\boldsymbol{\delta} = (\delta_0, \delta_1, \ldots \delta_\nu)$ and $\mathbf{T} = (T_0, T_1, \ldots, T_\nu)$ are fixed *densities* and *temperatures*, Λ is a ball centered at the origin and Z is the normalization factor.

With the above choice of initial data the physical requirement that the thermostats are in a configuration with densities and temperatures assigned is realized at time 0. But the probability distribution is not invariant under time evolution: because the temperatures β_j are different and also because H_0 does not contain the interaction between the system and the thermostats and because on the system will be imgained to act nonconservative forces.

The equations of motion (see Fig.1) in $\Lambda = \Lambda_n$, with Λ_n being the ball of radius $2^n r_\varphi$ with r_φ a length unit that can be chosen to be the interaction range (see below), will be different in the *frictionless* thermostats and in the *isokinetic* thermostats. They will differ by the value of a parameter $a = 0, 1$:

$$m\ddot{\mathbf{X}}_{0i} = -\partial_i U_0(\mathbf{X}_0) - \sum_{j > 0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \boldsymbol{\Phi}_i(\mathbf{X}_0)$$

$$m\ddot{\mathbf{X}}_{ji} = -\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) - \alpha \alpha_j \dot{\mathbf{X}}_{ji} \quad (1.2)$$

where the first label, $j = 0$ or $j = 1, \ldots, \nu$ respectively, refers to the test system or to a thermostat, while the second indicates the components of the coordinates of the points located in the corresponding container and initially *in the regularization box* Λ_n (hence the labels i in the subscripts (j, i) have $N_j d$ values). Furthermore:

(1) the $\boldsymbol{\Phi}(\mathbf{X}_0)$ are, positional, *nonconservative*, smooth stirring forces, possibly vanishing;

(2) other forces are conservative and generated by a pair potential φ, with range r_φ, which couples all pairs in the same containers and all pairs of particles one of which is located in Ω_0 and the other in Ω_j (*i.e.* there is *no direct interaction* between the different thermostats).

(3) particles are repelled by the boundaries $\partial \Omega_j$ by a conservative force of potential energy ψ, of range $r_\psi \ll r_\varphi$, diverging at the walls. The potential energies will be $U_j(\mathbf{X}_j)$, $j \geq 0$, and $U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$: respectively denoting the internal energies of the various systems and the potential energy of interaction between the system and the thermostats.

$$U_j(\mathbf{X}) = \sum_{q \in \mathbf{X}_j} \psi(q) + \sum_{(q,q') \in \mathbf{X}_j, q \in \Lambda} \varphi(q - q')$$

$$U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) = \sum_{q \in \mathbf{X}_0, q' \in \mathbf{X}_j} \varphi(q - q') \quad (1.3)$$

(4) in the case $a = 0$ particles will be allowed to exit the regions $\Omega_j \cap \Lambda_n$ through the boundary of Λ_n while

if $a = 1$ they will be constrained to remain inside the container $\Omega_j \cap \Lambda_n$ by an elastic reflection on $\partial\Lambda_n$: this choice of the boundary conditions is imposed mainly to make possible references to [2].

(5) the α_j are determined so that the solution to the equations with $a = 1$ *keeps exactly the same kinetic energy it has at time* 0, *i.e.* $\frac{d}{2}N_j k_B T_j$, for $j > 0$, see Eq.(1.1); this means

$$\alpha_j = \frac{Q_j - \dot{U}_j}{N_j\, d\, k_B T_j} \qquad (1.4)$$

where $Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_{\mathbf{X}_j} U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$, is the *heat* ceded by the system to the j-th thermostat.

(6) The potentials φ, ψ have been chosen j–independent for simplicity. The pair potential φ will be supposed smooth, ≥ 0, with finite range $r_\varphi > 0$, setting $\varphi(0) \stackrel{def}{=} \varphi_0 > 0$; the wall potential ψ will also be supposed smooth at a distance $r > 0$ from the walls, ≥ 0, with range r_ψ, and diverging proportionally to $r^{-\alpha}$ as $r \to 0$, for some $\alpha > 0$.

Hypothesis: *The initial state distributions* μ_{Λ_n} *are assumed to satisfy a large deviations property for the total potential energy* $U_{j,\Lambda_n}(x)$; *in the sense that for* $C > 0$ *there is* $c > 0$ *such that:*

$$\mu_{\Lambda_n}\left(\left\{x\,\middle|\,\left|\frac{U_{j,\Lambda_n}(x)}{|\Omega_j \cap \Lambda_n|} - u_j\right| > \frac{C\,\varphi_0}{N_j^\varepsilon}\right\}\right) < e^{-c2^{n(1-2\varepsilon)d}} \qquad (1.5)$$

for suitable $u_j \in \mathbb{R}, \varepsilon \in [0,1)$. *This is a "no phase transition" assumption (satisfied in the cluster expansion region of the parameters* $\mathbf{T}, \boldsymbol{\lambda}$ *as discussed in* [3, 4]). Notice that the volume $|\Omega_j \cap \Lambda_n|$ is $O(2^{nd})$.

The analysis will be restricted to the geometries in Fig.1 if $d = 1, 2$ and only in the second of Fig.1 if $d = 3$.

II. TIME EVOLUTION

Infinite systems are idealizations, not uncommon in statistical mechanics, that must be considered as limiting cases of large, yet finite, systems. We therefore call *regularized* equations of motion the Eq.(1.2) and denote $S_t^{(n,a)}x$, or also $x^{(n,a)}(t)$, their solutions with data randomly chosen with the distribution in Eq.(1.2).

Solutions exist (for all data in $\mathcal{H}(\Lambda)$, see the initial data hypothesis in Sec.I) by the standard existence and uniqueness theorems for ordinary differential equations in the case $a = 0$.

The case $a = 1$ involves elastic reflections on $\partial\Lambda$ and a proof of existence of the evolution requires (by adapting the analysis in [5], see [2, Appedix I]) obtaining exixtence and uniqueness for all initial data *outside a set of* μ_{Λ_n}-*probability* 0.

We shall discuss results that hold uniformly in the size n provided it is large enough. The results can be conveniently formulated in terms of quantities defined below.

Let $v_1 \stackrel{def}{=} \sqrt{\frac{\varphi_0}{m}}$, $|x_i - x_i'| \stackrel{def}{=} \frac{|\dot{q}_i - \dot{q}_i'|}{v_1} + \frac{|q_i - q_i'|}{r_\varphi}$, and

$$W(x;\xi,R) \stackrel{def}{=} \frac{1}{\varphi_0} \sum_{q_i \in \mathcal{B}(\xi,R)} \left(\frac{m\dot{q}_i^2}{2}\right.$$
$$\left. + \frac{1}{2}\sum_{j;j\neq i} \varphi(q_i - q_j) + \psi(q_i) + \varphi_0\right) \qquad (2.1)$$

$\mathcal{N}_i(x) \stackrel{def}{=}$ number of particles within r_φ of q_i,

Let $\log_+ z \stackrel{def}{=} \max\{1, \log_2 |z|\}$, $g_\zeta(z) = (\log_+ z)^\zeta$, $\rho_n(q)$ = distance of q from $\cup_j(\partial\Omega_j \cup \partial\Lambda_n)$ and call $\mathcal{X}_E \stackrel{def}{=} \{x\,|\,\mathcal{E}(x) \leq E\}$ with

$$\mathcal{E}(x) \stackrel{def}{=} \sup_\xi \sup_{R > g_{1/d}(x/r_\varphi)} \frac{W(x;\xi,R)}{R^d} \qquad (2.2)$$

The set $\mathcal{X}_E$ has μ_{Λ_n}–probability approaching 1 as $E \to \infty$ *uniformly in* n (see, for instance, [2, Eq.(9.2)] choosing $c = E$ and $c' = 1, \gamma(c) = c - c_0$):

$$\mu_{\Lambda_n}(\mathcal{X}_E) \geq 1 - \overline{C}e^{-\overline{c}E} \qquad (2.3)$$

for suitably chosen $\overline{C}, \overline{c} > 0$.

Let $d \leq 3$, then given an initial datum x the motion $S_t^{(n,a)}x$ exists for μ_{Λ_n}–almost all $x \in \mathcal{H}_{1/d}$ and $\forall t \geq 0$. Fixed *arbitrarily* an observation time $\Theta < \infty$ the main result will be

Theorem 1: *If* $x \in \mathcal{H}(\Lambda_n) \cap \mathcal{X}_E$ *and* $0 \leq t \leq \Theta$ *there are* $c = C(E,\Theta) < \infty$, $c' = C'(E,\Theta) > 0, 1 > \gamma > 1/2$ *such that, for particles which at time 0 are in* Λ_k, *i.e.* $q_i(0) \in \Lambda_k$. *Consider, for* $n > k$, *the events*

(1) $|\dot{q}_i^{(n,0)}(t)| \leq c\, v_1\, k^{\frac{1}{2}}$,

(2) $\rho_n(q_i^{(n,0)}(t)) \geq c'\, r_\varphi\, k^{-\frac{1}{\alpha}}$, $\qquad (2.4)$

(3) $\mathcal{N}_i(S_t^{(n,0)}x) \leq c\, k^{1/2}$,

(4) $|(S_t^{(n,0)}x)_i - (S_t^{(n+1,0)}x)_i| \leq e^{-c'2^{n/2}}$, $n > k$,

(5) $|(S_t^{(n,0)}x)_i - (S_t^{(n,1)}x)_i| \leq e^{-c'(\log n)^\gamma}$, $k < (\log n)^\gamma$.

The events (1-4) are realized for all $x \in \mathcal{X}_E$, *while the event (5) is realized with* μ_{Λ_n}-*probability* π_n *and* $|\mu_{\Lambda_n}(\mathcal{X}_E) - \pi_n| \leq c\,e^{-c'(\log n)^{2\gamma}}$.

This means that, if Λ_n is large, motion of the particles close to the test system is largely independent on the regularization size n. And thermostatted motion and frictionless motions, near the test system, are also very close.

The uniformity in n of the constants c, c' is the really interesting part of the statement.

Items (1-4) are proved in [2, theorem 5, sec.6] for $d = 1, 2, 3$ (and for $d = 1, 2$, only, in [1, theorem 7] via a

different method). Therefore *the novelty in the present paper will be the proof of item (5)*: it will heavily rely on [2, Sec.VII].

For later reference it is convenient to introduce a few more notations.

Let C_ξ the cube with side r_φ centered at a point ξ in the lattice $r_\varphi \mathbb{Z}^d$. Let Δ be a subset of $\mathbb{R}^d$ and, using the definitions in Eq.(2.1),

$$N_\Delta(x) \overset{def}{=} \sum_{q \in \Delta} 1, \qquad V_\Delta \overset{def}{=} \max_{q \in \Delta} \frac{|\dot q|}{v_1}$$

$$\|x\|_n \overset{def}{=} \max_{\xi \in \Lambda_n} \frac{\max(N_{C_\xi}(x), \varepsilon_{C_\xi}(x))}{g_{1/2}(\xi/r_\varphi)}, \tag{2.5}$$

where $\varepsilon_{C_\xi}(x) \overset{def}{=} \sqrt{e_{C_\xi}(x)}$, $e_C(x) = \max_{q \in C}(\frac12 \dot q^2 + \psi(q))$.

III. THERMOSTATTED EVOLUTIONS

Thermostatted evolution can now be studied by comparison with the frictionless one.

The problem will be studied by restricting attention to a suitable subset of the set $\mathcal{X}_E \overset{def}{=} \{x \mid \mathcal{E}(x) \le E\}$.

Consider the bands of points ξ at distance $\rho_0(\xi)$ within r_φ and $2r_\varphi$ from the boundary $\partial\Omega_0$ of Ω_0:

$$\Lambda_* \overset{def}{=} \{q : \rho_0(q) \le r_\phi\}, \ \Lambda_{**} \overset{def}{=} \{q : \rho_0(q) \le 2r_\phi\} \tag{3.1}$$

By items 1,2,3 theorem 1 in Sec.II (which can be taken for granted by the remark following theorem 1) there is $C_* > 0$ (depending on E) so that, for all $x \in \mathcal{X}_E$ and with the notations Eq.(2.5), for n large enough:

$$\max_{t \le \Theta} \max\{N_{\Lambda_{**}}(S_t^{(n,0)}x), V_{\Lambda_{**}}(S_t^{(n,0)}x)\} < C_* \tag{3.2}$$

Fixed γ once and for all, arbitrarily with $\frac12 < \gamma < 1$, let Σ' be the set where are realized the events delimiting the *stopping time* $T_n(x)$

$$T_n(x) \overset{def}{=} \{\max t : t \le \Theta, \forall \tau < t, \tag{3.3}$$

$$\left|\frac{U_{j,\Lambda_n}(S_\tau^{(n,1)}x)}{|\Omega_j \cap \Lambda_n|} - u_j\right| < \frac{\varphi_0}{N_j^\varepsilon}, \|S_\tau^{(n,1)}x\|_n < (\log n)^\gamma\}.$$

see Eq.(1.5) and Eq.(2.5) for notations. Split $\mathcal{X}_E = \mathcal{A}_n \cup \mathcal{B}_n$ with

$$\mathcal{B}_n \overset{def}{=} \{x \in \mathcal{X}_E : T_n(x) \le \Theta\} : \tag{3.4}$$

Theorem 2: *There are positive constants C, C', c depending only on E such that for all n large enough:*

(1) *if $t \le T_n(x)$, $S_t^{(n,0)}x$ and $S_t^{(n,1)}x$ are close in the sense that for $q_i(0) \in \Lambda_{(\log n)^\gamma}$*

$$|q_i^{(n,1)}(t) - q_i^{(n,0)}(t)| \le C r_\varphi e^{-(\log n)^\gamma c},$$
$$|\dot q_i^{(n,1)}(t) - \dot q_i^{(n,0)}(t)| \le C v_1 e^{-(\log n)^\gamma c}. \tag{3.5}$$

Furthermore with the notations in Eq.(3.1), (3.2), for n large enough and for all $t \le T_n(x)$:

$$N_{\Lambda_*}(S_t^{(n,1)}x) \le C_*, \ V_{\Lambda_*}(S_t^{(n,1)}x) \le C_* + 1 \tag{3.6}$$

(2) *the set $\mathcal{B}_n$ has μ_{Λ_n} –probability bounded by*

$$\mu_{\Lambda_n}(\mathcal{B}_n) \le C e^{-c(\log n)^{2\gamma} + C'}. \tag{3.7}$$

Remarks: (1) The Eq.(3.5) together with the first four items of theorem 1 imply Eq.(3.6).

(2) A sequence of initial data $\{x\} = (x_1, x_2, \ldots)$ sampled randomly and independently with the distributions μ_{Λ_n}, *i.e.* with the distribution $\mu_0(d\{x\}) \overset{def}{=} \prod_{n=1}^\infty \mu_{\Lambda_n}(dx_n)$, will consist of configurations $x_n \notin \mathcal{B}_n$ for all n large enough, by Borel-Cantelli's lemma and Eq.(3.7), because $\gamma > 1/2$.

(3) To prove item (1) and Eq.(3.6) we shall compare the evolutions $x^{(n,1)}(t)$ with $x^{(n,0)}(t)$, at same initial datum $x \in \mathcal{X}_E$ and $t \le T_n(x)$, the latter being the stopping time defined in Eq.(3.3).

Two preliminary results are necessary, namely that there is $C > 0$ so that for all n large enough the following holds.

Lemma 1: *Let $x \in \mathcal{X}_E$, $t \le T_n(x)$, see Eq.(3.3), and $k \ge (\log n)^\gamma$, then*

$$|\dot q_i^{(n,1)}(t)| \le C v_1 (k \log n)^\gamma,$$
$$|q_i^{(n,1)}(t)| \le r_\varphi (2^k + C (k \log n)^\gamma). \tag{3.8}$$

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

This lemma is needed because, otherwise, the positions and speed at time t cannot be controlled in terms of the norms $\|x\|_n$ at time 0: since the particles move they must be followed (a "Lagrangian" viewpoint).

A corollary of the above will be:

Lemma 2: *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*

$$\mathcal{N} \le C (k \log n)^{d\gamma}, \ \rho \ge c (k \log n)^{-2(d\gamma+1)/\alpha} \tag{3.9}$$

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

Remarks: (1) α is the power which controls the divergence rate of the wall potentials.
(2) The proof of the lemmas is in [2, Appendix L].

Proof (of theorem 2): The proof of the key "entropy bound" Eq.(3.7) is essentially identical to the proof of the corresponding statement in [2] and is reproduced in the Appendix A, because it requires some changes with respect to the analysis in [2] where the stopping time definition was based on the kinetic energy rather then on the potential energy as in Eq.(3.3).

We shall now bound $\delta_i(t,n) \overset{def}{=} |q_i^{(n,1)}(t) - q_i^{(n,0)}(t)|$ again following [2]. Let f_i be the acceleration of the particle i, with $q_i^{(n,a)}(t) \in \Lambda_{k+1}$, $t \leq T_n(x)$, and $k \overset{def}{=} (\log_+ n)^\gamma$, due to the other particles and to the walls.

If $q_i = q_i(0) \in \Lambda_k$, $|f_i| \leq C \ (k \log n)^{\eta'}$, $\eta' \overset{def}{=} (2d\gamma + 1)(1 + \frac{1}{\alpha})$ by Eq.(3.9). Consider the two evolutions, for $a = 0, 1$ respectively,

$$
q_i^{(n,a)}(t) = q_i(0) + \int_0^t \left(e^{-\int_0^\tau a\alpha_j(x^{(n,a)}(s))ds} \dot{q}_i(0) \right.
$$
$$
\left. + \int_0^\tau ds\, e^{-\int_s^\tau a\alpha_j(x^{(n,a)}(s'))ds'} f_i(x^{(n,a)}(s)) \right) d\tau \qquad (3.10)
$$

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).

Subtracting the Eq.(3.10) for $a = 0$ and $a = 1$ it follows that for any $q_i \in \Lambda_k$ (possibly close to the origin hence very far from the boundary of Λ_k if n is large, because $k = (\log_+ n)^\gamma$)

$$
\delta_i(t,n) \leq C \ (k \log n)^{\eta'} 2^{-n\varepsilon d} \qquad (3.11)
$$
$$
+ \Theta \int_0^t |f_i(q^{(n,1)}(\tau)) - f_i(q^{(n,0)}(\tau))| \, d\tau.
$$

provided $|\int_{t_1}^{t_2} \alpha_j ds|$ is bounded proportionally to $2^{-n\varepsilon d}$ for $[t_1, t_2] \subset [0, T_n(x)]$.

From the definition Eq.(1.4) of α_j the bound of $|\int_{t_1}^{t_2} \alpha_j ds|$ with $[t_1, t_2] \subset [0, T_n(x)]$ is split into a bound on $\int_0^{T_n(x)} \beta_j \frac{|Q_j|}{dN_j} dt$ and a bound on $\beta_j \frac{|U_j(S_{t_2}^{(n,1)}x) - U_j(S_{t_1}^{(n,1)}x)|}{dN_j}$.

The first bound can be derived from the inequality $\|S_t^{(n,1)}x\|_n < (\log n)^\gamma$ (*i.e.* for $t \leq T_n(x)$) and it is $\leq C (k \log n)^\gamma 2^{-nd}$. This requires using lemmata 1,2 because $\|S_t x\|_n$ only gives information about the particle that at time 0 are close to the test system, while the i-particle might be close to $\mathcal{C}_0$ at time t but not at time 0.

The second bound also follows from the definition of the stopping time, which implies the validity of the inequality $\frac{|U_j(S_{t_2}^{(n,1)}x) - U_j(S_{t_1}^{(n,1)}x)|}{dN_j} \leq C 2^{-n\varepsilon d}$. This also makes use of lemmata 1,2 (for the same reason as above).

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

$$
2^{k_\ell} = 2^k + \ell \, C \, (k \log n)^\gamma \qquad (3.12)
$$

and $u_{k_\ell}(t,n)$ the max of $\delta_i(t,n)$ over $|q_i| \leq 2^{k_\ell}$.

The difference in the accelerations is bounded, by lemma 2, by the maximum number $(k \log n)^{\gamma d}$ of the particles which can interact with $q_i(t,n)$ times $\max |\partial^2 \varphi|$, plus a term proportional to $(k \log n)^{(2d\gamma+1)(1+2/\alpha)}$ due to the walls potential. Then by Eq.(3.11) and writing $\eta'' \overset{def}{=} (2d\gamma + 1)(1 + \frac{2}{\alpha})$,

$$
\frac{u_{k_\ell}(t,n)}{r_\varphi} \leq C \, (k \log n)^{\eta'} 2^{-n\varepsilon d}
$$
$$
+ C \, (k \log n)^{\eta''} \int_0^t \frac{u_{k_{\ell+1}}(s)}{r_\varphi} \frac{ds}{\Theta}. \qquad (3.13)
$$

for $\ell \leq \ell^* = 2^k / ((k \log n)^\gamma C)$, the latter being the largest ℓ such that $2^{k_\ell} \leq 2^{k+1}$. By Eq.(3.13)

$$
u_k(t,n) \leq e^{C \, (k \log n)^{\eta''}} C (k \log n)^{\eta'} 2^{-n\varepsilon d}
$$
$$
+ \frac{(C \, (k \log n)^{\eta''})^{\ell^*}}{\ell^*!} \, C \, (k \log n)^\gamma. \qquad (3.14)
$$

Thus for n large enough $u_k(t,n)$ is bounded by the r.h.s. of the first of Eq.(3.5); analogous argument shows that also the velocity differences are bounded as in Eq.(3.5) which is thus proved for all $t \leq T_n(x)$.

It follows that, for $n > e^{k_0^{1/\gamma}}$ and i fixed, given $q_i(0)$ with $|q_i(0)|/r_\varphi \leq 2^{k_0}$ it is $|q_i^{(n,1)}(t) - q_i^{(n,0)}(t)| < u_{(\log n)^\gamma}(t,n) \leq Ce^{-c(\log n)^\gamma}$, *i.e.* for n large $q_i^{(n,1)}(t)$ is closer than r_φ to $q_i^{(n,0)}(t)$.

Remarking that we know "everything" about the Hamiltonian motion we can use such knowledge by applying Eq.(3.5) to particles which are initially within a distance $r_\varphi 2^{k_0}$ of the origin, with k_0 fixed arbitrarily, for all large n.

Therefore the number of particles in $q_i^{(n,1)}(t)$ which are in Λ_* is smaller than the number of particles of $q_i^{(n,0)}(t)$ in Λ_{**} which is bounded by C_*.

An analogous argument for the velocities allows to complete the proof of Eq.(3.6), given the closeness of the positions and speeds of the motions with $a = 0, 1$, see Eq.(3.5). Hence $T_n(x) \equiv \Theta$ unless $x \in \mathcal{B}_n$ and the proof of theorem 3, hence of theorem 1, is complete.

IV. APPENDIX A: ENTROPY

Entropy production per unit time, in a configuration x, is naturally defined in terms of $Q_j = -\dot{\mathbf{X}}_j \cdot \partial_{\mathbf{X}_j} U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$, interpreted as the *heat* ceded by the system to the thermostats and it is given by:

$$\sigma_0(x) = \sum_{j>0} \beta_j Q_j(x) \qquad (4.1)$$

In the isokinetic thermostat model, $a = 1$, and *if the volumes in phase space are measured by the distribution* μ_{Λ_n}, a direct computation shows that this quantity differs from the *contraction rate* of the phase space volume by $\beta_0(Q_0 + \Phi(X_0) \cdot X_0) \equiv \beta_0(\dot{K}_0 + \dot{U}_0)$ (Q_0 being $-\dot{\mathbf{X}}_0 \cdot \partial_{X_0} U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$) and by a further "small correction" $-\frac{Q_j + \dot{U}_j}{dN_j}$, see also [6]. It is:

$$\sigma(x) = \sigma_0(x) - \sum_{j>0} \beta_j \frac{\dot{U}_j + Q_j}{dN_j} + \beta_0(\dot{K}_0 + \dot{U}_0). \quad (4.2)$$

The Eq.(3.6) yields a bound $|\sigma_0(x)| \le C$, $\frac{|Q_j|}{N_j} \le C2^{-nd} \le C$ and also the last term in Eq.(4.2) gives a similar bound (because the number of particles in Ω_0 is bounded in terms of E and $\dot{K}_0 + \dot{U}_0$ equals $Q_0 + \Phi(\mathbf{X}_0) \cdot \dot{\mathbf{X}}_0$ is bounded by Eq.(3.6) and, via the comparison with the frictionless motion in Eq.(3.5) and the first four items in theorem 1).

Furthermore by the definition of the stopping time it is $\int_{t_1}^{t_2} \frac{\dot{U}_j}{N_j} dt \le C 2^{-n\varepsilon d}$: so that there is C' and

$$\int_{t_1}^{t_2} |\sigma(S_t^{(n,1)} x)| dt \le C', \qquad \forall t_1 \le t_2 \le T_n(x) \quad (4.3)$$

Writing k_ξ for the smallest integer $\ge (\log n)^\gamma g_\gamma(\xi/r_\phi)$ (here g_γ is chosen instead of the natural $g_{1/2}$ in order to simplify the formulae: recall that by definition $\gamma > 1/2$), then codimension 1 surface containing 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

$$\begin{aligned}
\mathcal{S}_\xi^1 &= \{y \in \Sigma' : |y \cap C_\xi| = k_\xi, |y \cap \partial C_\xi| = 1\} \\
\mathcal{S}_\xi^2 &= \{y \in \Sigma' : y \cap C_\xi \ni (q, \dot{q}), \varepsilon(q, \dot{q}) = \tilde{\varepsilon}_\xi\} \\
\mathcal{S}_\pm^3 &= \{y \in \Sigma' : \frac{U_{j,\Lambda_n}(x)}{|V_n|} - u_j = \pm \frac{\varphi_0}{2^{n\varepsilon d}}\}
\end{aligned} \quad (4.4)$$

if $\tilde{\varepsilon}_\xi \overset{def}{=} ((\log n)^\gamma g_\gamma(\xi/r_\phi))^2$ and $V_n \overset{def}{=} \Omega_j \cap \Lambda_n$.

By the assumption Eq.(1.5) it is not restrictive to suppose that at $t = 0$ it is $\left| \frac{U_{j,\Lambda_n}(x)}{|V_n|} - u_j \right| < \frac{1}{2} \frac{\varphi_0}{2^{n\varepsilon d}}$}.

Abridge $\Delta_{j,n} \overset{def}{=} \frac{U_{j,\Lambda_n}(x)}{|V_n|} - u_j$ and consider first the case of $\mathcal{S}_+^3$. Let $D \subset \mathcal{S}_+^3$ be the set of the x which satisfy $\Delta_{j,n}(x) = \varphi_0 2^{-n\varepsilon d}$ for a given $j > 0$ while $\Delta_{j',n} U(x) < \varphi_0 2^{-n\varepsilon d}$ for $j' > 0$, $j' \ne j$.

Then the probability $\mu_{\Lambda_n}(D)$ can be bounded, see Eq.(3.2), by

$$e^{C'} \int \mu_{\Lambda_n}(dx) \, \Theta \, \delta(\Delta_{j,n} - G) \, |\widehat{G}| \, \chi(N \le \rho 2^{nd}) \ (4.5)$$

where G is any value between $\frac{1}{2} \frac{\varphi_0}{|V_n|}$ and $\frac{\varphi_0}{|V_n|}$ and $\widehat{G}(x)$ is the derivative $\dot{\Delta}_{j,\Lambda}$ *i.e.*, from the equations of motion,

$$\widehat{G}(x) \overset{def}{=} \frac{1}{|V_n|} \left(\sum_{q,q'} (\dot{q} - \dot{q}') \partial_q \varphi(q - q') + \sum_q \dot{q} \partial_q \psi(q) \right) \ (4.6)$$

and $e^{C'}$ takes into account the entropy estimate *i.e.* the bound Eq.(4.3) of the non-invariance of μ_{Λ_n}.

Averaging the bound in Eq.(4.6) over G between $\frac{1}{2} \frac{\varphi_0}{|V_n|}$ and $\frac{\varphi_0}{|V_n|}$, our bound is

$$e^{C'} \frac{|V_n|}{\varphi_0} \int \mu_{\Lambda_n}(dx) |\widehat{G}(x)| \chi_x \qquad (4.7)$$

where χ_x is the characteristic function of the set where $|\Delta_{j,n}(x)| \in [\frac{1}{2} \frac{\varphi_0}{|V_n|}, \frac{\varphi_0}{|V_n|}]$. By Schwartz's inequality this is

$$\le e^{C'} \frac{|V_n|}{\varphi_0} (\mu_{\Lambda_n}(\widehat{G}^2)^{1/2} \mu_{\Lambda_n}(\chi_x)^{1/2}) \qquad (4.8)$$

By superstability and the integral can be bounded above by C while the second integral estimates the square root of a probability of a lage deviation and is therefore bounded by by $e^{-c2^{n(1-2\varepsilon)d}}$. Hence the contribution of $\mathcal{C}_3$ to the bound on $\mu_{\Lambda_n}(\mathcal{B})$ is (amply) bounded by the *r.h.s.* of Eq.(3.7).

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

$$\mu_{\Lambda_n, \Sigma'}(\mathcal{S}_\xi^i) \le C \sqrt{n} e^{-c[(\log n)^\gamma g_\gamma(\xi/r_\varphi)]^2}, \qquad (4.9)$$

(for suitable C, c, functions of E), also summable in n: this bound can be taken from Appendix J in [2] where it is derived in detail in the text following Eq.(9.41).

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