I. THERMOSTATS

A test system of particles in a container $\Omega_0$ and $\nu$ systems of particles in containers $\Omega_1, \ldots, \Omega_\nu$ interact and define a model of a system in interaction with $\nu$ 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:

Fig.1: The $1+\nu$ finite boxes $\Omega_j \cap \Lambda$, $j = 0, \ldots, \nu$, are marked $C_0, C_1, \ldots, C_\nu$ and contain $N_0, N_1, \ldots, N_\nu$ particles out of the infinitely many particles with positions and velocities denoted $X_0, X_1, \ldots, X_\nu$, and $\bar{X}_0, \bar{X}_1, \ldots, \bar{X}_\nu$, respectively, contained in $\Omega_j$, $j \geq 0$ 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, $\Omega_1, \Omega_2$ occupy half-spaces adjacent to $\Omega_0$.

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.

Considering external thermostats as correctly representing the physics of the interaction of a system in contact with external reservoirs has been introduced in [3]. Their analysis was founded on the grounds of (1) identity, in the thermodynamic limit, of the evolution with and without thermostats (2) identity of the phase space contraction of the thermostatted systems with the physical entropy production (up to a time derivative).

Here we follow their strategy. 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 $\Lambda$ is a ball centered at the origin the space $H(\Lambda)$ will be the space of the finite configurations $(X, \dot{X})$ with $X \subset \bigcup_{j \geq 0} \Omega_j \cap \Lambda$.

Referring to Fig.1 denote by $K_j(\dot{X}_j) = \frac{1}{2} \dot{X}_j^2$ the kinetic energy of the particles in the $j$-th container (assuming the particles mass = 1), by $U_j(\bar{X}_j)$ their potential energy (more explicitly expressed in Eq.(1.3)).

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

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

with $H_0(x) = \sum_{j=0}^\nu \beta_j (K_j(\dot{X}_j) + U_j(\bar{X}_j))$, and $N_j = \delta_j |\Lambda \cap \Omega_j|$ with $\beta_j = \frac{1}{k_B T_j} > 0$, $\delta_j > 0$, $j > 0$ ; 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 $\delta = (\delta_0, \delta_1, \ldots, \delta_\nu)$ and $T = (T_0, T_1, \ldots, T_\nu)$ are fixed densities and temperatures, $\Lambda$ is a ball centered at the origin and $Z$ is the normalization.

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 $\beta_j$ 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 imagined to act nonconservative forces.

The equations of motion (see Fig.1) in $\Lambda = \Lambda_n$, with $\Lambda_n$ being the ball of radius $2^n r_\varphi$ with $r_\varphi$ 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 $a = 0, 1$:

$$m \ddot{X}_{0i} = -\partial_i U_0(X_0) - \sum_{j>0} \partial_i U_{0,j}(X_0, X_j) + \Phi_i(X_0)$$

$$m \ddot{X}_{ji} = -\partial_i U_j(X_j) - \partial_i U_{0,j}(X_0, X_j) - a \alpha_{ij} \dot{X}_{ji} \quad (1.2)$$

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 $\Lambda_n$ (hence the labels $i$ in the subscripts $(j, i)$ have $N_j d$ values). Furthermore:

(1) the $\Phi_i(X_0)$ are, positional, nonconservative, smooth stirring forces, possibly vanishing;

(2) other forces are conservative and generated by a pair potential $\varphi$, with range $r_\varphi$, which couples all pairs in the same containers and all pairs of particles one of which is located in $\Omega_0$ and the other in $\Omega_j$ (i.e. there is no direct interaction between the different thermostats).

(3) particles are repelled by the boundaries $\partial \Omega_j$ by a conservative force of potential energy $\psi$, of range $r_\psi \ll r_\varphi$,
diverging at the walls. The potential energies will be
$U_j(X_j)$, $j \geq 0$, and $U_{0,j}(X_0, X_j)$: respectively denoting
the internal energies of the various systems and the poten-
tial energy of interaction between the system and the
thermostats.

\[
U_j(X) = \sum_{q \in X_j} \psi(q) + \sum_{(q',q') \in X_j \times X_j} \varphi(q - q')
\]
\[
U_{0,j}(X_0, X_j) = \sum_{q \in X_0, q' \in X_j} \varphi(q - q')
\]
(1.3)

In the case $a = 0$ particles will be allowed to exit
the regions $\Omega_j \cap \Lambda_n$ through the boundary of $\Lambda_n$ 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].

The analysis will be restricted to the geometries in
the regions $\Omega_j \cap \Lambda_n$ through the boundary of $\Lambda_n$ 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 $\alpha_j$ 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. $\frac{d}{dt}N_j k_B T_j$, for $j > 0$, see
Eq.(1.1); this means

\[
\alpha_j = \frac{Q_j - \dot{U}_j}{N_j d k_B T_j}
\]
(1.4)

where $Q_j \triangleq - \dot{X}_j \cdot \partial_X U_{0,j}(X_0, X_j)$, is the heat
ceded by the system to the $j$-th thermostat.

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

**Hypothesis:** The initial state distributions $\mu_{\Lambda_n}$ 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:

\[
\mu_{\Lambda_n} \left( \{ x \mid U_{j,\Lambda_n}(x) - u_j > \frac{C \varphi_0}{N_j^2} \} \right) < e^{-c n^{(1-2\alpha)d}}
\]
(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 $T, \Lambda$ as discussed in [4, 5]). Notice that the
volume $|\Omega_j \cap \Lambda_n|$ is $O(2^d)$.

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
$S_{i}^{(n,a)} x$, or also $x^{(n,a)}(t)$, their solutions with data ran-
domly chosen with the distribution in Eq.(1.2).

Solutions exist (for all data in $H(\Lambda)$, 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 [6], see [2, Appendix I]) obtaining existence
and uniqueness for all initial data outside a set of $\mu_{\Lambda_n}$-
probability $0$.

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

Let $v_1 \triangleq \sqrt{\frac{2}{m_1}} |x_i - x_j| \triangleq \frac{|q_i - q_j|}{v_1} + \frac{|q_i - q_j|}{r_\psi}$, and

\[
W(x; \xi, R) \triangleq \frac{1}{\varphi_0} \sum_{q_i \in R(\xi, R)} \left( \frac{m_i^2}{2} \right) + \frac{1}{2} \sum_{j,j \neq i} \varphi(q_i - q_j) + \psi(q_i) \varphi_0 \right)
\]
(2.1)

\[
N_i(x) \triangleq \text{number of particles within } r_\psi \text{ of } q_i.
\]

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

\[
\mathcal{E}(x) \triangleq \sup_{\xi} \sup_{R > \rho_n(x)/r_\psi} \frac{W(x; \xi, R)}{R^d}
\]
(2.2)

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

\[
\mu_{\Lambda_n}(\mathcal{X}_E) \geq 1 - C e^{-cE}
\]
(2.3)

for suitably chosen $C, c > 0$.

Let $d \leq 3$, then given an initial datum $x$ the motion
$S_{i}^{(n,a)} x$ exists for $\mu_{\Lambda_n}$–almost all $x \in H_{1/2}$ and $\forall t \geq 0$.
Fixed arbitrarily an observation time $\Theta < \infty$ the main
result will be

**Theorem 1:** If $x \in H(\Lambda_n) \cap \mathcal{X}_E$ 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 $\Lambda_k$, i.e.
$q_i(0) \in \Lambda_k$. Consider, for $n > k$, the events

\[
|q_i^{(n,0)}(t)| \leq c v_1 k^{d'},
\]
(1)

\[
\alpha_j \geq c v_1 k^{-\frac{d}{2}},
\]
(2)

\[
N_i(S_{i}^{(n,0)} x)_i \leq c k^{1/2},
\]
(3)

\[
|S_{i}^{(n,0)} x)_i - S_{i}^{(n+1,0)} x)_i| \leq e^{-c' n^{2/3}},
\]
(4)

\[
|S_{i}^{(n,0)} x)_i - S_{i}^{(n,1)} x)_i| \leq e^{-c'(\log n)\gamma},
\]
(5)

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

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

This means that, if \( \Lambda_n \) 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 \( C \xi \) the cube with side \( r_\varphi \) centered at a point \( \xi \) in the lattice \( r_\varphi \mathbb{Z}^d \). Let \( \Delta \) be a subset of \( \mathbb{R}^d \) and, using the definitions in Eq.(2.1),

\[
N_\Delta(x) \overset{\text{def}}{=} \sum_{\eta \in \Delta} 1, \quad V_\Delta \overset{\text{def}}{=} \max_{\eta \in \Delta} \frac{|\eta|}{v_1} \quad (2.5)
\]

\[
\|x\|_n \overset{\text{def}}{=} \max_{\xi \in \Lambda_n} \frac{1}{\min(N_{C_\xi}(x), \varepsilon_{C_\xi}(x))}, \quad (2.6)
\]

where \( \varepsilon_{C_\xi}(x) \overset{\text{def}}{=} \sqrt{eC_\xi(x)}, \varepsilon_C(x) = \max_{\eta \in C} (\frac{1}{2} \eta^2 + \psi(\eta)) \).

### 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 \( \mathcal{X}_E \overset{\text{def}}{=} \{ x | E(x) \leq E \} \).

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

\[
\Lambda_\varphi \overset{\text{def}}{=} \{ q : \rho_0(q) \leq r_\varphi \}, \Lambda_{\varphi s} \overset{\text{def}}{=} \{ q : \rho_0(q) \leq 2r_\varphi \} \quad (3.1)
\]

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.(2.6), for \( n \) large enough:

\[
\max_{\xi \in \Theta} \max_{\xi \in \Lambda_{\varphi s}} \{ N_{\Lambda_{\varphi s}}(S_t^{(n,0)} x), V_{\Lambda_{\varphi s}}(S_t^{(n,0)} x) \} < C_* \quad (3.2)
\]

Fixed \( \gamma \) once and for all, arbitrarily with \( \frac{1}{2} < \gamma < 1 \), let \( \Sigma' \) be the set where are realized the events delimiting the stopping time \( T_n(x) \)

\[
T_n(x) \overset{\text{def}}{=} \left\{ \max_{t} : t \leq \Theta, \forall \tau < t, \left| \frac{U_{\Lambda_n}(S_t^{(n,0)} x) - u_j}{|\Omega_{\varphi n(\Lambda_n)}|} \right| < \frac{r_\varphi}{N_j}, \|S_t^{(n,1)} x\|_n < (\log n)^{\gamma} \right\}. \quad (3.3)
\]

see Eq.(1.5) and Eq.(2.6) for notations. Split \( \mathcal{X}_E = A_n \cup \mathcal{B}_n \) with

\[
\mathcal{B}_n \overset{\text{def}}{=} \{ x \in \mathcal{X}_E : T_n(x) \leq \Theta \} \quad (3.4)
\]

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

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

\[
|q_i^{(n,1)}(t) - q_i^{(n,0)}(t)| \leq C r_\varphi e^{-c (log n)^{\gamma}} c, \quad (3.5)
\]

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

\[
N_{\Lambda_{s}}(S_t^{(n,1)} x) \leq C_*, \quad V_{\Lambda_{s}}(S_t^{(n,1)} x) \leq C_* + 1 \quad (3.6)
\]

(2) the set \( \mathcal{B}_n \) has \( \mu_{\Lambda_n} \)-probability bounded by

\[
\mu_{\Lambda_n}(\mathcal{B}_n) \leq C e^{c (log n)^{2\gamma}} + C'. \quad (3.7)
\]

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 \( \mu_{\Lambda_n} \), i.e. with the distribution \( \mu_0(d\{x\}) \overset{\text{def}}{=} \prod_{n=1}^{\infty} \mu_{\Lambda_n}(dx_n) \), 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 \( t \leq T_n(x) \), 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 \( x \in \mathcal{X}_E, t \leq T_n(x) \), see Eq.(3.3), and \( k \geq (log n)^{\gamma} \), then

\[
|q_i^{(n,1)}(t)| \leq C v_1 (k log n)^{\gamma}, \quad |q_i^{(n,1)}(t)| \leq r_\varphi (2^k + C (k log n)^{\gamma}). \quad (3.8)
\]

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

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 \( N \) and \( \rho \) be the maximal number of particles which at any given time \( \leq T_n(x) \) interact with a particle \( q_j \) initially in \( \Lambda_{k+1} \), and, respectively, the minimal distance of a particle from the walls. Then

\[
N \leq C (k \log n)^d \gamma, \quad \rho \geq C (k \log n)^{-2(d+1)/\alpha} \tag{3.9}
\]

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

Remarks: (1) \( \alpha \) is the power which controls the divergence rate of the wall potentials.

(2) The proof of the lemmas is in [2, Appendix A].

Proof (of theorem 2): The proof of the key “entropy bound” Eq.(3.7) is similar 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 than on the potential energy as in Eq.(3.3). In this appendix we make essential use of the hypothesis at the end of Sec.1.

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

If \( q_i = q_i(0) = q_i((t) \in \Lambda_{k+1}, t \leq T_n(x), \text{and} \ k \equiv (\log_n)^\gamma \),

\[
q_i(t, n) = q_i(0) + \int_0^t \left( e^{-\int_0^s \alpha(x_n(a)) ds} q_i(0) + \int_0^s ds e^{-\int_0^s \alpha(x_n(a)) ds} f_i(n, a)(s) \right) dt, \tag{3.10}
\]

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 \( \Lambda_k \) if \( n \) is large, because \( k = (\log_n)^\gamma \))

\[
\delta_i(t, n) \leq C (k \log n)^\gamma (\log n)^{2-nd} \tag{3.11}
\]

\[
+ \Theta \int_0^t \left| f_i(q_i(n, 1)(\tau)) - f_i(q_i(n, 0)(\tau)) \right| d\tau.
\]

provided \( \int_0^t \alpha ds \) is bounded proportionally to \( 2^{-nd} \) for \( [t_1, t_2] \subset [0, T_n(x)] \).

From the definition Eq.(1.4) of \( \alpha_j \) the bound of the integral \( \int_0^t \alpha_j ds \) with \( [t_1, t_2] \subset [0, T_n(x)] \) is split into a bound on \( \int_0^T \beta_j dN \) and a bound on the ratio

\[
\beta_j \frac{[U_j(S(x, n)) - U_j(S(x, n))]}{dN} \tag{3.12}
\]

The first bound can be derived from the inequality \( ||S(x, n)|| < (\log n)^\gamma (i.e. \text{for} \ t \leq T_n(x)) \) and it is \( \leq C (k \log n)^\gamma (\log n)^{2-nd} \). This requires using lemma 1,2 because \( ||S(x, n)|| \) only gives information about the particle that at time \( 0 \) are close to the test system, while the \( i \)-particle might be close to \( C_0 \) 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

\[
\frac{|U_j(S(x, n)) - U_j(S(x, n))|}{dN} \leq C 2^{-nd} \tag{3.13}
\]

This also makes use of lemma 1,2 (for the same reason as above).

Let \( \ell \) be a non-negative integer, \( k \) such that

\[
2^k = 2^k + \ell C (k \log n)^\gamma \tag{3.14}
\]

and \( u_k(t, n) \) 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 \( max |F(\varphi)| \), plus a term proportional to \( (k \log n)^{2d+1}(1/2+\alpha) \) to the walls potential. Then by Eq.(3.11) and writing \( \eta^\gamma = (2 \cdot d \cdot \gamma + 1)(1 + \frac{2}{\gamma}) \),

\[
\frac{|u_k(t, n)|}{r_x} \leq C (k \log n)^\gamma 2^{-nd} + C (k \log n)^\gamma \int_0^t \frac{u_k(x, s)}{r_x} ds, \tag{3.15}
\]

for \( \ell \leq \ell^* \leq (k \log n)^\gamma C \), the latter being the largest \( \ell \) such that \( 2^k \leq 2^{k_0} \). By Eq.(3.13)

\[
u_k(t, n) \leq e C (k \log n)^\gamma C (k \log n)^\gamma 2^{-nd} + \frac{(C (k \log n)^\gamma 2^{-nd}) \tilde{C}}{\ell!} \tag{3.16}
\]

Thus for \( n \) large enough \( u_k(t, n) \) is bounded by the r.h.s. of the first of Eq.(3.15); analogus argument shows that also the velocity differences are bounded as in Eq.(3.15) which is thus proved for all \( t \leq T_n(x) \).

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

Remark: 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 \( r_x \cdot 2^{k_0} \) of the origin, with \( k_0 \) fixed arbitrarily, for all large \( n \).

Therefore the number of particles in \( q_i(1)(t) \) which are in \( \Lambda_k \) is smaller than the number of particles of \( q_i(0)(t) \) in \( \Lambda_k \), which is bounded by \( C_4 \).

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 \( x \in B \) 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 $Q_j = -X_j \cdot \partial X_j U_{0,j}(X_0, X_j)$, interpreted as the heat ceded by the system to the thermostats and it is given by:

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

(4.1)

In the isokinetic thermostat model, $\alpha = 1$, and if the volumes in phase space are measured by the distribution $\mu_{\Lambda_n}$, a direct computation shows that this quantity differs from the contraction rate of the phase space volume by

$$\beta \dot{\sigma}_0 = \frac{\beta_j Q_j}{dN_j}$$

and by a further “small correction” $-\frac{Q_j+\hat{U}_j}{dN_j}$, see also [7]. It is:

$$\sigma(x) = \sigma_0(x) - \sum_{j>0} \beta_j \frac{\hat{U}_j + Q_j}{dN_j} + \beta_0(K_0 + \hat{U}_0).$$

(4.2)

The Eq.(3.6) yields a bound $|\sigma_0(x)| \leq C, |\frac{Q_j}{N_j}| \leq C 2^{-nd} \leq C$ and also the last term in Eq.(4.2) gives a similar bound (because the number of particles in $\Omega_0$ is bounded in terms of $E$ and $K_0+\hat{U}_0$ equals $Q_0+\Phi(X_0)$). $X_0$ 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

$$\int_{t_1}^{t_2} \frac{\hat{U}_j + Q_j}{dN_j} dt \leq C 2^{-nd}:$$ so that there is $C'$ and

$$\int_{t_1}^{t_2} |\sigma(\Sigma^{n,1}_x)| dt \leq C', \quad \forall t_1 \leq t_2 \leq T_n(x)$$

(4.3)

Writing $k_{\xi}$ for the smallest integer $\geq (\log n)^2 g_1(\xi/r_0)$ (here $g_1$ is chosen instead of the natural $g_1/2$ in order to simplify the formula: recall that by definition $\gamma > 1/2$, then codimension 1 surface containing $\Sigma'$ splits into an union over $\xi \in \Lambda_n \cap r_\varphi Z^d$ of the union of $S_1^1 \cup S_2^2 \cup S_3^3$, where

$$S_1^1 = \{ y \in \Sigma' : |y| \cap C_\xi = k_{\xi}, |y| \cap \partial C_\xi = 1 \}$$

$$S_2^2 = \{ y \in \Sigma' : y \cap C_\xi \ni (q, \tilde{q}), \tilde{e}(q, \tilde{q}) = \tilde{\xi} \}$$

$$S_3^3 = \{ y \in \Sigma' : \frac{U_j X_0(x)}{|V_n|} - u_j = \pm \frac{\tilde{\varphi}_n}{2\pi n^2} \}$$

(4.4)

if $\tilde{\varphi}_n \stackrel{def}{=} (\log n)^2 g_1(\xi/r_0)\}^2$ and $V_n \stackrel{def}{=} \Omega_j \cap \Lambda_n$.

By the assumption Eq.(1.5) it is not restrictive to suppose that at $t = 0$ it is $|\frac{U_j X_0(x)}{|V_n|} - u_j| < \frac{1}{2} \frac{\varphi_0}{2\pi n^2}$.

Abridge $\Delta_{j,n} \stackrel{def}{=} \frac{U_j X_0(x)}{|V_n|} - u_j$ and consider first the case of $S_1^1$. Let $D \subset S_1^1$ be the set of the $x$ which satisfy $\Delta_{j,n}(x) = \varphi_0 2^{-nd}$ for a given $j > 0$ while $\Delta_{j',n}(U(x)) < \varphi_0 2^{-nd}$ for $j' > 0, j' \neq j$.

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

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

(4.5)

where $G$ is any value between $\frac{1}{2} \frac{\varphi_0}{|V_n|}$ and $\frac{\varphi_0}{|V_n|}$ and $\hat{G}(x)$ is the derivative $\Delta_{j,n}$ i.e., from the equations of motion,

$$\hat{G}(x) \stackrel{def}{=} \frac{1}{|V_n|} (\sum_{q, q'} (\dot{q} - \dot{q'}) \partial q \varphi(q, q') + \sum_{q} q \dot{\partial q} \psi(q))$$

(4.6)

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

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

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

(4.7)

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

$$\leq e^{C'} |\frac{|V_n|}{\varphi_0} (\mu_{\Lambda_n}(\hat{G})^2)^{1/2} (\mu_{\Lambda_n}(\chi_x)^{1/2})$$

(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 large deviation and is therefore bounded by $e^{-2\rho 2^{nd}}$. Hence the contribution of $C_3$ to the bound on $\mu_{\Lambda_n}(B)$ is (amply) bounded by the $r.h.s.$ of Eq.(3.7).

Similarly, the surface areas $\mu_{\Lambda_n, \Sigma}(S_2^2)$ and $\mu_{\Lambda_n, \Sigma}(S_3^3)$ induced by $\mu_{\Lambda_n}$ on $S_1^1, S_2^2$ induced by $\mu_0$ are bounded by

$$\mu_{\Lambda_n, \Sigma}(S_2^2) \leq C \sqrt{n} e^{-2(\log n)^2 g_1(\xi/r_0)^2},$$

(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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