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Stationary States for a Mechanical System with Stochastic Boundary Conditions

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We consider a system of Newtonian particles, with a long-range repulsive pair potential, moving in a cavity whose surface temperature is spatially varying. When a particle hits the surface, it is "thermalized" at the temperature of the collision point. We prove that this system has a unique stationary ensemble, to which any initial distribution converges for large times. We show that this stationary ensemble depends continuously on the surface temperature profile.

KEY WORDS: Nonequilibrium steady state; Newtonian Markov process; stationary probability measure; heat flow.

1. INTRODUCTION

An outstanding problem in nonequilibrium statistical mechanics is that of finding a canonical description, analogous to that provided by the Gibbs state for equilibrium, for steady state nonequilibrium phenomena, such as the steady state heat flow produced when the walls confining a gas are maintained at different temperatures.[7–10] The simplest way to classically model such a gas is by requiring that whenever a particle hits a wall its velocity is "thermalized" according to the temperature of the wall at the point of collision. In this paper we establish the existence and uniqueness of a stationary microscopic state for such a system. We are, however, very far from the sort of understanding of this state which would be required to attain a *canonical* description of the steady state.

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We consider a system of N particles of unit mass moving inside a bounded region $\Lambda \subset \mathbb{R}^3$ according to the Hamiltonian equations

$$\begin{cases} \dot{q}_i = p_i \\ \dot{p}_i = -\sum\limits_{j \neq i} \operatorname{grad}_i U(|q_j - q_i|), \qquad i = 1,..., N \end{cases} \tag{1.1}$$

where $U(r)$, $r \geqslant 0$, describes a spherically symmetric repulsive smooth potential; more precisely, U is a C^2 function, $U'(0) = 0$, and $U'(r) < 0$ for $r > 0$. Each point q of the boundary $\partial \Lambda$ is connected to a reservoir at temperature $T(q)$. The interaction between particles and wall is described in the following way: if (q, p) is the position velocity of the particle before the collision with the wall, after the collision it takes a new velocity v which is randomly chosen according to the distribution

$$R_{\beta(q)}(dv) = Z_{\beta(q)}^{-1} 1_{\{v \cdot n(q) > 0\}} v \cdot n(q) \exp\left[-\beta(q) \frac{|v|^2}{2} \right] dv$$

where $n(q)$ is the inward normal to the boundary at q, $\beta(q) = 1/KT(q)$, and $Z_{\beta(q)}$ is a normalizing factor to make the integral of $R_{\beta(q)}$ equal to 1; 1_A is the indicator function of the set A.

We thus obtain a Markov process for the evolution of our system. Note that if the system is in contact with a thermal reservoir at constant temperature T, then the Gibbs state at temperature T is stationary (see Appendix). This will, of course, not be true if the temperature varies along the boundary. Nontheless, we establish the existence and uniqueness of a stationary probability measure and show that any initial distribution converges to it for large times; we prove also a result on the stability of the stationary measure (Theorems 3.1 and 3.2 of Section 3).

We remark that the state space of the Markov process contains points from which the evolution is trivial, namely, points for which all particles are coincident with zero speed. There are other configurations in which "focusing" occurs and no convergence to equilibrium is possible. The previously mentioned theorems refer to the process defined on a subset Ω of $(\Lambda \times \mathbb{R}^3)^N$ whose complement has vanishing Lebesgue measure.

We are not able to perform the thermodynamical limit of the unique stationary measure when the temperature varies along the boundary: unfortunately the techniques used in our proofs do not tell us anything about the detailed structure of the stationary state.

In Ref. 1 the proofs of similar results were sketched, but with additional unpleasant conditions. Λ was assumed to be convex, with a smooth boundary, while the temperature was assumed to be continuous along the boundary. Thus, for example, the cases in which Λ is bounded by concentric spheres or is a cube (with, say, opposite walls at different temperatures) were not covered.

Our methods do not apply to systems with hard cores. Related results for simple systems with hard cores have been obtained in Refs. 2, 3, and 6.

2. EXISTENCE OF THE PROCESS. DISCRETE TIME SKELETON

We will first define carefully the process which was described, somewhat heuristically, in the previous section. Denote by a configuration x a collection of N positions and velocities $x = \{(q_1, p_1),..., (q_N, p_N)\}$ where for all i $q_i \in \Lambda$. Set $\Omega = \{x \in (\Lambda \times \mathbb{R}^3)^N\colon\ p(x) = \sum p_i \neq 0\}$ and $\hat{\Omega} = \{x \in \Omega\colon q_i \in \partial\Lambda$ for some $i \in 1,..., N$ and $n(q_i) \cdot p_i > 0$ for all $q_i \in \partial\Lambda\}$.

We define a Markov kernel P on $\hat{\Omega}$ by the following: for $x \in \hat{\Omega}$, the system of the Hamiltonian equations has a unique solution $t \to x(t)$ with $x(0) = x$. Because $p(x)$ is not zero, this solution must exit from $(\Lambda \times \mathbb{R}^3)^N$. Set $\tau = \inf\{t\colon x(t) \notin (\Lambda \times \mathbb{R}^3)^N\}$ and set $y = x(\tau)$. Suppose that $\{q_{i_j}\}_{j=1,...,l}$, $l \leqslant N$, arc the positions of the particles in the configuration y that are at the boundary $\partial\Lambda$. Choose now $v_1,..., v_l$ independently, according to the law $R_{\beta(q_{i_j})}(dv)$ and call x_1 the configuration obtained by replacing the velocities of the particles at the boundary by the corresponding v's while leaving all the other coordinates unchanged. $P(x, dx_1)$ is then the distribution of x_1. Of course $P(x, dx_1)$ is well defined (as a probability Kernel on $\hat{\Omega}$) since for all $x \in \hat{\Omega}$ $P(x, \hat{\Omega}) = 1$ because the law $R_{\beta(q)}(dv)$ is absolutely continuous with respect to dv.

Given an $x_0 \in \Omega$ the continuous time process is defined in an obvious manner from the discrete time skeleton. (Ambiguities can be removed by deleting points with $n(q_i) \cdot p_i \leqslant 0$ and by requiring, for instance, right continuity of sample paths). In order to check that this process is well defined for all times we only need to check that almost surely we have $\sum \tau_i = \infty$ if τ_i are the successive waiting times before collisions. Notice that if $\sum \tau_j < \infty$, then at least one of the particle of our system must have an infinite number of collisions in a finite time. This means that if σ_i are the return times to the boundary for this particle, we have $\sum \sigma_j < \infty$. However it is easy to see that if the outgoing velocity v satisfies

(A) $v \cdot n(q) \geqslant \beta$ and $K_0 \leqslant |v| \leqslant 2K_0$ for some number K_0 and $\beta > 0$

then the σ that follows this collision is bounded away from zero independently of the hitting point q. Besides, the set (A) of outgoing velocities has a probability bounded away from zero uniformly in q. Therefore we have that $\sum \sigma_j = \infty$ almost surely.

We will denote by $P_t(x, dy)$ the continuous time Markov semigroup of this process.

There is a natural one-to-one correspondence between the invariant measure for P on $\hat{\Omega}$ and the invariant measure for P_t on Ω.

This correspondence can be most easily described in terms of a special flow representation[4] of the Markov process evolution on Ω. Given $x \in \Omega$, take the $\xi \in \hat{\Omega}$ such that x belongs to the trajectory of ξ [i.e., the Hamiltonian evolution starting from ξ reaches x before $\tau(\xi)$] and call $t(x)$ the time necessary to go from ξ to x.

Set $M = \{(\xi, t) \in \hat{\Omega} \times \mathbb{R}_+ : 0 \leqslant t < \tau(\xi)\}$ M is naturally isomorphic to Ω. Under this isomorphism the evolution on Ω becomes a flow "upwards"away from the base $\hat{\Omega}$ until the ceiling $\{t = \tau(\xi)\}$ is reached, followed by a return to the base at a random point via P. A minimal condition for a measure μ to be invariant under this process is that its image under the isomorphism be of the form $d\hat{\mu} \times dt$ (where $d\tilde{\mu}$ is a measure on the base $\hat{\Omega}$) but of course this is not sufficient. In fact, we have the following:

Proposition 2.1. (1) μ is P_t invariant iff $\tilde{\mu}$ is P invariant; (2) $\int \tilde{\mu}(d\xi)\, \tau(\xi) < \infty$ iff μ has finite mass.

However in our case, owing to the form of the stochastic boundary reflections, the second condition in always satisfied.

Proposition 2.2. If $\tilde{\mu}$ is a $P(x, dy)$-invariant probability, it satisfies

$$\int \tau(x)\, \tilde{\mu}(dx) < \infty$$

Proof. If $\tilde{\mu}$ is P invariant,

$$\int \tau(y)\, \tilde{\mu}(dy) = \int \tilde{\mu}(dx)\, P(x, dy)\, \tau(y)$$

But, of course $\tau(y) \leqslant N\, |\text{diam}\, \Lambda| / |p(y)|$, where $p(y)$ is the total momentum of the configuration y. We may assume that y is such that particle "1" is on the boundary, i.e., that $y = \{(q_1, v), (q_2, p_2),..., (q_N, p_N)\}$ so that $p(y) = \sum_2^N {}_i p_i + V$. Provided the temperature at the boundary is bounded below and above, the function defined on $\mathbb{R}^6$, $(q, v) \to f(q, v) = Z_{\beta(q)}^{-1} 1_{v \cdot n > 0} v \cdot n \exp[-\beta(q)(|v|^2/2)]$ is bounded, so that $f(q, v)(1/|\sum p_i + v|)\, dv$ is bounded uniformly in $\sum p_i$ and therefore $\int P(x, dy)\, \tau(y)$ is bounded uniformly in x. ∎

3. MAIN RESULTS

Theorem 3.1. Suppose that Λ is a closed region of $\mathbb{R}^3$ such that $\mathring{\Lambda}$ is connected and the boundary $\partial\Lambda$ is a finite disjoint union of C^2-compact manifolds and that there exist two strictly positive, finite constants a and b such that $a \leqslant \beta(q) \leqslant b$ for all $q \in \partial\Lambda$. Then there exists α unique, nontrivial invariant probability measure μ_β for the Markov process P_t defined above. Moreover, this unique invariant probability measure is equivalent to the Lebesgue measure on the state space of the process $(\Lambda \times \mathbb{R}^3)^N$ and any probability measure on $(\Lambda \times \mathbb{R}^3)^N$ converges in variation norm to μ_β under the time evolution.

Theorem 3.2. The unique invariant measure μ_β associated to a given temperature profile β at the boundary depends continuously in variation norm on β.

To prove Theorems 3.1 and 3.2, we need Theorems 3.3 and 3.4 below that we will prove in the next section. We note that by Proposition 2.1 it is enough to prove that the process at the collisions has a unique invariant probability measure.

Definition (Strong Doeblin condition). We will say that a Markov kernel $P(x, dy)$ satisfies the strong Doeblin condition (SD) iff there exist a nontrivial measure $v(dy)$ and an integer n such that for all $x \in \hat{\Omega}$

$$P^n(x, dy) \geqslant v(dy)$$

In this case, we say that P is v-SD.

Theorem 3.3. There exist an integer n, a constant $\delta > 0$ and a set $A \subset \hat{\Omega}$ of strictly positive Lebesgue measure, such that for all $x \in \hat{\Omega}$

$$P^n(x, dy) \geqslant \delta 1_A(y)\, dy$$

Moreover the set A is independent of the temperature profile on the boundary and δ depends only on a and b.

Remark. In the previous theorem dy is the product of the surface area measure for the position of the particle on $\partial\Lambda$ and the Lebesgue measure for the other coordinates. (The set of configurations in $\hat{\Omega}$ which has more than one particle in $\partial\Lambda$, has zero dy measure).

We also need a result on the continuous time process.

Let P_t be the transition probability for the continuous time process. For each $\tau > 0$ let $P_{m\tau}$ be the Markov chain obtained observing the process only at times $t = m\tau$.

Theorem 3.4. For each $\tau > 0$, $P_{m\tau}$ is an ergodic, aperiodic Harris chain.

Proof of Theorem 3.1. Theorem 3.1 follows from Theorems 3.3 and 3.4. More precisely it follows from the three following propositions.

Proposition 3.5. If P is ν-SD then (a) there exists a unique invariant probability measure $\tilde{\mu}_\beta$ for P, and (b) for any probability measure $\tilde{\pi}$ on $\hat{\Omega}$ we have

$$\|\tilde{\pi}P^K - \tilde{\mu}_\beta\| \leqslant 2[1 - \nu(\hat{\Omega})]^{\gamma K}$$

where $\gamma > 0$ and $\| \ \|$ denotes the variation norm of the measure.

Proof. Both (a) and (b) follow from the fact that if $\tilde{\pi}_1$ and $\tilde{\pi}_2$ are two probability measures on $\hat{\Omega}$, then

$$\|\tilde{\pi}_1 P^n - \tilde{\pi}_2 P^n\| \leqslant [1 - \nu(\hat{\Omega})] \ \|\tilde{\pi}_1 - \tilde{\pi}_2\|$$

Proposition 3.6. For any probability measure π on Ω we have

$$\|\pi P_t - \mu_\beta\| \to 0 \qquad \text{as} \quad t \to \infty$$

Proof. Proposition 3.6 follows immediately from Theorem 2.4.

Proposition 3.7. For any temperature profile, the invariant probability measure is equivalent to the Lebesgue measure λ on $(\Omega \times \mathbb{R}^3)^N$ provided there exist a and b such that $0 < a \leqslant \beta(q) \leqslant b < \infty$.

Proof. Note first, via the correspondence between μ and $\tilde{\mu}$, that μ is equivalent to the Lebesgue measure on Ω iff $\tilde{\mu}$ is equivalent to the Lebesgue measure on $\hat{\Omega}$. Moreover we know that the Gibbs state γ_a at temperature $T = 1/ka$ is invariant for the evolution P_0 with boundary temperature T (Appendix); hence if A is a subset of the phase space of Lebesgue measure zero, then $\gamma_a(A) = 0$ and

$$0 = \gamma_a(A) = \int \gamma_a(dx) \, P_0(x, dy) \, 1_A(y)$$

Hence $P_0(x, A) = 0$ almost everywhere and consequently the same is true of $P(x, A)$. This proves that P transforms any measure absolutely continuous with respect to the Lebesgue measure into a measure also absolutely continuous. Now take the invariant measure μ for P and decompose it in $\tilde{\mu}_1 + \tilde{\mu}_2$, where $\tilde{\mu}_1 \perp \tilde{\lambda}$ and $\tilde{\mu}_2 \ll \tilde{\lambda}$. Since $\tilde{\mu} = \tilde{\mu}_1 + \tilde{\mu}_2 = (\tilde{\mu}_1 + \tilde{\mu}_2) P$ we see that $\tilde{\mu}_1$ must also be invariant. On the other hand the density cannot vanish on a set of strictly positive Lebesgue measure: If A is the set on which the density is positive, $\gamma_a^A(.) = \gamma_a(. \cap A)$ is invariant for P_0. Applying Proposition 3.5 to P_0, for which we know that γ_a is invariant, we see that $\tilde{\lambda}(\hat{\Omega} \backslash A) = 0$. ∎

Proof of Theorem 3.2. For any β: $\partial \Lambda \to [a, b]$ denote by $P_\beta(\xi, d\eta)$ the associated Markov kernel and by $\tilde{\mu}_\beta$ its invariant probability measure. For any fixed ξ in $\hat{\Omega}$

$$\|\tilde{\mu}_{\beta_K} - \tilde{\mu}_\beta\| \leqslant \|\tilde{\mu}_{\beta_K} - P^n_{\beta_K}\| + \|P^n_{\beta_K} - P^n_\beta\| + \|P^n_\beta - \mu_\beta\|$$

By Theorem 3.3, δ is independent of the profile β and the first and the third terms are small for n large enough. On the other hand we have that for n large enough

$$\sup \|P^n_{\beta_K} - P^n_\beta\| \leqslant n \left[\int d\tilde{\mu}_{\beta_K} \, \|P_{\beta_K} - P_\beta\| + \varepsilon \right]$$

Besides if ξ is a configuration in which only one particle is on the boundary at position q

$$\begin{aligned} \|P_{\beta_K} - P_\beta\| &= \int v \cdot n \, 1_{v \cdot n > 0} \left| \frac{\exp[-\beta_K(q)(|v|^2/2)]}{Z_{\beta_K(q)}} - \frac{\exp[-\beta(q)(|v|^2)]}{Z_{\beta(q)}} \right| dv \\ &\leqslant C \, |\beta_K(q) - \beta(q)| \end{aligned}$$

So when $\{\beta_K\}$ converges in (Lebesgue) measure to β, $\tilde{\mu}_{\beta_K} \to \tilde{\mu}_\beta$ in variation norm. ∎

Remark. The previous result implies that the invariant measure μ_β for the continuous time process depends continuously, in variation norm, on β.

4. PROOFS OF THEOREMS 3.3 AND 3.4

4.1. Sketch of the Proof

We first give the outline of the proof . There are three basic ingredients:

(1) For free motion ($U = 0$) the conclusion of Theorem 3.3 is easy to establish in two steps:

There exists a point $\eta_0 \in \hat{\Omega}$, a neighborhood Δ of η_0, and an open set A such that (a) for any $\eta \in \Delta$, $P^{2N}(\eta, d\xi) \geqslant \delta 1_A(\xi) \, d\xi$ and (b) for any initial point $\xi \in \hat{\Omega}$, the process evolves into Δ with a probability and in a time for which we have bounds that are uniform in ξ.

(2) If the speeds of the particles are sufficiently large, the motion is well approximated by free motion. Therefore in view of (1), it will suffice to show the following.

(3) From any initial point $\xi \in \hat{\Omega}$, the process evolves into the set on which all speeds are "fast" with a probability and in a time (i.e., number of collisions) for which we have bounds that are uniform in ξ.

In making the above precise, we proceed as follows: We first establish (2) via some approximation lemmas which imply that the actual motion is sufficiently well approximated by free motion provided the speeds are large enough. This is done by comparing the free motion with the rescaled actual motion. The time is rescaled in such a way that velocities of order unity, under the rescaled motion, correspond to large velocities in the original motion. The key to this comparison is that the rescaling greatly diminishes the strength of the interaction between particles.

We then establish (1), (a) above not only for free motion, but also for the actual motion, as long as the speeds are sufficiently large. Later in the proof we will explain how we prove (3) and (1), (b) both for free and actual motion.

4.2. The Rescaled Motion

The rescaling we exploit arises from the change of time variables $t \to \lambda t$, where λ should be regarded as small. We must consider the rescaled motion of a single particle, with position in $\Lambda \subset \mathbb{R}^3$, and the rescaled motion of our system of particles, with position in $\Lambda^N \subset \mathbb{R}^{3N}$. To handle both cases simultaneously, consider any motion $t \to q(t) \in \mathbb{R}^M$; $M = 1, 2,...$

Then the motion q_λ rescaled by λ is given by

$$q_\lambda(t) = q(\lambda t) \tag{4.1}$$

If $q(t)$ satisfies

$$\begin{aligned} \frac{dq}{dt} &= p \\ \frac{dp}{dt} &= F(q, t) \end{aligned} \tag{4.2}$$

then $q_\lambda(t)$ satisfies

$$\begin{aligned} \frac{dq_\lambda}{dt} &= p_\lambda \\ \frac{dp_\lambda}{dt} &= \lambda^2 F(q_\lambda, \lambda t) \end{aligned} \tag{4.3}$$

where

$$p_\lambda(t) = \lambda p(\lambda, t) \tag{4.4}$$

Thus under the λ rescaling, if $F = F(q)$, the vector field $X(q, p) = (p, F(q))$ is transformed into the vector field $X_\lambda(q, p) = (p, \lambda^2 F(q))$. Note that if X is $\mathscr{C}^1$, then X_λ is $\mathscr{C}^1$ in (q, p, λ).

4.3. Approximation Lemmas

Suppose $(q(t), p(t))$ is a solution of (4.2), with $F(q, t) \equiv F(t)$ depending explicitly only on t in a continuous manner. We wish to compare the λ-rescaled motion $(q_\lambda(t), p_\lambda(t))$ defined by (4.3) with the free motion $(q_0(t), p_0(t))$ given by (4.3) with $\lambda = 0$ starting from the same initial point $(\bar{q}, \bar{p})$.

In the following, $\|.\|$ refers to the Euclidian norm and $\|F\|_\infty = \sup_{0 \leqslant t < \infty} \|F(t)\|$.

Lemma 4.1. (i) $\|p_\lambda(t) - p_0(t)\| \leqslant \lambda^2 \|F\|_\infty t$, (ii) $\|q_\lambda(t) - q_0(t)\| \leqslant (\lambda^2/2) \|F_\infty\| t^2$.

Proof. The lemma follows immediately from the integral form of (4.3)

$$q_\lambda(t) = \int_0^t p_\lambda(s)\, ds$$

$$p_\lambda(t) = \lambda^2 \int_0^t F(\lambda s)\, ds \quad \blacksquare$$

Let $\mathscr{M}$ be a submanifold of $\mathbb{R}^M$ of dimension $M - 1$; τ_λ, the hitting time for $\mathscr{M}$, is given by

$$\tau_\lambda = \inf\{t > 0 : q_\lambda(t) \in \mathscr{M}\}, \qquad \lambda \geqslant 0$$

Lemma 4.2. Suppose that $\bar{q} \in \mathscr{M}$, $\bar{p}$ is transverse to $\mathscr{M}$ at $\bar{q}$, $\tau_0 < \infty$ and $p_0(\tau_0)$ is transverse to $\mathscr{M}$ at $q_0(\tau_0)$. Then the mapping $\lambda \to (q_\lambda(\tau_\lambda), p_\lambda(\tau_\lambda), \tau_\lambda)$ is continuous at $\lambda = 0$.

Proof. By Lemma 4.1 for λ sufficiently small, $q_\lambda(\tau_\lambda)$, the point of return to $\mathscr{M}$, is near $q_0(\tau_0)$ and the lemma thus follows easily. $\blacksquare$

Remark. We will use Lemmas 4.1 and 4.2 primarily for the case $M = 3$ with $\mathscr{M} \subset \partial\Lambda$.

Suppose now that $(q_\lambda(t), p_\lambda(t))$ is a solution of (4.3) with $F = F(q_\lambda)$ a $\mathscr{C}^1$ function. Let $\Phi(\lambda, q, p, t)$ be the solution map:

$$\Phi(\lambda, \bar{q}, \bar{p}, t) = (q_\lambda(t), p_\lambda(t))$$

Lemma 4.3. The map Φ is $\mathscr{C}^1$.

Proof. Let $\hat{\xi}(t) = (\lambda, q(t), p(t))$. Then $\hat{\xi}(t)$ is a solution of $d\hat{\xi}/dt = (0, p, \lambda^2 F(q))$ if $(q(t), p(t))$ satisfies (4.2). Since the vector field on the right is $\mathscr{C}^1$, it follows from the usual theorem on ODE's that $\hat{\xi}(t)$, and hence $(q(t), p(t))$, depends in a $\mathscr{C}^1$ manner on t and the initial conditions $\lambda, \bar{q}, \bar{p}$. ∎

Now let $\mathscr{M}$ be a submanifold of $\mathbb{R}^{2M}$ of dimension $2M-1$, let τ_λ be the hitting time of $\mathscr{M}$ and let $\tilde{\Phi}$ be the return map on $\mathscr{M}$ defined on the domain $\tilde{D}$ of initial points (λ, q, p) with $\xi = (q, p) \in \mathscr{M}$, $X_\lambda(\xi)$ transverse to $\mathscr{M}$ at ξ, and $X_\lambda(\xi_\lambda(\tau_\lambda))$ transverse to $\mathscr{M}$ at $\xi_\lambda(\tau_\lambda)$.

Writing $\tau(\lambda, \xi) = \tau_\lambda$ (τ_λ depends upon the initial point ξ), $\tilde{\Phi}$ is given by

$$\tilde{\Phi}(\lambda, \xi) = \Phi(\lambda, \xi, \tau(\lambda, \xi)) \tag{4.5}$$

Lemma 4.4. The map $\tilde{\Phi}$ is $\mathscr{C}^1$.

Proof. By (4.5) and Lemma 4.3 it will suffice to show that $\tau(\lambda, \xi)$ is $\mathscr{C}^1$. We may assume that there exists a real-valued function f: $\mathbb{R}^M \to \mathbb{R}$ nonsingular (i.e., $df \neq 0$) on $\mathscr{M}$, such that

$$\mathscr{M} = \{\xi \in \mathbb{R}^{2M}: f(\xi) = 0\}$$

Let $\tilde{f}(\lambda, \xi, t) = f(\phi(\lambda, \xi, t))$. $\tilde{f}$ is $\mathscr{C}^1$.

Note that τ_λ satisfies $\tilde{f}(\lambda, \xi, \tau_\lambda) = 0$. Moreover, by the continuity in λ and t of $\xi_\lambda(t)$ and the smoothness of $X_\lambda(\xi)$ in λ and ξ, it follows from the transversality at the initial point and at $\xi_\lambda(\tau_\lambda)$ that $\xi_\lambda(\tau_\lambda)$ is continuous in λ. In fact, for any $\varepsilon > 0$

$$\|\xi_\lambda(t) - \xi_{\lambda'}(t)\| \leqslant \int_0^t |X_\lambda(\xi_\lambda(s)) - X_{\lambda'}(\xi_{\lambda'}(s))| \, ds \leqslant \varepsilon \qquad \text{for } t < 1$$

and λ close to λ'. (This precludes return to $\mathscr{M}$ for small t.) By the transversality at $\xi_\lambda(\tau_\lambda)$, we have that $\partial\tilde{f}/\partial t = \partial f/\partial\xi \, d\xi/dt \neq 0$ at the point $(\lambda, \xi, \tau(\lambda, \xi))$. Hence, by the implicit function theorem, τ is a $\mathscr{C}^1$ function ∎

We now focus on the system of interest. Thus $M = 3N$ and $F = -\sum_{i,j,i \neq j} \operatorname{grad} U(q_i - q_j)$.

Recall that $\Omega = \{\xi \in (\Lambda \times \mathbb{R}^3)^N: \sum p_i \neq 0\}$ and that $\hat{\Omega}$ is the set of points $\xi \in \Omega$ for which at least one particle is in $\partial\Lambda$ and all particles in $\partial\Lambda$ have position and velocity (q, p) satisfying $n(q) \cdot p > 0$. Let $\hat{\Omega}_0$ be the set of points $\xi \in \Omega$ for which exactly one particle is in $\partial\Lambda$. If the ith particle is in $\partial\Lambda$ one writes (q_0, p_0) for its phase coordinates.

$\hat{\Omega}_0$ is a submanifold of $\hat{\Omega}$ of dimension $M-1$. Let Φ and $\tilde{\Phi}$ be defined as before, with $\mathscr{M}=\hat{\Omega}_0$. We are interested in $\tilde{\Phi}$ only on the domain $D_{\tilde{\Phi}} \subset \tilde{D}$, where $D_{\tilde{\Phi}} = \{(\lambda, \xi) \in [0, \infty] \times \Omega_0 : n(q_0) \cdot p_0 > 0, n(q_0(\tau_\lambda)) \cdot p_0(\tau_\lambda) \neq 0\}$. τ_λ is defined as $\tau_\lambda = \inf\{t : q_0(t) \in \partial \Lambda\}$, so this means that there is no multiple collision. By Lemma 4.4 $\tilde{\Phi}$ is $\mathscr{C}^1$ on $D_{\tilde{\Phi}}$.

Remark. At time τ_λ, the particle in $\partial \Lambda$ may be different from the particle in $\partial \Lambda$ at $t=0$.

We now define maps which take into account random "reflections" from $\partial \Lambda$.

Let $V=(v_1,..., v_n) \in \mathbb{R}^{3n}$ describe the velocities with which the particles leave $\partial \Lambda$ in successive collisions. A suitable choice of V determines the motion up to the time of the nth collision with $\partial \Lambda$. We wish to regard the first collision as occurring at $t=0$. Let $\bar{\Omega}_0$ be the set which describe only the position of the particle at the boundary (and not its velocity) as well as the position and velocity of the $N-1$ remaining particles. We therefore define the projection

$$\pi : \hat{\Omega}_0 \to \bar{\Omega}_0$$

Let $\psi : D_\psi \subset \bar{\Omega}_0 \times \mathbb{R}^3$ be the corresponding injection: ψ is defined on the set D_ψ of points (ξ, v) with $\xi \in \bar{\Omega}_0$ and $n(q_0(\xi)) \cdot v > 0$ and $\psi(\xi, v)$ is the point in $\hat{\Omega}_0$ for which the particle at the boundary has phase coordinates $(q_0(\xi), v)$ and all the other particles are described by the remaining coordinates of ξ. Clearly π and ψ are $\mathscr{C}^1$. We define by induction

$$\phi_n : D_n \subset [0, \infty] \times \bar{\Omega}_0 \times \mathbb{R}^{3n} \to \bar{\Omega}_0 \qquad \text{as follows:}$$

$$\phi_1(\lambda, \xi, v_1) = \psi(\xi, v_1) \qquad \text{on the domain } D_1 = [0, \infty] \times D_\psi$$

$$\phi_2(\lambda, \xi, v_1, v_2) = \psi(\pi(\tilde{\phi}(\lambda, \phi_1(\lambda, \xi, v_1))), v_2) \qquad \text{on the domain}$$

$$D_2 = \{(\lambda, \xi, v_1, v_2) : (\lambda, \xi, v_1) \in D_1, (\lambda, \phi_1(\lambda, \xi, v_1)) \in D_{\tilde{\phi}}$$
$$\text{and } (\pi(\tilde{\phi}(\lambda, \phi_1(\lambda, \xi, v_1))), v_2) \in D_\psi\}$$

$$\phi_n(\lambda, \xi, v_1,..., v_{n-1}, v_n) = \psi(\pi(\tilde{\phi}(\lambda, \phi_{n-1}(\lambda, \xi, v_1,..., v_{n-1}))), v_n)$$

on the domain

$$D_n = \{(\lambda, \xi, v_1,..., v_n) : (\lambda, \xi, v_1,..., v_{n-1}) \in D_{n-1}, (\lambda, \phi_{n-1}(\lambda, \xi, v_1,..., v_{n-1})) \in D_{\tilde{\phi}}$$
$$\text{and } (\pi(\tilde{\phi}(\lambda, \phi_{n-1}(\lambda, \xi, v_1,..., v_{n-1}))), v_n) \in D_\psi\}$$

Remark. D_n is the domain on which the phase point ξ_j after the jth collision is such that $(\lambda, \xi_j) \in D_{\tilde{\phi}}$, $j=1,..., n-1$, and $\xi_n \in \hat{\Omega}_0 \cap \hat{\Omega}$.

By induction, we have as an immediate consequence of Lemma 4.4:

Lemma 4.5. The map ϕ_n is $\mathscr{C}^1$ on D_n. ∎

We also need a continuous time version of ϕ_n. Let

$$\tilde{\phi}_n(\lambda, \xi, v_1,..., v_n, t) = \phi(\lambda, \phi_n(\lambda, \xi, v_1,..., v_n), (t - \tau_n))$$

where τ_n is the time of the nth collision.

Let $\tilde{D}_n = \{(\lambda, \xi, v_1,..., v_n, t) \in D_n \times [0, \infty]: t > \tau_n\}$ We easily obtain the following:

Lemma 4.6. The map $\tilde{\phi}_n$ is $\mathscr{C}^1$ on $\tilde{D}_n$.

Remark. By the continuity of the map ϕ_n, the D_n's are open.

We will apply Lemmas 4.5 and 4.6 to the case $n = 2N$.

4.4. Jacobian Estimates and Absolute Continuity

We will establish the existence of a nonempty open set $\Delta \subset \bar{\Omega}_0$, a nonempty open set $A \subset \bar{\Omega}_0$, and a $\delta > 0$ such that

$$\Pi^{2N}(\eta, d\xi) \geqslant \delta\, 1_A(\xi)\, d\xi \qquad \text{for all} \quad \eta \in \Delta$$

where Π is a Markov kernel on $\bar{\Omega}_0$. (The P and the Π are related in an obvious manner.) We do this by establishing a similar result for the rescaled motion. For this purpose, let η_0 be a point of $\bar{\Omega}_0$ such that there exists a choice $V_0 \equiv (V_1^{(0)},..., V_{2N}^{(0)}) = (u_0, v_0)$, $u_0 = (u_1^{(0)},..., u_N^{(0)})$, $v_0 = (v_1^{(0)},..., v_N^{(0)})$ for which $(0, \eta_0, V_0) \in D_{2N}$ and each particle collides with $\partial \Lambda$ exactly twice under the motion arising from V_0 starting from η_0 with the ith particle at $\partial \Lambda$ at the ith and the $N + i$th collision. Since D_{2N} is open, there exists an open set

$$\tilde{\mathscr{N}} = \tilde{\mathscr{O}}_0 \times \tilde{\Lambda} \times \mathscr{O}_{V_0}$$

satisfying $(0, \eta_0, V_0) \in \tilde{\mathscr{N}} \subset D_{2N}$.

By shrinking $\tilde{\mathscr{O}}_0$, $\tilde{\Lambda}$, and $\mathscr{O}_{V_0}$, if necessary, we may assume that the closure of $\tilde{\mathscr{N}} \subset D_{2N}$, and that it is compact. We assume that $\tilde{\mathscr{N}}$ has been chosen small enough so that the ith particle is on $\partial \Lambda$ at the ith and the $N + i$th collision for all $(\lambda, \eta, V) \in \tilde{\mathscr{N}}$. Since the Nth particle must "spread" in only $2N - 1$ dimensions, we write $u_N = (\sigma_N, \rho)$ in spherical coordinates and $u_N^{(0)} = (\sigma_N^{(0)}, \rho^{(0)})$; $\sigma_N = u_N / |u_N|$ is a point on the unit sphere and $\rho = |u_N|$.

Set $\tilde{V} = (u_1,..., u_{N-1}, \sigma_N, v_1,..., v_N)$, so that $V = (\tilde{V}, \rho)$ and write

$$\bar{\Phi}(\lambda, \rho, \eta, \tilde{V}) = \Phi_{2N}(\lambda, \eta, V)$$

We may assume that $\mathcal{O}_{V_0} = \mathcal{O}_{\tilde{V}_0} \times \mathcal{O}_{\rho^{(0)}}$ in the $(\tilde{V}, \rho)$ coordinates, and that $\mathcal{U} = \mathcal{O}_{\tilde{V}_0}$ is an open disk. By Lemma 4.6 $\bar{\Phi}$ is $\mathscr{C}^1$ on

$$\tilde{\mathcal{N}} = \tilde{\mathcal{O}}_0 \times \mathcal{O}_{\rho^{(0)}} \times \tilde{\Delta} \times \mathcal{U}$$

Define $\Phi_{\lambda,\rho,\eta}\colon \mathcal{U} \to \mathscr{A}_{\lambda,\rho,\eta} \equiv \Phi_{\lambda,\rho,\eta}(\mathcal{U})$ for $\lambda \in \tilde{\mathcal{O}}_0$, $\rho \in \theta_{\rho^{(0)}}$, and $\eta \in \tilde{\Delta}$ by

$$\Phi_{\lambda,\rho,\eta}(\tilde{V}) = \bar{\Phi}(\lambda, \rho, \eta, \tilde{V})$$

We wish to estimate the normalized Jacobian determinant $J_{\lambda,\rho,\eta}(\tilde{V})$ of $\Phi_{\lambda,\rho,\eta}$.

By this we mean the following. $\hat{\Omega}$ and $\{\tilde{V}\}$ have natural geometrical measures: $d\xi$, "Lebesgue measure," on $\hat{\Omega}$ and $du_1,..., du_{N-1}$, $d\sigma_N$, $dv_1,..., dv_N$ for $\{\tilde{V}\}$, where $d\sigma_N$ is the solid angle measure (surface area of the unit sphere).

Similarly for any funtion described in coordinates $x \to y$ by $y_u(x_1,..., x_m)$, $i = 1,..., m$ the normalized Jacobian $J(y; x) = \partial(y_1,..., y_m)/\partial(x_1,..., x_m)$ satisfies $dy = J(y; x)\, dx$, where dy and dx are the measures geometrically appropriate to the coordinates. $J_{\lambda,\rho,\eta}$ satisfies

$$d\xi = J_{\lambda,\rho,\eta}(\tilde{V})\, d\tilde{V} \qquad \text{for} \quad \xi = \Phi_{\lambda,\rho,\eta}(\tilde{V})$$

Since $\Phi_{\lambda,\rho,\eta}$ is a $\mathscr{C}^1$ map depending continuously on λ, ρ, η, it follows that $J_{\lambda,\rho,\eta}(\tilde{V})$ is a continuous function of $\lambda, \rho, \eta, \tilde{V}$. We estimate it by perturbing around $\lambda = 0$. Let $\Phi_0 = \phi_{0,\rho^{(0)},\eta_0}$, let $\mathscr{A}_0 = \mathscr{A}_{0,\rho^{(0)},\eta_0}$, and $J_0 = J_{0,\rho^{(0)},\eta_0}$.

Lemma 4.7. $\Phi_0\colon \mathcal{U} \to \mathscr{A}_0$ is a $(\mathscr{C}^1)$ diffeomorphism. Moreover there exist constants c_1, c_2, $0 < c_1 < \infty$, $0 < c_2 < \infty$ such that

$$c_1 \leqslant J_0(\tilde{V}) \leqslant c_2 \qquad \text{for all} \quad \tilde{V} \in \mathcal{U}$$

Proof. It is obvious that Φ_0 is a $\mathscr{C}^1$ bijection. It remains to compute the Jacobian. For this purpose we will sometimes use "special flow" coordinates for a point $(q, p) \in \Lambda \times \mathbb{R}^3$

$$(q, p) \leftrightarrow (\bar{\bar{q}}, s, p) \qquad \text{where} \quad \bar{\bar{q}} \in \partial\Lambda,\ s > 0, \qquad \text{and} \quad q = \bar{\bar{q}} + sp$$

We will use "spherical coordinates" to describe $u_i = (\sigma_i, \rho_i)$. We wish to compute the normalized Jacobian determinant $J(q_1,..., \bar{\bar{q}}_N, p_1,..., p_N; u_1,..., u_{N-1}, \sigma_N, v_1,..., v_N)$ for the map Φ_0. Under Φ_0, $(\bar{\bar{q}}_N, p_N)$ depends only upon (σ_N, v_N), while (q_i, p_i) depends only on (u_i, v_i) $i = 1,..., N-1$

and on (σ_N, v_N). Therefore J_0 is upper block triangular, with blocks corresponding to the particles, so that

$$J_0 = \prod_{i=1}^{N} J_0^{(i)} \qquad \text{where} \quad J_0^{(i)} = J(q_i, p_i; u_i, v_i), \qquad i = 1,..., N-1$$

and

$$J_0^{(N)} = J(\bar{\bar{q}}_N, p_N; \sigma_N, v_N)$$

But, since $(q_i, p_i) \leftrightarrow (\bar{\bar{q}}_i, s_i, p_i)$ and $(u_i) \leftrightarrow (\sigma_i, \rho_i)$ $i = 1,..., N-1$, we have that $p_i = v_i$, $i = 1,..., N$, $\bar{\bar{q}}_i$ depends only on σ_i, and s_i depends only on (σ_i, ρ_i) (as well as on σ_N).

Thus, for $i = 1,..., N-1$:

$$dq_i\, dp_i = p_i \cdot n(\bar{\bar{q}}_i)\, d\bar{\bar{q}}_i\, ds_i\, dp_i = J_0^{(i)}\, du_i\, dv_i$$

and

$$J_0^{(i)} = v_i \cdot n(\bar{\bar{q}}_i) \left|\frac{\partial \bar{\bar{q}}_i}{\partial \sigma_i}\right| \cdot \left|\frac{\partial s_i}{\partial \rho_i}\right| \cdot \left|\frac{\partial(\sigma_i, \rho_i)}{\partial u_i}\right|$$

Let $\bar{q}_i$ be the position the ith particle at the first of its two collisions with $\partial \Lambda$. Then

$$\left|\frac{\partial \bar{\bar{q}}_i}{\partial \sigma_i}\right| = \frac{|\bar{q}_i \bar{\bar{q}}_i|^3}{n(\bar{\bar{q}}_i) \cdot \bar{q}_i \bar{\bar{q}}_i}, \qquad \left|\frac{\partial s_i}{\partial \rho_i}\right| = \frac{|\bar{q}_i \bar{\bar{q}}_i|}{\rho_i^2}\ (\bar{q}_i \bar{\bar{q}}_i = \bar{\bar{q}}_i - \bar{q}_i)$$

and $du_i = \rho_i^2\, d\sigma_i\, d\rho_i$.

We thus obtain that

$$J_0^{(i)} = \frac{v_i \cdot n(\bar{\bar{q}}_i)}{\bar{q}_i \bar{\bar{q}}_i \cdot n(\bar{\bar{q}}_i)} \cdot \frac{|\bar{q}_i \bar{\bar{q}}_i|^4}{\rho_i^4}, \qquad i = 1,..., N-1$$

and similarly

$$J_0^{(N)} = \frac{|\bar{q}_N \bar{\bar{q}}_N|^3}{\bar{q}_N \bar{\bar{q}}_N \cdot n(\bar{\bar{q}}_N)}. \quad \blacksquare$$

Lemma 4.8. There exist open sets Δ', $\mathcal{O}'_{\rho^{(0)}}$, and $\mathcal{O}_0$ with $\eta_0 \in \Delta' \subset \tilde{\Delta}$ $\rho^{(0)} \in \mathcal{O}'_{\rho^{(0)}} \subset \mathcal{O}_{\rho^{(0)}}$ and $0 \in \mathcal{O}_0 \subset \tilde{\mathcal{O}}_0$ such that $\Phi_{\lambda,\rho,\eta}\colon \mathcal{U} \to \mathcal{A}_{\lambda,\rho,\eta}$ is a diffeomorphism for all $\lambda \in \mathcal{O}_0$, $\rho \in \mathcal{O}'_{\rho^{(0)}}$, and $\eta \in \Delta'$. There exists a constant C, $0 < C < \infty$ such that

$$J_{\lambda,\rho,\eta}(\tilde{V}) \leqslant C \tag{4.6}$$

for all $\lambda \in \mathcal{O}_0$, $\rho \in \mathcal{O}'_{\rho^{(0)}}$, $\eta \in \Delta'$, and $\tilde{V} \in \mathcal{U}$. Moreover $\mathcal{A}'$, defined as the interior of the intersection for $\lambda \in \mathcal{O}_0$, $\eta \in \Delta'$, $\rho \in \mathcal{O}'_{\rho^{(0)}}$ of $\mathcal{A}_{\lambda,\rho,\eta}$, is nonempty.

Proof. Since Φ is $\mathscr{C}^1$ on $\mathcal{N}$, for every $\varepsilon > 0$ there exist open sets Δ', $\mathcal{O}'_{\rho^{(0)}}$ and $\mathcal{O}_0$ with $\eta_0 \in \Delta' \subset \Delta$, $\rho^{(0)} \in \mathcal{O}'_{\rho^{(0)}} \subset \mathcal{O}_{\rho^{(0)}}$, $0 \in \mathcal{O}_0 \subset \tilde{\mathcal{O}}_0$ such that for $\lambda \in \mathcal{O}_0$, $\rho \in \mathcal{O}'_{\rho^{(0)}}$, and $\eta \in \Delta'$

$$\sup_{\tilde{V} \in \mathcal{U}} |\Phi_{\lambda,\rho,\eta}(\tilde{V}) - \Phi_0(\tilde{V})| < \varepsilon \tag{4.7}$$

and

$$\sup_{\tilde{V} \in \mathcal{U}} \left\| \frac{\partial \phi_{\lambda,\rho,\eta}}{\partial \tilde{V}} - \frac{\partial \phi_0}{\partial \tilde{V}} \right\| < \varepsilon \tag{4.8}$$

where $\| \ \|$ denotes the sup$| \ |$ over all matrix elements (of the difference of two Jacobian matrices). From (4.8) and Lemma 4.7, it follows that for ε sufficiently small $\mathcal{A}'$ is nonempty, since $\mathcal{A}'$ contains all points of $\mathcal{A}_0$ at a distance greater than ε from the boundary of $\mathcal{A}_0$. ∎

Now choose any $\lambda_0 \in \mathcal{O}_0$ and let $\mathcal{V} = \mathcal{U}/\lambda_0$, $\Delta = \Delta'/\lambda_0$ $\tilde{\mathcal{O}}_{\rho^{(0)}} = \mathcal{O}'_{\rho^{(0)}}/\lambda_0$, $\mathcal{A} = \mathcal{A}'/\lambda_0$. Here $\cdot/\lambda_0$ indicates scaling the velocities by λ_0; e.g., $\mathcal{A} = \{(q, p/\lambda_0): (q, p) \in \mathcal{A}'\}$. For any $\rho \in \tilde{\mathcal{O}}_{\rho^{(0)}}$ and $\eta \in \Delta$ let $\mu_{\rho,\eta}$ be the image under $\Phi_{1,\rho,\eta}(\lambda = 1$ corresponds to the actual unscaled motion) of the measure $d\tilde{V}$ on $\mathcal{V}$.

Lemma 4.9. For all $\rho \in \tilde{\mathcal{O}}_{\rho^{(0)}}$ and $\eta \in \Delta$

$$\mu_{\rho,\eta}(d\xi) \geqslant \frac{1}{C\lambda_0^{3(N-1)}} 1_{\mathcal{A}}(\xi)\, d\xi$$

where C is as in Lemma 4.8.

Proof. This is an immediate consequence of Lemma 4.8 and the fact that $\phi_{1,\rho/\lambda_0,\eta/\lambda_0}(\tilde{V}) = \Phi_{\lambda_0,\rho,\eta}(\lambda_0 \tilde{V})/\lambda_0$ for all $\rho \in \mathcal{O}'_{\rho^{(0)}}$, $\eta \in \Delta'$, and $\tilde{V} \in \mathcal{V}$. ∎

For $\eta \in \Delta$ let μ_η be the image under the map $V = (\tilde{V}, \rho) \to \Phi_{1,\rho,\eta}(\tilde{V})$ of the measure $dV(dV = \rho^2 d\tilde{V} d\rho)$ on the set, in $\tilde{V}$, ρ coordinates, $\mathcal{V} \times \tilde{\mathcal{O}}_{\rho^{(0)}}$.

Lemma 4.10. For all $\eta \in \Delta$

$$\mu_\eta(d\xi) \geqslant \frac{\sigma}{C\lambda_0^{3N}} 1_{\mathcal{A}}(\xi)\, d\xi$$

where $0 < \sigma = \int_{\mathcal{O}'_{\rho^{(0)}}} \rho^2\, d\rho = \lambda_0^3 \int_{\mathcal{O}_{\rho^{(0)}}} \rho^2\, d\rho$.

Proof:

$$\mu_\eta = \int_{\tilde{\mathcal{O}}_{\rho^{(0)}}} \rho^2\, d\rho\, \mu_{\rho,\eta}. \quad ∎$$

Lemma 4.11. There exists a $\delta > 0$ such that

$$\Pi^{2N}(\eta, d\xi) \geqslant \delta\, 1_{\mathscr{A}}(\xi)\, d\xi \tag{4.9}$$

for all $\eta \in \Delta$.

Proof. Let $\gamma_1 = \sup\{|V|: \lambda_0 V \in \mathcal{O}_{V_0}\} < \infty$ and $\gamma_2 = (1/\lambda_0) \inf\{V_i \cdot n(\tilde{q}_i): i = 1,..., 2N,\ \eta \in \Delta',\ V \in \mathcal{O}_{V_0}\}$, where $\tilde{q}_i$ is the position of the particle at $\partial\Lambda$ after the ith collision. Note that γ_2 is strictly positive. Then (4.9) follows from Lemma 4.10 by taking into account the expression for $R_{\beta(q)}$; we obtain (4.9) with $\delta = \gamma_3 \gamma_2^{2N} e^{-b\gamma_1^2/2}(\sigma/\lambda_0^{3N})$. ∎

4.5. Completion of the Proof

Recall now that Δ was constructed as a small neighborhood of a point $\eta_0 \in \bar{\Omega}_0$ provided this point satisfied a certain number of conditions which involve only the free motion and are therefore purely geometrical in nature. (These conditions in particular enable us to construct also the set A and to compute δ.)

We will prove in Lemma 5.1 the existence of a point $q_0 \in \partial\Lambda$ such that the surface near q_0 looks like a "piece of sphere." From this, we can construct an η_0 that satisfies our assumptions as follows: because of the properties of $\partial\Lambda$ at q_0, we know that the surface near q_0 is close to the osculating ellipsoid at q_0 so that there exist at least two points $\bar{q}$ and $\bar{\bar{q}}$ of $\partial\Lambda$ such that the segments $\bar{q}q_0$ and $\bar{\bar{q}}q_0$ are contained in $\mathring{\Lambda}$ and the tangent planes at $\bar{q}$, q_0, and $\bar{\bar{q}}$ are transverse to the directions $\bar{q}q_0$ or $\bar{\bar{q}}q_0$. We then set the positions of the particles in η_0 as $(q_0, q_1,..., q_{N-1})$ with all q_i's on the segment $\bar{q}q_0$; we also take for common direction of the velocities $(u_0^0,..., u_{N-1}^0)$ the direction $\bar{q}q_0$ and choose the speeds so that the order of the collisions is the one prescribed for η_0. The direction of $(v_0^0,..., v_{N-1}^0)$ is chosen equal to $q_0\bar{\bar{q}}$ and the speeds similarly adjusted.

Now it remains to prove steps (3) and (1), (b) of Section 4.1 for the actual as well as free motion. We proceed as follows: we prove (3), i.e., that for any K there exist an integer n and an $\alpha > 0$ such that for every $\xi \in \hat{\Omega}$ $P^n(\xi, \mathscr{H}_K) > \alpha$, where $\mathscr{H}_K$ is the set of configurations of $\hat{\Omega}$ for which all particles have velocity larger than K.

Then we prove that there exist an integer m and an $\bar{\alpha} > 0$ such that for every $\xi \in \mathscr{H}_K$, $P^m(\xi, \Delta) > \bar{\alpha}$.

Lemmas 4.12, 4.13, and 4.14 below imply this last proposition and Lemma 4.15 completes step (3). In the proofs the reader should bear in mind the approximation lemmas.

Let N_ε be a small enough neighborhood of $\bar{q}$ obtained by looking at all points q of Λ such that $n(\bar{q})\cdot q \leqslant n(\bar{q})\cdot \bar{q}+\varepsilon$ for ε small enough. Moreover let Γ be the set of points $\xi \in \bar{\Omega}_0$ such that for all i $q_i \in N_\varepsilon$ and if $q_i \notin \partial\Lambda$ then $n(\bar{q})\cdot p_i < 0$ and $|p_i| > K_2$. We have the following:

Lemma 4.12. Suppose that there exist an integer M and a constant α_1 such that for all configurations $\xi_0 \in \bar{\Omega}_0$ there exists an integer $m(\xi_0)$ such that $\Pi^{m(\xi_0)}(\xi_0, \Gamma) \geqslant \alpha_1$. Then for a certain constant $\bar{\alpha} > 0$ and for all $\xi_0 \in \hat{\Omega}$

$$P^{M+N}(\xi_0, \Delta) \geqslant \bar{\alpha} \tag{4.10}$$

Proof. Of course, the problem is to have exactly $M+N$ collisions, since to end up in Δ one needs only to aim at q_0 with correct velocities. To get the desired number of collisions, send the particle hitting at the $[m(\xi_0)]$th collision to and fro between $\bar{q}$ and q_0 until it has made the necessary number of collisions. The condition on the curvature at $\bar{q}$ allows us to avoid any problem of periodicity. Also choose the velocities after the extra collision of this last particle to be so large that the real time necessary to perform these collisions is so small that the first particles hardly moved. ∎

Define for K_3 large enough $\mathscr{Y}_{K_3}$ to be the set of configuration $\xi \in \hat{\Omega}$ such that the velocities of all particles that are not on $\partial\Lambda$ is larger than K_3. Then, provided K_3 is large enough, we have the following.

Lemma 4.13. Suppose that there exist an integer $\bar{M}$ and an $\alpha_2 > 0$ such that for all $\xi \in \bar{\Omega}_0$ there exists an $m_0(\xi) \leqslant \bar{M}$ for which $\Pi^{m_0(\xi)}(\xi, \mathscr{Y}_{K_3}) \geqslant \alpha_2$. Then there exist an integer M and $\alpha_1 > 0$ such that for an $m(\xi) \leqslant M$

$$\Pi^{m(\xi)}(\xi, \Gamma) \geqslant \alpha_1 \tag{4.11}$$

Proof. Recall that to be in Γ a configuration must fulfill the following conditions:

$$n(\bar{q})\cdot q_i \leqslant n(\bar{q})\cdot \bar{q}+\varepsilon, \qquad i=1\cdots N \tag{4.12a}$$

and

$$n(\bar{q})\cdot p_i < 0,\ |p_i| \geqslant K_2, \qquad \text{if} \quad q_i \notin \partial\Lambda \tag{4.12b}$$

It is easy to fulfill (4.12) by shooting the particles from any "good point" (see definition in Section 5), for instance, from q_0, with large enough velocities. However to fulfill (4.12a) it is sufficient to restrict these velocities to a range $[K_2, K_2']$ so that the delay between the first and the last particle is controlled, provided all the particles start from q_0 at almost the same moment. It is indeed enough to know that, given a neighborhood of q_0, under approximate free motion a particle goes from any point of the boundary to this neighborhood in a bounded number ν of collisions with uniformly bounded below probability (Lemma 5.3). Indeed the claim follows by imposing on each particle a velocity large than K_4 and the total delay at q_0 is less than $2(L/K_4 + L/K_3)$. (L is the width of the box.)

It now remains to prove that our system evolves into a set in which all particles are fast in a time and with a probability which are uniform in ξ.

We will first set some notations (see Fig. 1):

1. Choose a unit vector u for which Lemma 4.1 holds. Call q_M (resp. q_m) the corresponding point of $\partial\Lambda$ which realizes $\sup_{q\in\partial\Lambda} u\cdot q$ (resp. $\inf_{q\in\partial\Lambda} u\cdot q$) and R the distance $q_M q_m$.

2. For $\lambda > u\cdot q_m$ define

$$A_\lambda = \{q\in\Lambda : u\cdot q>\lambda\}$$

3. For $u\cdot q_m < \nu < \mu < u\cdot q_M$ define

$$S_{\mu,\nu} = \{q\in\Lambda : \nu\leqslant u\cdot q\leqslant\mu\}$$

and

$$\sum_{\mu,\nu} = \{q\in\partial\Lambda : \nu\leqslant q\cdot u\leqslant\mu\}$$

We further restrict μ and ν to be close enough to $u\cdot q_m$ so that $\sum_{\mu,\nu}$ does not contain any point of an inner boundary.

4. For any $\lambda > u\cdot q_m$ define the function

$$\varphi_\lambda(q) = \sum_{i=1}^{N} (u\cdot q_i - \lambda)\, 1_{A_\lambda}(q_i)$$

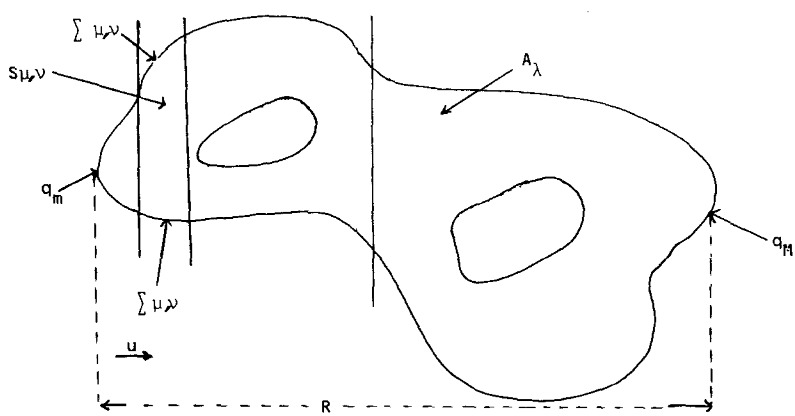

Figure 1

Notice that until a particle in A_λ hits the wall this function is continuous under the mechanical motion, and moreover its right derivative in time exists and is equal to $\varphi_\lambda(q, p) = \sum p_i \cdot u \, 1_{A_\lambda}(q_i)$.

It has a finite number of positive jumps, since particles leaving and entering A_λ contribute a nonnegative quantity.

In each of the intervals between the jumps, the function ψ_λ itself has a derivative equal to

$$\psi'_\lambda = -\sum_{i \neq j} 1_{A^c_\lambda(q_i)} 1_{A_\lambda(q_j)} U'(|q_i - q_j|) \frac{(q_j - q_i) \cdot u}{|q_j - q_i|}$$

This function is nonnegative and if we define for $\lambda > \mu$

$$\alpha(\lambda, \mu) = \inf_{q_1 \in A^c_\mu, q_2 \in A_\lambda} |U'(|q_2 - q_1|)| \frac{(q_2 - q_1) \cdot u}{|q_2 - q_1|}$$

which is strictly positive by the long-range assumption, a lower bound for this function ψ'_λ is

$$\alpha(\lambda, \mu) \left[\sum 1_{A_\lambda}(q_i) \right] \left[\sum 1_{A^c(q_i)} \right]$$

Therefore if we force the fast particle to remain in A^c_μ, ϕ_λ satisfies

$$\phi_\lambda(t) \geqslant \phi_\lambda(0) + \psi_\lambda(0) \, t + \alpha(\lambda, \mu) \, t^2/2$$

until a collision occurs in A_λ or all the particles leave A_λ. Besides note that the function ϕ_λ must remain smaller than $N(R - \lambda)$ (otherwise one of the particles would be outside our region). In this sense $(R - \lambda) N$ is the critical value for ϕ_λ.

Lemma 4.14. For all μ and v close enough to $u \cdot q_m$, every $T > 0$, and all k_4, there exist an integer $\tilde{n}$ and an $\alpha_3 > 0$ such that if a particle is colliding in $\sum_{\mu,v}$ at time 0, then the probability that it will remain in $S\mu,v$ up to time T, having less than $\tilde{n}$ collisions and keeping a velocity larger than k_4, is larger than α_3.

Proof. By choosing μ and v close enough to $u \cdot q_m$, we can ensure by Lemma 5.1 that $\sum_{\mu,v}$ looks like a "slice of sphere."

From any point of $\sum_{\mu,v}$, we can therefore "aim" at $\sum_{\mu,v}$. By choosing the direction σ of the post collision velocity at site q in the cone $u \cdot n(q) \geqslant \gamma$ for any given $\gamma > 0$ and the speed p between two constants k_5 and k_6 large enough, we bound away uniformly from zero the time it takes before the next recollision of this fast particle while uniformly controlling the probability of these events. ∎

We observe now that because $\sum p_i \neq 0$, one particle will hit the boundary in a finite time (that we do not control). We have the following:

Lemma 4.15. For any given k_4, there exist an integer n and an $\alpha_4 > 0$, such that for any configuration $\xi \in \bar{\Omega}_0$, the probability that at a collision before the nth collision all the particles have velocity larger than k_4 is larger that α_4.

Proof. The proof will be by induction on the number of fast particles one can create. Of course the probability that the particle initially at $\partial\Lambda$ bounces off with a velocity larger than a given k_5 is bounded away from zero independently of the hitting place. We will now explain how a particle should move, according to the state of the system, to create another collision. For this purpose, we define

$$U_1^\lambda = \{\xi : \varphi_\lambda(q) > 0, \psi_\lambda(\xi) \geqslant 0\}$$
$$U_2^\lambda = \{\xi : \varphi_\lambda(q) > 0, \psi_\lambda(\xi) \leqslant -\bar{K}\}$$
$$U_3^\lambda = \{\xi : \varphi_\lambda(q) > 0, -\bar{K} \leqslant \psi_\lambda(\xi) < 0\}$$
$$U_4^\lambda = \{\xi : \varphi_\lambda(q) = 0\}$$

and we will choose $\bar{K}$ such that a particle with initial velocity $\bar{K}/N$ will travel a distance at least R in the direction of its initial velocity against any force applied to it by the other $(N-1)$ particles. In this case the time needed to travel this far is bounded. We will now take $v < \mu < \lambda$, and these values will be fixed later. When the first particle to collide hits the boundary we take it to $\sum_{\mu,v}$ using Lemma 5.3.

If no collision (of another particle) occurred by this time, compute φ_λ and ψ_λ at the moment when the fast particle first hits $\sum_{\mu,v}$.

If we are in U_1^λ, then by the remark following the definition of φ_λ and ψ_λ, use Lemma 4.14 to keep the fast particle in $S_{\mu,v}$. By doing so we will have a collision in A_λ before the time necessary for φ_λ to reach its critical value (which is bounded). Thus the number of collisions of the fast particle is bounded and the probability is uniformly bounded away from zero.

If we are in U_2^λ, then at least one particle has a velocity p such that $u \cdot p \leqslant -\bar{K}/N$, so that also another collision must occur.

If we are in U_3^λ, then after a fixed time determined by $\bar{K}$ (provided we keep the fast particle in $S_{\mu,v}$) ψ_λ must be nonnegative unless another particle collided. Therefore we end up either in U_1^λ or in U_4^λ.

We therefore only need to consider the case when the configuration is in U_4^λ, which means that all the particles are in A_λ^c. At this point compute k_λ such that if a particle has velocity p satisfying $u \cdot p \geqslant k_\lambda$, independently of its position in A_λ^c and against any force applied to it by the $(N-1)$ other particles it will enter A_λ. The time t_λ needed for that to happen is bounded. It is easy to see that both k_λ and t_λ tend to zero as λ tends to $u \cdot q_m$.

If one of the particles (different form the fast one) satisfies $u \cdot p \geqslant k_\lambda$ then we end up in U_1^λ.

Now if all the slow particles satisfy $u \cdot p \leqslant k_\lambda$, we will define new functions $\bar{\varphi}$ and $\bar{\psi}$ analogous to φ and ψ but constructed near q_M, instead of near q_m. For ρ close to $u \cdot q_M$

$$B_\rho = \{q \in \Lambda : u \cdot q \leqslant \rho\}$$

and

$$\bar{\varphi}_\rho(q) = \sum_{i=1}^{N} (\rho - u \cdot q_i)\, 1_{B_\rho}(q_i)$$

so that the critical value for this function is now $(N-1)(\rho - u \cdot q_m)$. Its value is initially larger than $(N-1)(\rho - \lambda)$, which is close to the critical value, and by moving rapidly the fast particle to B_ρ^c we do not much alter this initial value. Besides, $\bar{\psi}_\rho$ is larger than $-(N-1)\, k_\lambda$ and is also only slightly perturbed by the time the fast particle gets to B_ρ^c.

Of course we might be in a situation of the type $\bar{U}_2$ for $\bar{\varphi}$, but we will argue now that by an appropriate choice of λ we cannot end up in $\bar{U}_4$. The reason for this is that because all the particles are close to q_m and have small velocities, the time necessary (in the worst possible case) for a particle to escape from B_ρ is bounded below, while the time necessary for $\bar{\varphi}_\rho$ to reach its critical value tends to zero as λ tends to $u \cdot q_m$. This proves the lemma. ∎

Lemmas 4.15, 4.14, 4.13, 4.12, and 4.11 imply Theorem 3.3, in view of the obvious relation between Π and P.

Let Π_t be the continuous time kernel on $\bar{\Omega}_0$. Then by an argument very similar to the proof of Lemma 4.11, using Lemma 4.6 and letting (η, t) play the role previously played by η, we obtain the following.

Lemma 4.16. There exist a time t_0, an interval I_0 around t_0, a nonempty open set $\bar{A} \subset \bar{\Omega}_0$, and a $\delta > 0$ such that

$$\Pi_t(\eta, d\xi) \geqslant \delta 1_{\bar{A}}(\xi)\, d\xi$$

for all $\eta \in \Delta$, $t \in I_0$. Here $d\xi$ is the usual Lebesgue measure on $\mathbb{R}^{6N}$.

Proof of Theorem 3.4. Lemmas 4.15, 4.14, 4.13, 4.12, and 4.16 imply Theorem 3.4, in view of the obvious relation between Π and P. ∎

5. GEOMETRICAL LEMMAS

We used in the proof of Lemma 4.14 that there exists a direction u such that if q_M (resp. q_m) denotes the point of $\partial \Lambda$ which realizes the supremum of $u \cdot q$ for $q \in \partial \Lambda$ (resp. the infimum), there exists a "stripe" $S_{\mu,v}$ for all μ and v close enough to $u \cdot q_m$ but different from the supremum of $u \cdot q$ (resp. the infimum), such that a particle can bounce to and fro inside this stripe.

Of course if we can find a direction u such that at both q_M and q_m the quadratic forms appearing in the Taylor expansion of the surface at these points are nondegenerate, the planes tangent to the surface at a point of a neighborhood of both q_M and q_m are close to the planes tangent to the osculating ellipsoid. The existence of such a direction is proved in Lemma 5.1 below.

Lemma 5.1. Let $\partial \Lambda$ be a finite disjoint union of $\mathscr{C}^2$-compact submanifolds of $\mathbb{R}^3$. Then for almost all directions u the surface at q_M and q_m is nondegenerate.

Proof. The problem is local so by taking an open covering of $\partial \Lambda$ we can consider that our surface is given by an application $F\colon \mathbb{R}^2 \to \mathbb{R}^3$. Consider now the subset A of $\mathbb{R}^2 \times \mathbb{R}^3$ of those (x, u) such that the tangent plane to $\partial \Lambda$ at $F(x)$ is orthogonal to u. This is a $\mathscr{C}^1$ submanifold of $\mathbb{R}^5$ of dimension 3, a parametrization of which is given by $\varphi\colon (x, \lambda) \in \mathbb{R}^2 \times \mathbb{R} \to [x, \lambda n(F(x))]$. Of course for any direction u of $\mathbb{R}^3$, the points $(F^{-1}(q_M), u)$ and $(F^{-1}(q_m), u)$ belong to this submanifold. Introduce now the application $\pi\colon A \to \mathbb{R}^2$ which is the restriction to A of the canonical projection of $\mathbb{R}^2 \times \mathbb{R}^3$ on $\mathbb{R}^3$, and note that $\pi \circ \varphi$ is an application from $\mathbb{R}^3 \to \mathbb{R}^3$ which is of maximal rank if and only if $\pi \circ \varphi\colon (a, b, \lambda) \to (a, b, \lambda n(F(a, b)))$ is such that $[n(F(a, b)), \partial n/\partial a, \partial n/\partial b]$ have a nonvanishing determinant. An easy computation shows that this last condition is equivalent to the quadratic form at $F(x)$ being nondegenerate. Since $\pi \circ \varphi$ is $\mathscr{C}^1$, it follows from Sard's Lemma[5] that the set of directions for which the quadratic form at q_M or q_m is degenerate has zero Lebesgue measure. ∎

Let Λ be as in the assumptions of Theorem 3.1. Define an admissible trajectory from x to y (both in $\partial \Lambda$) as a path contained in Λ that links x to y, made of straight lines inside $\mathring{\Lambda}$ and changing direction only at the points on $\partial \Lambda$, but such that at a point on $\partial \Lambda$ both the incoming and the outgoing directions are not tangential to $\partial \Lambda$. An outgoing direction which is not tangential will be called a good direction.

Lemma 5.2. For every pair of points x and y in $\partial\Lambda$ there exists an admissible trajectory linking x to y.

Proof. We introduce the following relation: $x\mathscr{R}y \Leftrightarrow x$ is linked to y by an admissible trajectory. Of course $x\mathscr{R}y$ if and only if $y\mathscr{R}x$ and also $x\mathscr{R}y$ and $y\mathscr{R}z$ imply $x\mathscr{R}z$. We want to prove $x\mathscr{R}x$ (which is not obvious since constant trajectories are not admissible). Now by Sard's lemma, there exists a point z on the boundary such that the line $\overline{xz}$ is in $\mathring{\Lambda}$ and the direction xz is good for both x and z. We therefore have $x\mathscr{R}z$ and $z\mathscr{R}x$ hence $x\mathscr{R}x$. So $\mathscr{R}$ is an equivalence relation. Besides it is easy to see that if $x\mathscr{R}y$ then for all y' close enough to y we also have $x\mathscr{R}y'$. Indeed take an admissible trajectory from x to y and by slightly perturbing the last good direction we can reach any point in a neighborhood of y. Since $\mathscr{R}$ is an equivalence relation we see that any connected component of the boundary is either made of points all $\mathscr{R}$ equivalent to a given x_0 or that no point of this component is $\mathscr{R}$ equivalent to x_0. It remains to prove that the second case cannot occur if $\mathring{\Lambda}$ is connected. We will prove that the equivalence class (denoted by C_1) of the outer boundary is all $\partial\Lambda$. Argue by contradiction and assume that C_2 is the union of all the equivalence classes different from C_1. Take any direction u and define m as the point of C_2 such that $u\cdot x$ is maximized at m when x varies in C_2. Look now at the half-space $H=\{y\in\mathbb{R}^3: u\cdot y>u\cdot m\}$. Because $\mathring{\Lambda}$ is connected the intersection of this half-space with $\mathring{\Lambda}$ must contain $H\cap\{y: \|y-m\|\leqslant\varepsilon\}$ for a small ε. (This means that Λ^c is around m at the left of m and not at the right of it; otherwise there would be another point in the same connected component containing m further to the right.) Therefore the point m satisfies $m\mathscr{R}z$ at least on z of C_1. This proves that C_2 is empty.

Consider now the stochastic motion of a single particle, initially at $x\in\partial\Lambda$, defined by the probability kernel $\mathscr{R}_{\beta(q)}(dv)$ and the force $F\equiv F(t, x, v_0, v_1,...)$: the particle leaves $x=X_0$ with velocity v_0 and moves under the influence of F until it again reaches $\partial\Lambda$, at X_1, where it acquires a new velocity v_1 with distribution $\mathscr{R}_{\beta(X_1)}(dv)$, and so on. Suppose that if the $(m+1)$th collision with $\partial\Lambda$ has not yet occurred by time t then $F(t,...)$ depends only upon x and $v_1,..., v_m$.

Let $\Xi=(\mathbb{R}^3)^\infty=\{\xi=(v_0, v_1,...)\}$. For given x and F a point $\xi\in\Xi$ determines a trajectory and the process starting from x with force F may thus be realized on the space (Ξ, P_x^F) with P_x^F a probability measure on Ξ.

For $\xi=(v_0, v_1,...)\in\Xi$, let $\xi_n=(v_0,..., v_n)$. The motion up to the $(n+1)$th collision is determined by x, F, and ξ_n and thus $X_j=X_j(F, x, \mathbf{v})$ $j=0,..., n+1$ are well-defined for all $\mathbf{v}=(v_1,..., v_n)\in(\mathbb{R}^3)^n$. We call $(F, x, \mathbf{v})$ acceptable if $v_i\cdot n(X_i)>0$ for all $i=0,..., n$.

With $\|F\|=\sup_{t,x,\xi}|F(t, x, \xi)|$ we have the following.

Lemma 5.3. Suppose that Λ satisfies the conditions of Theorem 3.1. Then for every open set $\mathcal{O} \subset \partial\Lambda$ there exists an integer $N < \infty$, an $\varepsilon > 0$, and $\alpha > 0$ such that

$$P_x^F\{\xi \mid \exists n \leqslant N \text{ such that } X_n \in \mathcal{O}\} \geqslant \alpha$$

provided $\|F\| < \varepsilon$.

Proof. The proof is based on a compactness argument. From Lemma 5.2 it follows that given $x \in \partial\Lambda$, there exists a sequence of points $x = x_0, x_1, ..., x_{n(x)}$ such that $x_{n(x)} \in \mathcal{O}$ and all the directions $x_i x_{i+1}$ are good for both x_i and x_{i+1}. Therefore there exists an $\varepsilon = \varepsilon(x) > 0$ and sets $U_x, V_0, ..., V_{n(x)}$, where U_x is a neighborhood of x on $\partial\Lambda$ and $V_i \subset \mathbb{R}^3$ is a neighborhood of $x_i x_{i+1}/\|x_i x_{i+1}\|$ such that for every $(y, \mathbf{v}) \in U_x \times V_0 \times \cdots \times V_{n(x)}$, $(F, y, \mathbf{v})$ is acceptable and $X_n(F, y, \mathbf{v}) \in \mathcal{O}$ provided $\|F\| < \varepsilon(x)$. It follows that there exists an $\alpha(x) > 0$ such that for all $y \in \mathcal{U}_x$

$$P_y^F\{\xi \in \Xi \mid \xi_{n(x)} \in V_0 \times \cdots \times V_{n(x)}\} \geqslant \alpha(x)$$

provided $\|F\| < \varepsilon(x)$. Since U_x is an open covering of $\partial\Lambda$ (which is compact) we can extract a finite subcovering, and the lemma follows.

APPENDIX

Let γ_a the Gibbs measure at temperature $T = 1/K_a$. First, we note that the projection $\tilde{\gamma}_a$ of γ_a on $\hat{\Omega}_0$ is absolutely continuous with respect to $d\tilde{\xi}$, $\tilde{\xi} \in \hat{\Omega}_0$, with density proportional to the usual Gibbs factor multiplied by $n(q_0) \cdot p_0$ (see the special flow representation, Section 2) Thus writing $\tilde{\xi} = (\hat{\xi}, p_0)$, $\hat{\xi} \in (\Lambda \times \mathbb{R}^3)^{N-1} \times \partial\Lambda$ $\tilde{\gamma}_a$ is of the form

$$\tilde{\gamma}_a(d\tilde{\xi}) = v_a(d\hat{\xi})\, R_a(dp_0)$$

for some measure v_a. It follows that

$$\tilde{\gamma}_a R_a = \tilde{\gamma}_a$$

Moreover, since $\tilde{\gamma}_a$ is preserved by the Hamiltonian flow on Ω, given by (1.1) together with elastic reflection from $\partial\Lambda$, it follows that $\tilde{\gamma}_a \tau = \tilde{\gamma}_a$, where τ is the return map for this flow regarded as a stochastic kernel $[\tau(\xi, d\eta) = \delta_{\tau\xi}(d\eta)$ the unit measure at $\tau\xi]$. Since $P = \tau R_a$ [i.e., $P(\xi, d\eta) = \int_{\eta'} \tau(\xi, d\eta')\, R_a(\eta', d\eta)$] it follows that

$$\tilde{\gamma}_a P = (\tilde{\gamma}_a \tau)\, R_a = \tilde{\gamma}_a R_a = \tilde{\gamma}_a$$

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