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Ergodic Properties of the Multidimensional Rayleigh Gas with a Semipermeable Barrier

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We consider a multidimensional system consisting of a particle of mass M and radius r *(molecule)*, surrounded by an infinite ideal gas of point particles of mass m *(atoms)*. The molecule is confined to the unit ball and interacts with its boundary *(barrier)* via elastic collision, while the atoms are not affected by the boundary. We obtain convergence to equilibrium for the molecule from almost every initial distribution on its position and velocity. Furthermore, we prove that the infinite composite system of the molecule and the atoms is Bernoulli.

KEY WORDS: Rayleigh gas; Bernoulli flow; Harris chain.

1. INTRODUCTION

Several efforts have been made to understand the dynamical theory of Brownian motion at least for simplified models. A unified theory for the Rayleigh gas, i.e., for the case when the Brownian heavy particle interacts with an ideal gas, is outlined in ref. 5. (A good survey of results and conjectures can be found in ref. 6.) These efforts were made toward limit theorems for the motion of the heavy particle. A related direction of research is aimed at the ergodic properties of the same system. The simplest one-dimensional case is discussed in ref. 3, when the heavy particle is confined to the unit interval. The semi-infinite case is investigated in ref. 1, whose method can be generalized to a wide class of systems where the heavy particle is subject to an external potential (ref. 4). All these models were one-dimensional; however, in ref. 6 a short section is devoted to the multidimensional case. In a recent paper we generalize the method and results of ref. 3 to a multidimensional system. We hope that our result may

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stimulate similar progress toward ergodic properties and limit theorems for multidimensional systems (maybe with an external potential), as was the case for the one-dimensional ones.

2. DESCRIPTION OF THE MODEL AND RESULTS

Consider the following dynamical system describing an infinite number of particles moving in d-dimensional real space. A particle of mass M and radius r moves in the unit ball $B(0, 1) \subset \mathbf{R}^d$ centered at the origin. It is in contact with an ideal gas of point particles of mass m $(M > m)$ which interact with the molecule through elastic collision. The molecule also interacts with the wall of the ball through elastic reflection. The wall does not affect the atoms. Between collisions, the particles move freely.

Suppose that this infinite system is in equilibrium at temperature $T = (k\beta)^{-1}$ and density ρ, i.e., the particles are distributed according to the appropriate infinite-volume Gibbs state μ. Let $\mathscr{A} = (\Omega, \mu, \phi_t)$ denote our system, where Ω is the phase space and ϕ_t is the time evolution. Following the idea of ref. 3, we show that $\mathscr{A}$ is a Bernoulli flow.

Denoting by $X(t)$ the position and $V(t)$ the velocity of the molecule at time t, we have a stochastic process $Y(t) = (X(t), V(t)) \in B(0, 1) \times \mathbf{R}^d$ on (Ω, μ). Let $\mathscr{B}$ denote this process. This process inherits an equilibrium distribution $\nu(dX, dV) \propto e^{-(1/2)\beta M V^2}\, dX\, dV$ for the molecule. We prove that for a.e. $Y_0 = (X_0, V_0)$ the conditional distribution $\nu^t_{Y_0}$ of $Y(t)$ given $Y(0) = Y_0$ converges to ν in variation norm.

Let $\mathscr{M} = (Z(t))_{t \in \mathbf{R}}$ denote the process obtained by observing only the particles in $B(0, 1)$, that is, $Z(t) \in \Omega|_{B(0,1)}$, where $\Omega|_{B(0,1)}$ denotes the phase space of $\mathscr{M}$.

Clearly $\mathscr{M}$ is Markovian with stationary distribution $\sigma(dz) = \mu(Z(0) \in dz)$. Let $P^t(z, dz') = \mu(Z(t) \in dz' \mid Z(0) = z)$ be the transition probability for the process $\mathscr{M}$. For each $\tau > 0$, let $\mathscr{M}_\tau = (\Omega|_{B(0,1)}, \sigma, P^\tau)$ denote the stationary Markov chain obtained by observing Z only at times $n\tau$ $(n \in \mathbf{N})$.

Theorem 1. For any $\tau > 0$, $\mathscr{M}_\tau$ is an ergodic aperiodic Harris chain. (For relevant definitions see ref. 3.)

The key lemma is the following.

Main Lemma. There exists a set $\bar{\Omega} \subset \Omega|_{B(0,1)}$, $\sigma(\bar{\Omega}) = 1$, such that for any $z, z' \in \bar{\Omega}$, $P^t(z, \cdot)$ and $P^t(z', \cdot)$ are overlapping for t sufficiently large.

Since $\sigma(\cdot) = \int P^t(z, \cdot)\, \sigma(dz)$, it follows from the Main Lemma that $\sigma(\cdot)$ and $P^t(z, \cdot)$ are overlapping for all $z \in \bar{\Omega}$ and for t sufficiently large. From

this we get the proof of Theorem 1 following the proof of Theorem 1 in ref. 3. Moreover, we have the analogue of Corollary 1 of ref. 3.

Corollary 1. (i) $\|P^t(z, \cdot) - \sigma(\cdot)\| \to 0$ in variation norm as $t \to \infty$ for σ a.e. $z \in \Omega|_{B(0,1)}$.

(ii) There exists a set $\tilde{\Omega} \subset \Omega|_{B(0,1)}$, $\sigma(\tilde{\Omega}) = 1$ such that $\|\gamma P^t - \sigma\| \to 0$ as $t \to \infty$ for any probability measure γ on $\Omega|_{B(0,1)}$ with $\gamma(\tilde{\Omega}) = 1$.

Restricting this collorary to $\mathscr{B}$, we have a similar convergence to equilibrium theorem for $\mathscr{B}$. (See Theorem 2 in ref. 3.) Using Appendix B of ref. 3, we obtain the following result.

Corollary 2. The process $\mathscr{M}$ and, hence, $\mathscr{A}$ and $\mathscr{B}$ are Bernoulli.

The Bernoulliness of $\mathscr{A}$ in the one-dimensional model follows from the fact that the process $\mathscr{B}$ is equivalent to $\mathscr{A}$ in an abstract sense, since from the knowledge of $\mathscr{B}$ one can recover the process $\mathscr{A}$ (see ref. 3). Here this conclusion does not follow, since certain atoms may never get inside the ball. But they develop independently from one another and from $\mathscr{M}$. Thus, $\mathscr{A}$ can be factorized into two subsystems: one contains all atoms which ever get inside the ball; the other contains the rest. The first is Bernoulli for the same reason as in ref. 3. The second is an ideal gas in $\mathbf{R}^d \setminus B(0, 1)$; thus, it is Bernoulli itself (see ref. 2, p. 199). Since the two factors are independent, we get the Bernoulliness of $\mathscr{A}$.

3. PROOF OF THE MAIN LEMMA

The proof consists of three parts. In the first part we prove that for almost all $z \in \mathscr{M}$, one can "sweep out" all atoms from the ball by choosing an appropriate "environment"; that is, there exists a suitable phase point in $\Omega|_{B(0,1)^c}$ such that after awhile there is no atom in the ball (Lemma 1). Lemma 2 shows that a small perturbation of the environment yields essentially the same "sweeping out"; thus, it occurs with positive probability. Lemma 3 asserts the overlapping of the measures $P^t(z, \cdot)$ and $P^t(z', \cdot)$ if z and z' consist of the molecule only. From these lemmas the Main Lemma follows.

Lemma 1. For almost all phase points

$$Z = Z(0) = ((X(0), V(0)), (\xi_i(0), \eta_i(0)), i = 1, 2, \ldots, n) \in \mathscr{M}$$

there exists a time t and a phase point with finitely many atoms

$$\bar{Z} = \bar{Z}(0) = ((\bar{\xi}_i(0), \bar{\eta}_i(0)), |\bar{\xi}_i(0)| > 1, i = 1, 2, \ldots)$$

such that $\phi^t(Z \cup \bar{Z})|_{B(0,1)}$ consists of the molecule only.

Proof. We have to sweep out all atoms of Z (which we will call Z-atoms) from the ball. The idea is that suitably chosen outside atoms ($\bar{Z}$-atoms) colliding with the molecule can arbitrarily change its velocity. We will use a very fast $\bar{Z}$-atom to make the molecule push out the nearest Z-atom. To guarantee that these atoms leave the ball freely (i.e., they do not meet the molecule again), we stop the molecule by an other $\bar{Z}$-atom. The later possible collisions with other Z-atoms cannot speed up the molecule too much. During the whole procedure we shall take care to avoid multiple collisions. Since almost all phase points Z have finitely many atoms, the repetition of this procedure works.

Let Z contain n atoms. We prove by induction on n. Let E denote the full energy of this phase point, $E=\frac{1}{2}(MV^2+\sum m_i\eta_i^2)$. Let us allow the system to develop freely for time 1 and consider the phase point $Z(1)$. If during this time the number of Z-atoms decreased, then we are done. So we can assume that $Z(1)$ has n atoms. Let ε be the minimal distance between the Z-atoms and the boundary of the ball at time 1. With probability one, $\varepsilon>0$. Let H_s be the following set (see Fig. 1):

$$H_s=\left\{x\in B\left(0,1-\frac{\varepsilon}{2}\right): s\right.$$
$$\left.=\min\left\{s': \exists y, |y|\leqslant 1-\frac{\varepsilon}{2}-r, |y-x|=r, |y-X(1)|=s'\right\}\right\}$$

In other words, these points form the "front" of the molecular radius of action, that is, the molecule has to fly a distance of at least s to hit the points of H_s if the molecule is not allowed outside $B(0, 1-\varepsilon/2)$ (ε is introduced to avoid the simultaneous collisions with the wall and the atom). Of

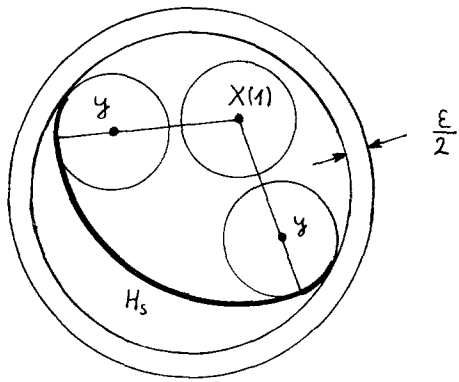

Fig. 1. The "front' of the molecular radius of action.

course, $B(0, 1-\varepsilon/2) = \bigcup_{0 \leqslant s \leqslant 2} H_s$. Let $s_0 = \min\{s: \exists i \leqslant n, \xi_i(1) \in H_s\}$, that is, the ith atom can be hit with the shortest molecular flying distance (this atom is called the target, since it will be pushed out first). With probability one, $s_0 > 0$, and the index i is unique, i.e., there is no Z-atom in $\bigcup_{s \leqslant s_0 + \delta} H_s$ except for the ith one if $\delta > 0$ is small enough. Let even $\delta < s_0$. Thus, there exists a $t_0 > 1$ such that (1) there is no Z-atom in the time interval $[1, t_0]$ in $\bigcup_{s \leqslant s_0 + \delta/2} H_s$ except for the target; (2) the target remains at a distance at least $3\varepsilon/4$ away from the wall.

The first $\bar{Z}$-atom will hit the molecule at time 1 and will direct it to the target. Let t denote the time of collision between the target and the molecule (t will be chosen smaller than t_0). Let $s(t)$ be defined by $\xi_i(t) \in H_{s(t)}$, and if t is small enough, then $|s(t) - s_0| < \delta/2$ and $s(t) > \delta/2$. By the definition of $H_{s(t)}$ there is a $y(t)$ such that $|y(t) - X(1)| = s(t)$, $|\xi_i(t) - y(t)| = r$ and $|y(t)| \leqslant 1 - \varepsilon/2 - r$. Let $V'(1+0) = [1/(t-1)]$ $[y(t) - X(1)]$, the postcollision velocity of the molecule after the collision with the first $\bar{Z}$-atom at time 1. By the Proposition of the Appendix, there exists a suitable $\bar{Z}$-atom $(\bar{\xi}_1(0), \bar{\eta}_1(0))$ for this task, and if t is small enough, i.e., $V'(1+0)$ is large [since $|y(t) - X(1)| = s(t)$ is separated from zero], then $\bar{\eta}_1(1-0)$ must be greater than 2, i.e., $\bar{\xi}_1(0)$ is outside of the ball [see Proposition (i)]. If t is even smaller, then the postcollision velocity of this atom can be guaranteed to be greater than K [see Proposition (ii)], where

$$K = \max\left(\left[\left(\frac{4m}{M-m}\right)^2 + \frac{2E}{m}\right]^{1/2}, \left[\frac{4Em^2}{M(M+m)^2} + \frac{2E}{M}\right]^{1/2}\right)$$

Now we consider the second collision. We have

$$\eta_i^{\|}(t+0) = \frac{m-M}{m+M}\eta_i^{\|}(t-0) + \frac{2M}{m+M}V'^{\|}(t-0)$$

where $t-0$ and $t+0$ indicate the pre- and postcollision velocities, the parallel sign denotes the component parallel to the normal vector of incidence. Of course, $V'(t-0) = V'(1+0)$, since the choice of i and t_0 guarantees that no collision occurred in $[1, t]$.

If t is close enough to 1, then $|\eta_i^{\|}(t+0)| \geqslant K$ can be achieved, since $\eta_i^{\|}(t-0)$ does not depend on t and the angle $\alpha(t)$ between $V'(1+0)$ and $x_i(t) - X(t)$ is separated from $\pi/2$ by (2). Thus $|V'^{\|}(1+0)| \geqslant \varepsilon' |V'(1+0)|$ for a fixed $\varepsilon' > 0$ and $|V'(1+0)|$ can be arbitrarily large if t is close enough to 1, since $s(t)$ is separated from zero. Because of the choice of i and t_0, the molecule does not hit any other Z-atom in the interval $[1, t]$.

Now we need to guarantee that the molecule no longer hits either the first $\bar{Z}$-atom or the target (i.e., they fly away from the ball freely). These

two atoms have velocity larger than K, but actually the molecule can be faster. We need to slow it down by a second $\bar{Z}$-atom.

If the molecule is slower than $(K^2-2E/M)^{1/2}$ after the collision with the target, then the second $\bar{Z}$-atom is not necessary. In this case the molecule cannot accelerate to velocity K, since the total energy of the system consisting of the molecule and the other $n-1$ atoms is less than $\frac{1}{2}MK^2$. There are two fast atoms in the ball, but the molecule cannot reach them (and cannot get energy from them) since their velocities are greater than K and they are flying away from the point $X(t)$.

If $V^t(1+0)$ is at least $(K^2-2E/M)^{1/2}$, then we need a second $\bar{Z}$-atom to stop the molecule. After the collision with the target, let t_1 be the first time the molecule hits any atom or the wall. With probability one, $t_1>t$. We direct the second $\bar{Z}$-atom to stop the molecule at time $t_2=t+(t_1-t)/2$. By the Proposition it can be done by a suitable $\bar{Z}$-atom $(\bar{\xi}_2^t(0), \bar{\eta}_2^t(0))$. The collision yields

$$\bar{\eta}_2^t(0)=\bar{\eta}_2^t(t_2-0)=[(m-M)/2m]\ V^t(t+0)$$

thus, for the speed of the stopping atom we have that

$$|\bar{\eta}_2^t(0)|\geqslant\frac{M-m}{2m}\left(K^2-\frac{2E}{M}\right)^{1/2}\geqslant 2$$

because of the choice of K. Since $t>1$, this guarantees that at time 0 this atom was outside the ball.

On the other hand, we have to guarantee that the molecule would not affect the motion of the two $\bar{Z}$-atoms and that of the target.

The second $\bar{Z}$-atom cannot be affected, since its velocity

$$\begin{aligned}|\bar{\eta}_2^t(t_2+0)| &= \left|\frac{m-M}{M+m}\bar{\eta}_2^t(0)+\frac{2M}{M+m}V^t(t+0)\right| \\ &= \frac{M+m}{2m}|V^t(t+0)|\geqslant\frac{M+m}{2m}\left(K^2-\frac{2E}{M}\right)^{1/2}\end{aligned}$$

is greater than $(2E/M)^{1/2}$, which is the maximal velocity the molecule can gain from the rest of the Z-atoms.

To prove that the target cannot be affected, let us suppose that the hyperplane perpendicular to the normal vector of its collision with the molecule is moving together with the target. Between t and t_2 the molecule does not intersect this moving hyperplane.

After t_2 this hyperplane is moving away with speed at least K, which is greater than $(2E/M)^{1/2}$, the maximal molecular velocity; thus, the molecule never reaches the target.

At the end we have to prove that the first $\bar{Z}$-atom is not affected. But

$$V^{(1)}(t+0) = V^{(1)}(t_2-0) = \frac{M-m}{M+m} V^{(1)}(t-0) + \frac{2m}{M+m} \eta_i^{(1)}(t-0)$$

which points in the same direction as $V^{(1)}(t-0)$ if $V^{(1)}(t-0)$ is large enough, i.e., if t is close enough to 1 [here we used the fact that $\alpha(t)$ is separated from $\pi/2$]. This proves that between t and t_2 the molecule was moving away from the first $\bar{Z}$-atom. After t_2 the atom is moving faster than the molecule; therefore, they do not meet.

All we have to do is to wait until the target and the two $\bar{Z}$-atoms fly away from the ball. Then the new configuration has at most $n-1$ atoms and the induction works. After a finite time all atoms can be swept out from the ball.

Lemma 2. Given T_0, then for almost all phase points

$$Z = Z(0) = ((X(0), V(0)), (\xi_i(0), \eta_i(0)), i = 1, 2, \ldots, n)$$

there exists a moment T such that

$$\mu(\phi^\tau(Z \cup \bar{Z})|_{B(0,1)} \text{ has no atoms } |Z) > 0$$

for all $\tau \in [T, \max(T_0, T) + 3]$.

Proof. It follows from Lemma 1 that there exists a moment T and a phase point $\bar{Z} = \{\bar{\xi}_i(0), \bar{\eta}_i(0), |\bar{\xi}_i(0)| > 1, \ i = 1, 2, \ldots\}$ such that $\phi^\tau(Z \cup \bar{Z})|_{B(0,1)}$ contains no atoms for all $\tau > T$. (Originally it was proved for only one T, but clearly if $\bar{Z}$ consists of only those atoms which played a role in directing the molecule, then these atoms will never return to the ball; therefore, nothing will affect the molecule any more.)

We have to perturb this phase point $\bar{Z}$ such that it has positive probability. All we have to keep in mind is the following regularity property of the collisions.

Regularity Property (RP). With probability one, the following holds: Given a phase point at time t_0 such that on the surface of the molecule there is no atom, suppose that there is an atom $A = (\xi(t_0), \eta(t_0))$ inside or outside the ball such that it is to be collided with (not touched by) the molecule at time $t_0 + t$ and no other collisions or touches occur with any atom or with the wall in the time interval $[t_0, t_0 + t]$. This collision will be called regular, and it is continuous in the following sense. Given an arbitrary $\varepsilon > 0$, there exists $\delta > 0$ such that if $|t_0 - t_0'| < \delta$, $|\xi(t_0) - \xi'(t_0')| < \delta$, $|\eta(t_0) - \eta'(t_0')| < \delta$, $|X(t_0) - X'(t_0')| < \delta$, $|V(t_0) - V'(t_0')| < \delta$, then the perturbed molecule given by $(X'(t_0'), V'(t_0'))$

would hit the perturbed atom $(\xi'(t_0'), \eta'(t_0'))$ at time t' such that $|t'-t|<\varepsilon$, $|X'(t')-X(t)|<\varepsilon$, $|\xi'(t')-\xi(t)|<\varepsilon$, $|V'_+ - V_+|<\varepsilon$, $|\eta'_+ - \eta_+|<\varepsilon$, where $V_+, V'_+, \eta_+, \eta'_+$ are the postcollision velocities of the original and the perturbed molecule and atom, respectively. Moreover, by choosing δ small enough, we can assure that in the time interval $[t_0', t_0'+t']$ no other collisions occur. A similar RP can be stated for the collision with the wall. Furthermore, it follows from the differentiability of the collision equations that in case of regular collision the postcollision phase point depends on the precollision one in a differentiable way; i.e., we have:

(i) The positions $X(t)$ and $\xi(t)$ are differentiable functions of t, $X(t_0)$, $V(t_0)$, $\xi(t_0)$, and $\eta(t_0)$.

(ii) If the collision is regular, then the postcollision velocities are differentiable functions of the precollision ones and the collision point on the surface of the molecule.

Now we can prove Lemma 2. Attentively reading the proof of Lemma 1, one can observe that all collisions are regular. (That is why we had to define H_s in a bit smaller ball, and this is the reason for waiting for a while after hitting the target and before sending the stopping atom. We intentionally avoided multiple collisions and touches which cannot be perturbed.)

Because of the RP and the finiteness of $\bar{Z}$, we get that a small perturbation of $\bar{Z}$ yields the same order of collisions and almost the same hitting points and velocities. Considering the distribution of the ideal gas, we obtain that a small perturbation of $\bar{Z}$ has a positive probability provided that only these atoms are in the ball with radius $R_0 = \max\{|\bar{\xi}_i(0)|; \bar{\xi}_i \in \bar{Z}\} + 1$. But the probability that no other atoms enter the ball $B(0, R_0)$ in the time interval $[0, \max(T, T_0)+3]$ is clearly positive, and this proves Lemma 2.

Lemma 3. Given two phase points $Z_1(T) = (X_1(T), V_1(T))$, $Z_2(T) = (X_2(T), V_2(T))$ of $\Omega|_{B(0,1)}$ at the same time T such that they contain no atom and we suppose that $|X_i(T)|<1$, $X_i(T)\neq 0$, $V_i(T)\neq 0$ $(i=1,2)$, then the conditional measures $P^t_{Z_i}(\cdot) = P^t(\cdot \mid Z_i(T))$ $(i=1,2)$ are overlapping if $t \geqslant 3$.

Proof. Let $\mathscr{E}$ be the following event:

$$\mathscr{E} = \left\{ \begin{array}{l} \text{there is no atom in the ball at time } T \text{ and } T+3; \\ \text{in the time interval } [T, T+3] \text{ exactly two collisions} \\ \text{occur and the molecule does not hit the wall;} \\ |X(T+3)|<\delta, \quad |V(T+3)|<\delta \end{array} \right\}$$

($\delta > 0$ will be chosen later).

We have

$$P^3(X(T+3)\in dx,\ V(T+3)\in dv \mid Z_i(T)) = \mu(X(T+3)\in dx,\ V(T+3)\in dv \mid \mathscr{E}, Z_i(T)) \times \mu(\mathscr{E} \mid Z_i(T))$$

First, we have to prove that on the event $\mathscr{E}$ the measure

$$P^3_{\mathscr{E}}(dx, dv) = \mu(X(T+3)\in dx,\ V(T+3)\in dv \mid \mathscr{E}, Z_i(T))$$

and the Lebesgue measure

$$\Lambda^{(2d)}(dx, dv) = \Lambda^{(d)}(X(T+3)\in dx)\cdot \Lambda^{(d)}(V(T+3)\in dv)$$

are equivalent. (Here $\Lambda^{(d)}$ denotes the d-dimensional Lebesgue measure.) Second, we are to prove that $\mu(\mathscr{E} \mid Z_i(T)) > 0$ $(i=1, 2)$.

We introduce the following notations. Let $X_0 = X_i(T)$, $V_0 = V_i(T)$, $X_3 = X_i(T+3)$, $V_2 = V_i(T+3)$. Let $t_1 + T$ and $t_2 + T$ be the times and X_1 and X_2 the molecular positions of the collisions. Let V_1 and V_2 be the postcollision velocities and e_1, e_2 the unit normal vectors of the collisions. Let v_1, v_1^+ and v_2, v_2^+ denote the pre- and postcollision velocities of the atoms, and x_1, x_2 denote their positions at time T. Let $S = S_i \subset \mathbf{R}^{4d}$ be the following set:

$$S_i = \{(x_1, x_2, v_1, v_2)\text{: such that } \mathscr{E} \text{ is true under the condition that } Z_i(T) \text{ is given}\}$$

We know that the second correlation function of the Gibbs measure μ at (x_1, x_2, v_1, v_2) exists and it is positive, and its integral on S_i is equal to $P(\mathscr{E} \mid Z_i(T))$ due to the Poisson property of the Gibbs state. Summing up, we have to prove that the function $F(x_1, x_2, v_1, v_2) = (X_3, V_2)$ has full rank in S or in a subdomain of S with positive Lebesgue measure, since this proves that the distribution $P^3_{\mathscr{E}}$ of (X_3, V_2) in a subset of $[-\delta, \delta]^{2d}$ is equivalent to the Lebesgue measure.

First we prove that S_i is nonempty; moreover, there exists a

$$\bar{p} = (\bar{x}_1, \bar{x}_2, \bar{v}_1, \bar{v}_2)$$

such that $F(\bar{p}) = (0, 0)$. Then we are to prove that a small full-rank perturbation p of $\bar{p}$ yields a full-rank perturbation of the range F around $(0, 0)$. The RP guarantees that F is continuous; moreover, it is differentiable in a small neighborhood of $\bar{p}$. Therefore, we need only to prove that its Jacobian has full rank at point $\bar{p}$.

In order to prove that S_i is nonempty, we have to push the molecule to the origin and stop it there. It can be done by two suitably chosen

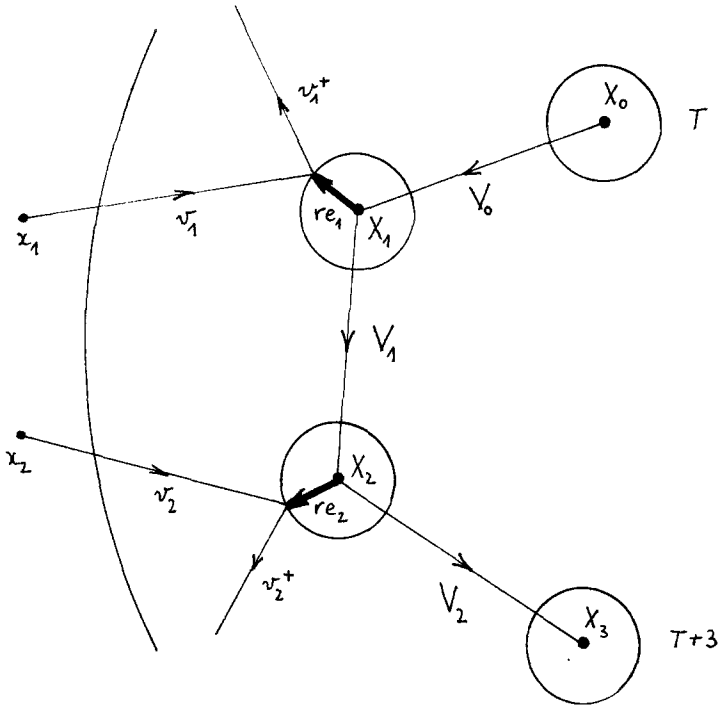

Fig. 2. Two consecutive collisions.

$\bar{Z}$-atoms (Fig. 2). Let $t_1 > 0$ be small enough so that the molecule neither hits the wall nor gets to the origin in $[T, T+t_1]$. Let $V_+ = -c \cdot X_i(T+t_1)$, $V_- = V_i(T+t_1)$, $X = X_i(T+t_1)$ and use the Proposition to obtain suitable hitting point x and velocity v_-. Let $\eta_1(T) = \eta_1(T+t_1) = v_-$ and $\xi_1(T) = x - v_- \cdot t_1$ be the phase point of the first atom. If c is large enough, then by (i) of the Proposition, v_- is larger than $2/t_1$, that is, $\xi_1(T)$ is outside the ball. If c is even larger, then (ii) and (iii) guarantee that $|v_+| > 2$, and v_- and v_+ are opposite, so in a unit of time after the collision this atom leaves the ball following the same path by which it entered. Its motion will no longer affect that of the molecule.

The second atom is used for stopping the molecule; therefore, it should hit the molecule exactly when it gets to the origin. The velocity v_- of this atom is equal to $-[(M-m)/2m]\, V_+$. If c is large enough, then $|v_-| \geqslant 2/t_1$, that is, $\eta_2(T) = v_-$, and

$$\xi_2(T) = -\frac{X_i(T+t_1)}{|X_i(T+t_1)|} \cdot r - v_- \left(t_1 + \frac{|X_i(T+t_1)|}{|V_+|} \right)$$

determines a point outside the ball.

Thus, the second atom stops the molecule and in a unit of time leaves the ball if c is large enough [Proposition (iv)]. Waiting until both atoms leave the ball, we get a phase point of $\mathcal{M}$ which consists of only the molecule standing in the origin and we need less than 3 units of time for this purpose. Thus S_i is nonempty, since $\bar{p} = (\xi_1(T), \xi_2(T), \eta_1(T), \eta_2(T)) \in S_i$, $F(\bar{p}) = (0, 0)$. We note that all collisions satisfy the RP, that is, a small perturbation of $\bar{p}$ yields the same order of collisions.

Now we turn to the Jacobian of F at point $\bar{p}$.

We have the following equations (see Fig. 2):

$$V_1 = V_0 + \frac{2m}{m+M} \cdot (v_1 - V_0, e_1) \cdot e_1 \tag{1}$$

$$V_2 = V_1 + \frac{2m}{m+M} \cdot (v_2 - V_1, e_2) \cdot e_2 \tag{2}$$

$$X_1 = X_0 + t_1 V_0 \tag{3}$$

$$X_2 = X_0 + t_1 V_0 + (t_2 - t_1) V_1 \tag{4}$$

$$X_3 = X_0 + t_1 V_0 + (t_2 - t_1) V_1 + (3 - t_2) V_2 \tag{5}$$

$$x_1 + v_1 t_1 = X_0 + t_1 V_0 + r e_1 \tag{6}$$

$$x_2 + v_2 t_2 = X_0 + t_1 V_0 + (t_2 - t_1) V_1 + r e_2 \tag{7}$$

Here (a, b) denotes the scalar product of the vectors a and b.

F is the composition of the following two functions, which are differentiable in a small neighborhood of $\bar{p}$ and $F_1(\bar{p})$, respectively:

$$F_1(x_1, x_2, v_1, v_2) = (v_1, v_2, t_1, t_2, e_1, e_2), \qquad F_1 : \mathbf{R}^{4d} \to \mathbf{R}^{2d} \times \mathbf{R}^2 \times \mathbf{R}^{2(d-1)}$$

$$F_2(v_1, v_2, t_1, t_2, e_1, e_2) = (X_3, V_2), \qquad F_2 : \mathbf{R}^{2d} \times \mathbf{R}^2 \times \mathbf{R}^{2(d-1)} \to \mathbf{R}^{2d}$$

The differentiability follows from the RP.

The Jacobian of F_1 has full rank at $\bar{p}$. Now, F_1 is invertible, since from (1), (6), (7), we have

$$x_1 = X_0 + t_1 V_0 + r e_1 - v_1 t_1$$

$$x_2 = X_0 + t_1 V_0 + (t_2 - t_1)\left(V_0 + \frac{2m}{m+M} (v_1 - V_0, e_1) \cdot e_1 \right) + r e_2 - v_2 t_2$$

Since F_1^{-1} is clearly differentiable, the Jacobian of F_1 at $\bar{p}$ is invertible, so it has full rank.

The Jacobian of F_2 has full rank at $F_1(\bar{p}) = (\bar{v}_1, \bar{v}_2, \bar{t}_1, \bar{t}_2, \bar{e}_1, \bar{e}_2)$. Again elementary calculation shows that subtracting $3 - t_2$ times the second d

rows from the first d rows of this Jacobian, we have the following simple matrix:

$$M=\begin{pmatrix}(t_2-t_1)\,dV_1/dv_1 & 0 & V_0-V_1 & V_1-V_2 & (t_2-t_1)\,dV_1/de_1 & 0\\ dV_2/dv_1 & dV_2/dv_2 & 0 & 0 & dV_2/de_1 & dV_2/de_2\end{pmatrix}_{F_1(\bar p)}$$

We prove that both matrices

$$M_1=\left(\frac{dV_1}{dv_1}\,\frac{dV_1}{de_1}\right)_{F_1(\bar p)} \qquad \text{and} \qquad M_2=\left(\frac{dV_2}{dv_2}\,\frac{dV_2}{de_2}\right)_{F_1(\bar p)}$$

have rank d and this proves that rank $M=2d$ ($t_2-t_1\neq 0$, because the time of the first collision can be chosen in such a way that, at t_1, the molecule is not at the origin, remembering that $X_0=0$, $V_0=0$ was excluded in Lemma 3).

Calculation shows that M_1 is

$$\frac{2m}{m+M}\begin{pmatrix}0 & 0\cdots 0 & (\bar v_1-\bar V_0,\bar e_1) & 0 & \cdots & 0\\ 0 & 0\cdots 0 & 0 & (\bar v_1-\bar V_0,\bar e_1) & \cdots & 0\\ \vdots & \vdots\ddots\vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0\cdots 0 & 0 & 0 & \cdots & (\bar v_1-\bar V_0,\bar e_1)\\ 0 & 0\cdots 1 & * & * & \cdots & *\end{pmatrix}$$

in a basis having $\bar e_2$ as its dth element ($\bar V_0$ denotes the appropriate value of V_0 at $\bar p$).

This matrix has rank d, since the collision was regular, i.e., $(\bar v_1-\bar V_0,\bar e_1)\neq 0$. Similarly, we get that rank $M_2=d$.

From these lemmas the Main Lemma follows. Given two phase points $z_1, z_2\in\mathscr{M}$, there exist times t_1, t_2 such that $z_1(\tau)$ and $z_2(\tau)$ contain no atom for $\tau\in[t, t+3]$ with positive probability, where $t=\max(t_1, t_2)$ (Lemma 2). Then by Lemma 3 the measures $P_{z_1}^{t+3}$, $P_{z_2}^{t+3}$ overlap.

Remark. Our proof can be generalized for barriers different from the unit ball. The same proof works if the molecule is confined to a convex domain whose curvature is uniformly smaller than that of the molecule. Otherwise, certain points of the domain cannot be reached by the molecule. During the procedure defined in the proof of Lemma 1, we have to avoid those phase points where the molecule has more than one point in common with the wall, since this collision is not regular and cannot be perturbed. But the set of these phase points has probability zero, and the proof of Theorem 1 works.

APPENDIX

Proposition. Given the precollision position (X, V_-) of the molecule and a velocity V_+, then there exist a point x on the surface of the molecule ($|x-X|=r$) and a velocity v_- parallel to $x-X$ such that if an atom is situated in x and its precollision velocity is v_-, then the postcollision velocity of the molecule is V_+. Furthermore, the following relations hold:

(i) $|v_-| \geq \dfrac{m+M}{2m}(|V_+| - 2|V_-|)$

(ii) $|v_+| \geq \dfrac{M-m}{2m}|V_+| - \dfrac{M+m}{2m}|V_-|$

(iii) if $\dfrac{M-m}{M+m}|v_-| > 2|V_-|$, then v_+ and v_- are opposite

(iv) if $V_+ = 0$, then $|v_+| = \dfrac{M+m}{2m}|V_-|$

Proof. The molecular velocity has two components: one is parallel to $x-X$, and the other is orthogonal to it. They are denoted by $\|$ and $\perp$. Thus we have

$$V_-^{\perp} = V_+^{\perp}, \qquad v_-^{\perp} = v_+^{\perp} = 0 \tag{A1}$$

$$V_+^{\|} = \frac{M-m}{M+m} V_-^{\|} + \frac{2m}{M+m} v_-^{\|} \tag{A2}$$

$$v_+^{\|} = \frac{m-M}{M+m} v_-^{\|} + \frac{2M}{M+m} V_-^{\|} \tag{A3}$$

Equation (A1) is equivalent to $(X-x) \| (V_+ - V_-)$; thus, we have two possibilities for x. For both choices, $V_+^{\|}$ and $V_-^{\|}$ are the same. Therefore Eq. (A2) determines v_-. Finally, v_- and $x-X$ must point in the same direction (to the center of the molecule) and this determines the point x uniquely. The relations (i)–(iv) can be obtained easily from (A1)–(A3).

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