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Author
Alexander, Roger Keith.

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Roger Keith Alexander
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The Infinite Hard-Sphere System

by

Roger Keith Alexander

ABSTRACT

We construct the time-evolution for the system of infinitely many particles in space interacting by the hard-sphere potential Φ:

$$\Phi(x) = \begin{cases} +\infty & |x| < a \\ 0 & |x| \geq a \end{cases}$$

Examples abound of configurations of the infinite system having more than one solution to the Newtonian equations of motion. We impose a regularity condition on the solutions we seek, which limits the growth of velocities and of the length of chains of particles close together as $|x| \to \infty$; we prove that through any point of the phase space there passes at most one regular solution.

Every point in a subset $\overline{\mathfrak{X}}$ of the phase space $\mathfrak{X}$ is the initial point of a regular solution which is defined for all time. The subset $\overline{\mathfrak{X}}$ is of full measure for every Gibbs state and is invariant under the one-parameter group T^t of shifts along solution trajectories. Moreover, the flow T^t leaves every Gibbs state invariant.

The solutions we construct are limits, as $R \to \infty$, of motions in which particles inside the sphere of radius R are elastically reflected from its boundary while those outside remain fixed. For this reason, we also study the motion of finite systems.

For finitely many hard-sphere particles in a region of space with piecewise smooth boundary, the set of points of the phase space through which solutions exist for all time without triple or grazing

collisions, is of full Lebesgue measure and is residual in the sense of Baire. Liouville's Theorem holds for the one-parameter group of shift-transformations T^t.

Finally, we give examples in which a single billiard moving in the plane is reflected infinitely often from a boundary curve in finite time, and we establish necessary conditions for such singularities to occur.

I. INTRODUCTION

A. The Problem

Systems of infinitely many particles are a first approximation to realistic systems with a finite but unmanageably large number of particles. Such systems were first studied extensively by O. Lanford [Lanford 1968, 1969] who proved existence of the time-evolution for one-dimensional systems of infinitely many particles interacting through finite-range, Lipschitz-continuous forces. Sinai constructed the time evolution for one-dimensional systems ([Sinai 1972]) and for ν-dimensional systems at low density ([Sinai 1974]) for finite range forces with hard cores, by showing that the particles break up into finite clusters which do not interact for short times. Lanford's 1974 Battelle Lectures [Lanford 1974] are in part devoted to his construction of time evolution for ν-dimensional infinite systems, where the superstable potential is allowed to have infinite range. An existence theorem for the dynamics for ν-dimensional systems with a finite-range, C^2 potential was obtained by Marchioro et al. [Marchioro et al. 1975a]. A summary of all these works is contained in Lanford's 1974 Battelle Lectures.

The purpose of the present work is to construct the time evolution for the infinite hard-sphere system in three-dimensional space.

Briefly, we have a configuration of the infinite system, that is, a sequence $\{(q_i, v_i\}_{i=1}^{\infty}$, the position and velocity of the i-th particle being given by $\mathscr{R}^3$ - vectors q_i, v_i respectively. Our object is to construct the motion of all, or almost all such configurations of particles interacting through the hard sphere potential:

$$\Phi (q_i - q_j) = \begin{cases} +\infty & |q_i - q_j| < a \\ 0 & \text{else} \end{cases}$$

(We require of the configuration $\{(q_i, v_i)\}_{i=1}^{\infty}$ that $|q_i - q_j| \geq a$ if $i \neq j$.)

The problems peculiar to infinite systems are described in Lanford's survey [Lanford 1974]. In fact one cannot hope to solve the equations of motion for all initial configurations, because it is easy to construct examples which reach a catastrophe in finite time. With hard spheres it is so simple the reader may do it himself, if he likes. Thus to make progress one must restrict the set of allowed initial configurations -- but not too severely: what remains should be large enough to support measures on the phase space which describe interesting statistical states of the system.

As usual, the hard sphere potential leads to some simplifications. All Boltzmann factors exp $[-\beta\Phi]$ are independent of the inverse temperature β and take only the values 0 and 1, simplifying many estimates. Moreover, the hard core condition guarantees that every bounded region of space will contain only finitely many particles.

On the other hand, there are difficulties peculiar to the hard-sphere system: the potential Φ is not differentiable, so there is not an honest differential equation to determine the motion. We resort to a prescription based on the elastic reflection law, but it is not clear then what to do about triple and higher multiple collisions.

A further problem is most simply illustrated by an example of a configuration having more than one solution to the equations of motion, which is complementary to the example given by Lanford [Lanford 1974]. Place an infinite sequence of billiard balls of diameter a in a straight line so that $\Sigma_{i \geq 1} (q_{i+1} - q_i - a) < \infty$. All $p_i = 0$. One solution is: all particles remain at rest forever. For a second solution, let particle i begin to move toward particle $i - 1$ with velocity v at time

$$t_i = \frac{1}{v} \sum_{j \geq i} (q_{j+1} - q_j - a)$$

and come to rest when it collides with particle $i - 1$ at time $t_i + (q_i - q_{i-1} - a)/v$.

This shows that in critical configurations a disturbance can be propagated over arbitrarily large distance in a given finite time. It is easy to see that by allowing a moderate growth in the velocity of the i^{th} particle as $i \to \infty$ one can eliminate the requirements that the particles lie in a straight line and that the sum of the interparticle distances be finite.

B. The Infinite System Phase Space

We specify once and for all that the hard sphere diameter is a fixed positive number denoted by a, and that the particles have mass $m = 1$.

Vectors in $\mathscr{R}^3$ giving positions, momenta or velocities of particles will be denoted by q,p,x,y, etc., subscripted or not. Points of the one-particle phase space $\mathscr{R}^3 \times \mathscr{R}^3$ are written as ordered pairs (q,p). Points of $\mathscr{R}^{3N}$ for N > 1 are written $\underline{q},\underline{p}$, and we think of them as N-tuples of points of $\mathscr{R}^3$: $\underline{q} = (q_1, q_2, \cdots, q_N)$ with $q_i \in \mathscr{R}^3$, $1 \leq i \leq N$.

The Euclidean scalar product is written $\langle \cdot , \cdot \rangle$, and when the dimension is not clear from the context it is given by a subscript: $\langle \cdot , \cdot \rangle_{\mathscr{R}^{3N}}$. The scalar product of a vector x with itself is written x^2.

For any set Ω and any subset $A \subset \Omega$, I_A denotes the indicator function of A, that is, the function on Ω which takes the value 1 on A and 0 on $\Omega \setminus A$.

The complement of a set A is written A^c when Ω is understood. In a topological space, the interior of A is denoted A^0. When the domain of a function is understood, we use the bracket notation for brevity, for example, if $f: \Omega \to \mathscr{R}$, then $[f > 0]$ is the set $\{\omega \in \Omega : f(\omega) > 0\}$.

For bounded measurable set $\Lambda \subset \mathscr{R}^3$, $|\Lambda|$ denotes volume of Λ.

The phase space $\mathscr{X}$ of the infinite hard-sphere system may be specified in several ways. The most naive way is to take all sequences $\{(q_i, p_i)\}_{i=1}^{\infty}$ of points of the 1-particle space $\mathscr{R}^3 \times \mathscr{R}^3$, for which $|q_i - q_j| \geq a$ if $i \neq j$, and say that two sequences define the same point of $\mathscr{X}$ if they differ only by permutation of the indices.

Alternatively, define $\mathscr{X}$ to be the set of all functions

$x: \mathscr{R}^3 \times \mathscr{R}^3 \to \{0, 1\}$ such that if $x(q,p) = 1 = x(q',p')$, then either $q = q'$ and $p = p'$ or $|q - q'| \geq a$.

We agree to the following abuse of notation: to each $x \in \mathscr{X}$ there is associated a unique function, which will also be called x, from $\mathscr{R}^3$ to $\{0, 1\}$ giving the positions of the particles of x: that is, $x(q) = 1$ if for some momentum p, $x(q,p) = 1$, otherwise $x(q) = 0$.

For any measurable $\Lambda \subset \mathscr{R}^3$ we obtain the space $\mathscr{X}_\Lambda$ of configurations of particles in Λ by restricting elements of $\mathscr{X}$ to $\Lambda \times \mathscr{R}^3$. Then $\mathscr{X}$ breaks up naturally into a product

$$\mathscr{X} = \mathscr{X}_\Lambda \times \mathscr{X}_{\mathscr{R}^3 \setminus \Lambda}$$

which is just a fancy way of saying that every configuration of the infinite system consists of the part inside Λ and the part outside Λ.

There is a natural way of defining a topology on $\mathscr{X}$ which makes it into a space with desirable measure-theoretic properties. For a continuous function $\Psi: \mathscr{R}^3 \times \mathscr{R}^3 \to \mathscr{R}$ whose support has a compact projection onto the first factor, define a function $\Sigma\Psi: \mathscr{X} \to \mathscr{R}$ by

$$\Sigma\Psi(x) = \sum_{x(q,p) \neq 0} \Psi(q,p).$$

Because of the hard core condition and the support properties of Ψ, only finitely many summands differ from 0. The $\mathscr{X}$ topology is the weakest topology making all functions $\Sigma\Psi$ continuous.

It can be proved ([Lanford 1969]) that $\mathscr{X}$ with this topology is a Polish space, that is, $\mathscr{X}$ has a countable dense subset and the topology is given by a metric in which $\mathscr{X}$ is complete.

The fact that $\mathscr{X}$ is a Polish space gives it very good measure-theoretic properties. The results we shall need about Borel probability measures on Polish spaces are summarized in the following theorem:

Theorem I.B.1 [Schwartz]

Every Borel probability measure P on $\mathscr{X}$ is inner regular and τ-continuous at zero. That is, for every Borel set A,

$$PA = \sup\{PK: A \supset K \text{ compact}\},$$

and for every generalized sequence of closed sets F_α decreasing to ϕ we have $\lim_\alpha PF_\alpha = 0$.

There is a one-to-one correspondence between Borel probability measures on $\mathscr{X}$ and positive linear functionals E on the space $C_\infty(\mathscr{X})$ of bounded continuous functions such that E(1) = 1 with the continuity property $\lim_\alpha E(f_\alpha) = 0$ for every generalized sequence of positive functions $f_\alpha \in C_\infty(\mathscr{X})$ decreasing to 0.

Thus a Borel probability measure on $\mathscr{X}$ is determined by the integrals of bounded continuous functions with respect to it.

C. Gibbs states

Equilibrium states of the infinite system are described by probability measures called Gibbs states. This section contains a summary of their basic properties, and proofs of some basic estimates which will be needed later. Fundamental papers with full details are [Lanford and Ruelle 1969], [Ruelle 1970]. [Lanford 1974] gives a thorough account; a concise summary is [Ruelle 1971].

Choose real numbers $\beta > 0$, $z > 0$; a Gibbs state for the infinite system with inverse temperature β and activity z is a Borel probability measure μ on $\mathscr{X}$ which satisfies the Equilibrium Equations:

Equilibrium Equations. Let Δ be a bounded Borel set of $\mathscr{R}^3$ and let $\Psi \in L^1(\mathscr{X}, \mathscr{B}, \mu)$. Then $\int_{\mathscr{X}} \Psi(x)\mu(dx)$

$$\sum_{n\geq 0} \frac{z^n}{n!} \left(\frac{\beta}{m\pi}\right)^{3n/2} \int_{\Delta^n \times \mathscr{R}^{3n}} d\underline{q}\, d\underline{p} \quad \exp\left(-\frac{\beta}{2m}\underline{p}^2\right) \prod_{1\leq i<j\leq n} I_{[|q_i - q_j| \geq a]}$$

$$\times \int_{\mathscr{X}_{\mathscr{R}^3\setminus\Delta}} \mu(dy) \prod_{\substack{1\leq i\leq n \\ y(q)\neq 0}} I_{[|q_i - q|\geq a]} \Psi(x,y) \;.$$

Here (x,y) is the decomposition of a configuration of $\mathscr{X}$ into the part inside Δ and the part outside. Also, $y \in \mathscr{X}_{\mathscr{R}^3\setminus\Delta}$ has only finitely many particles within distance a of Δ, so that only finitely many factors in the product in the second line differ from 1. Because of the hard-core condition, only finitely many terms in the sum over n are different from zero.

Here are several properties of Gibbs states which can easily be deduced from the definition:

1) For a bounded Lebesgue measurable set $\Delta \subset \mathscr{R}^3$ the random variable $n_\Delta(x) = \#\{\epsilon\Delta : x(q) \neq 0\}$ is bounded a.e. - μ by a constant times the volume of Δ because of the hard-core condition. Therefore the mean number of particles in Δ, $\int_{\mathscr{X}} n_\Delta d\mu$ is bounded by const $|\Delta|$.

The correlation functions for μ are defined by [Ruelle 1969]

$$\rho_n(\underline{q}) = z^n \int_{\mathscr{X}} \mu(dy)\, e^{-\beta U(\underline{q}) - \beta W(\underline{q},y)}$$

$$= z^n \prod_{1\le i<j\le n} I\,[\,|q_i - q_j| \ge a] \int_{\mathscr{X}} \mu(dy) \prod_{\substack{1\le i\le n \\ y(q)\ne 0}} I\,[\,|q_i - q| \ge a]$$

Since μ is a probability measure and the integrand is bounded by one, it is easy to see that [Ruelle 1969 Exercise 4.D]

$$\rho_n(\underline{q}) \le z^n \prod_{1\le i<j\le n} I\,[\,|q_i - q_j| \ge a]$$

and we refer to this fact as the basic inequality for correlation functions.

The correlation functions have the following interpretation: for a Lebesgue measurable set $E \subset \mathscr{R}^n$ the integral

$$\int_E \rho_n(\underline{q})\, d\underline{q}$$

is the mean number of n-tuples of particles in E.

3) The conditional distribution of the momenta given the positions is independent Gaussian with mean zero and variance $\frac{3}{m\beta}$. This Maxwellian velocity distribution leads to important bounds on the probability of occurrence of large velocities.

For a bounded Lebesgue-measurable set $\Lambda \subset \mathscr{R}^3$ define a random variable

$$v_{max} = v_{max}^{(\Lambda)} = 0 \vee \sup_{\substack{(q,p)\in \Lambda \times \mathscr{R}^3 \\ x(q,p) \neq 0}} |p/m| .$$

The square of the magnitude of the velocity of any particle has a Gamma distribution with parameters $\nu = 3/2$, $b = m\beta/2$.*

As before, let n_Λ denote the random variable which counts the number of particles in Λ. On the set $[n_\Lambda = k]$, v_{max} is the square root of the maximum of k independent random variables with this same Gamma distribution. Let $P_k(\lambda)$ be the probability that $v_{max} > \lambda$ given that there are k particles in Λ. Then for any $\gamma < \beta/(2m)$:

$$P_k(\lambda) = \mu[v_{max} \geq \lambda | \; n_\Lambda = k] = 1 - \left[\int_0^{\lambda^2} \frac{1}{\Gamma(3/2)} \left(\frac{\beta}{2m}\right)^{3/2} u^{1/2} e^{-\beta u/2m} du\right]^k$$

$$\leq k \int_{\lambda^2}^{\infty} \Gamma_{\nu,b}(x)dx \leq \text{const } k \exp(-\gamma\lambda^2) \text{ as } \lambda \to \infty.$$

Therefore for each bounded measurable Λ:

$$\mu[v_{max}^{\Lambda} > \lambda] \leq \sum_k \mu[n_\Lambda = k] \; P_k(\lambda) \leq \text{const } e^{-\gamma\lambda^2} \sum_k k \; \mu[n_\Lambda = k]$$

$$\leq \text{const } e^{-\gamma\lambda^2} |\Lambda|,$$

---

*A random variable has the Gamma distribution with parameters ν, b if it has the probability density function

$$\Gamma_{\nu,b}(x) = \frac{1}{\Gamma(\nu)} b^{\nu} x^{\nu-1} e^{-bx} I_{[x>0]}$$

[Feller p. 46].

because the last sum in the previous line is just the expectation of n_Λ .

It follows that $e^{\gamma v_{max}^2}$ is μ-integrable for any $\gamma < \frac{1}{2}\beta m$,

and

$$\int_{\mathscr{X}} \exp(\gamma v_{max}^2)\, d\mu \;\le\; M|\Lambda|$$

where M depends on γ but not on Λ.

To conclude this section we use the correlation functions to estimate the probability of having a long chain of particles lined up close together in some bounded region of space.

Proposition I.C.1 (Chain estimate)

Let μ be a Gibbs state for $\mathscr{X}$. Let Λ be a bounded measurable subset of $\mathscr{R}^3$. Let $0 < \varepsilon_i < 1$ $i = 1, 2, \cdots N-1$. Let F be the set of configurations in $\mathscr{X}$ in which there is a string of N particles with mutual distances $\varepsilon_i a$, that is

$$F = \{x \in \mathscr{X} \,|\, (*) \text{ holds}\}$$

$$(*) \quad \exists\, q_{i_1}, \cdots, q_{i_N} \in \Lambda, |q_{i_{j+1}} - q_{i_j}| \le (1 + \varepsilon_j)a \quad \text{for } 1 \le j \le N-1.$$

Then $$\mu F \le N!\, z^N |\Lambda| \left(\frac{28}{3}\pi a^3\right)^{N-1} \prod_{i=1}^{N-1} \varepsilon_i .$$

Proof: If Y denotes the integer-valued random variable defined by

Y(x) = number of N-tuples of particles of x satisfying(*)

then $F \subseteq [Y \geq 1]$, and $\mu F \leq \mu[Y \geq 1] \leq \int_{\mathscr{X}} Y d\mu$.

By the properties of correlation functions,

$$\int_{\mathscr{X}} Y\, d\mu = N! \int_{\substack{\underline{q}\in\Lambda^N: \\ |q_{i+1} - q_i| \leq (1+\varepsilon_i)a}} \rho_N(\underline{q})\, d\underline{q}$$

Insert the basic estimate for correlation functions,

$$\rho_N \leq z^N \prod_{1\leq i<j\leq N} I_{[\,|q_i - q_j| \geq a]}$$

into the integral above to get

$$\int_{\mathscr{X}} Y d\mu \leq N!\, z^N \int_{\substack{\underline{q}\in\Lambda^N: a \leq |q_{i+1}-q_i| \leq (1+\varepsilon_i)a, \quad 1\leq i\leq N-1 \\ a \leq |q_i - q_j|, \quad i \neq j}} d\underline{q}\, d\underline{y}$$

Change to difference variables $y_i = q_{i+1} - q_i$ $(1 \leq i \leq N-1)$; then

$$\int_{\mathscr{X}} Y d\mu \leq N!\, z^N \int_{\Lambda} dq_1 \int_{a \leq |y_i| \leq (1+\varepsilon_i)a} dy = N!\, z^N |\Lambda| \prod_{i=1}^{N-1} \frac{4}{3}\pi a^3 \left((1+\varepsilon_i)^3 - 1\right).$$

Since $(1+\varepsilon)^3 - 1 < 7\varepsilon$ if $0 < \varepsilon < 1$, the last expression is less than

$$N!\, z^N |\Lambda| \left(\frac{28}{3}\pi a^3\right)^{N-1} \prod_{i=1}^{N-1} \varepsilon_i$$

and the proof is terminated.

Subsequently, when this estimate is applied, we put

$$C_0 = \frac{28}{3} \pi a^3 \quad z^{N/N-1}$$

so that $\mu F \leq N! |\Lambda| C_0^{N-1} \prod_{i=1}^{N-1} \varepsilon_i$.

II. FINITELY MANY PARTICLES

This chapter is devoted to the study of systems consisting of finitely many hard sphere particles restricted to a bounded region of space by a piece-wise smooth, elastically reflecting boundary. The basic existence result of section B will be needed in Chapter III in the proof of the existence of the motion for the infinite system. A result analogous to that of our section B, for particles interacting by a C^2 potential bounded below, has been obtained by Marchioro, Pellegrinotti, Presutti and Pulvirenti [Marchioro et al. 1975b]. In section C we give examples in which a particle undergoes infinitely many reflections from the boundary in a finite time, and establish necessary conditions for such singularities to occur.

A. Phase space

Let Λ_1 be a bounded open region in space. To describe the motion of N hard spheres of diameter a in Λ_1, define Λ, the set of interior positions of a particle in Λ_1, by

$$\Lambda = \{q \in \Lambda_1 : d(q,\partial\Lambda_1) > \tfrac{1}{2} a\}$$

Λ is an open set of which, to avoid pathology, we require a few simple properties:

1) Λ is homeomorphic to an open ball.

2) There is a constant C_Λ such that for $\delta > 0$ sufficiently small

$$\int_{d(q,\partial\Lambda) < \delta} dq \leq C_\Lambda \delta \, |\Lambda|^{2/3};$$

3) $\partial\Lambda$ is contained in the union of finitely many surfaces for which

a) there is a constant ρ_0 such that at every point of each surface the radii of principal curvature are $\geq \rho_0$ or $\leq - \rho_0$;

b) the intersection of two of the surfaces is either empty or consists of a smooth rectifiable arc along which the angle between the surface normals is bounded away from 0 and $\pm \pi$.

Since the particles only see the part of Λ_1 they can get to, namely $\overline{\Lambda}$, we will mention only $\overline{\Lambda}$ in what follows. The N-particle phase-space is

$$\Gamma = \{\underline{x} = (\underline{q},\underline{p}) \varepsilon\ \overline{\Lambda}^N \times \mathscr{R}^{3N} : |q_i - q_j| \geq a \text{ if } i \neq j\} \subseteq \mathscr{R}^{6N}$$

Our goal is to construct the time development which is described informally by saying that the particles move freely in Λ, rebounding elastically at collisions with each other or the walls.

A collision-point is a point $\underline{x}\ \varepsilon\ \Gamma$ for which some $q_i\ \varepsilon\ \partial\Lambda$ or some $|q_i - q_j| = a$.

To describe the flow somewhat more precisely, suppose first that $\underline{x}\ \varepsilon\ \Gamma^0$, the interior of Γ considered as sitting in $\mathscr{R}^{6N}$; then there is a largest open interval about 0 for which $\underline{x}(=(\underline{q},\underline{p})) \rightarrow \underline{x}(t)(=(\underline{q}+t\underline{p},\underline{p}))$ is still in Γ, and this defines the flow for such points, in a neighborhood of $t = 0$.

When particle j strikes the wall $\partial\Lambda$, the point $(\underline{q},\underline{p})$ is to be instantaneously transformed to the point $(\underline{q},\underline{p}')$ given by

$$p' = p_i \qquad i \neq j$$

$$p_j' = p_j - 2 \left\langle p_j, n(q_j)\right\rangle \ n(q_j)$$

where the unit outward normal to the wall at q_j has been denoted by $n(q_j)$.

Similarly, when particle i collides with particle j, we interchange normal components of their momenta:

$$p_i' = p_i - \langle p_i - p_j, \hat{q} \rangle \hat{q}$$

$$p_j' = p_j - \langle p_j - p_i, \hat{q} \rangle \hat{q}$$

where $\hat{q} = (q_j - q_i)/a$ is the unit vector along the line of centers.

Notice that elastic reflection of particles appears in the motion of the phase point $\mathscr{X}$ as elastic reflection from the boundary of Γ. This is immediately obvious when a single particle hits the wall. Let $h_{ij}(\underline{q})$ be the function $(q_i - q_j)^2 - a^2$: then at a collision of particles i and j the phase point $\underline{x}$ strikes a point of the hypersurface $h_{ij}(q) = 0$ in $\partial\Gamma$. We have

$$\text{grad } h_{ij} = (0,\cdots,0,\underset{\uparrow i\text{th place}}{2\,(q_i-q_j)},0,\cdots,0,\underset{\uparrow j\text{th place}}{2\,(q_j-q_i)},0,\cdots,0),$$

so that the unit normal is $\underline{n} = \dfrac{1}{a\sqrt{2}}\,(0,\cdots,0,q_i-q_j,0,\cdots,0,q_j-q_i,0,\cdots,0)$, and the exchange of normal components of momenta of particles i and j is effected by the transformation

$$p \mapsto \underline{p}' = \underline{p} - 2\,\langle \underline{p},\underline{n}\rangle_{\mathscr{R}^{3N}}\ \underline{n}.$$

We look only at i,j components, since the others are obviously unchanged:

$$(p_i',p_j') = (p_i,p_j) - 2\,\left\langle (p_i,p_j), \frac{1}{a\sqrt{2}}\,(q_i-q_j,q_j-q_i)\right\rangle_{\mathscr{R}^6} \frac{1}{a\sqrt{2}}\,(q_i-q_j,q_j-q_i)$$

$$= (p_i,p_j) - \left\langle p_i-p_j, \frac{q_i-q_j}{a}\right\rangle_{\mathscr{R}^3} \left(\frac{q_i-q_j}{a}, \frac{q_j-q_i}{a}\right)$$

$$= \left(p_i - \langle p_i-p_j, \hat{q}\rangle_{\mathscr{R}^3}\,\hat{q},\ p_j + \langle p_i-p_j, \hat{q}\rangle_{\mathscr{R}^3}\,\hat{q}\right)$$

where $\hat{q} = (q_i - q_j)/a$.

It is easy to see that any number of simultaneous, separated collisions may be performed at once, since the reflection operators $I - 2 \langle \cdot, \underline{n}_1 \rangle \underline{n}_1$ and $I - 2 \langle \cdot, \underline{n}_2 \rangle \underline{n}_2$ commute in case $\underline{n}_1 \perp \underline{n}_2$, which will be true if $\underline{n}_1$, $\underline{n}_2$ are (parallel to) gradients of functions depending on distinct coordinates.

However, there are many cases not covered by our prescription, for example collisions involving three particles at once. Moreover grazing collisions can occur, after which the motion does not depend smoothly on the initial configuration.

Our approach will be to identify the subset of $\partial\Gamma$ corresponding to events such as these, and to discard from Γ all phase points which ever reach it. This will turn out to be no loss, for the excluded set is of first category and Lebesgue measure zero. On its complement solutions are defined for all time.

We identify the following sets of "bad" collision points:

$$\bigcup_{i,j,k} \{ |q_i - q_j| = |q_j - q_k| = a \} \text{ (triple collisions)}$$

$$\bigcup_{i,j,k} \{ q_i \varepsilon S_j, |q_i - q_k| = a \} \text{ (particle hits wall and second particle simultaneously)}$$

$$\bigcup_{i,j,k} \{ q_i \varepsilon S_j,\ q_i \varepsilon S_k \} \text{ (particle hits a corner curve in the wall)}^*$$

$$\bigcup_{i,j} \{ |q_i - q_j| = a, \langle p_i - p_j, q_i - q_j \rangle = 0 \} \text{ (grazing two-body collision)}$$

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*Notice that, if we like, we may leave in points where a particle hits a corner curve at an interior point in the curve of the set where the two surface normals n_j and n_k are perpendicular.

$\cup_{i,j} \{q_i \varepsilon S_j : \langle p_i, n_j(q_i) \rangle = 0\}$ (grazing collision with wall).

The union of all these sets is a closed subset of $\partial\Gamma$ which we call D. In fact D is a finite union of submanifolds of $\mathscr{R}^{6N}$, each of which has codimension at least two. This fact will be useful in section B.

It is possible to make the phase space into a manifold on which the trajectories have no corners. Let $\overline{M} = \Gamma \setminus D$. In $\overline{M}$ define an equivalence relation by

$$(\underline{q},\underline{p}) \sim (\underline{q}',\underline{p}') \quad \text{if either}$$

$$(\underline{q}.\underline{p}) = (\underline{q}',\underline{p}') \text{ or } \quad (\underline{q},\underline{p}),\ (\underline{q}',\underline{p}')\varepsilon\partial\Gamma$$

$$\underline{q} = \underline{q}'$$

$$\langle \underline{p},\underline{n}(\underline{q}) \rangle \neq 0$$

$$\text{and} \quad \underline{p}' = \underline{p} - 2 \langle \underline{p},\underline{n}(\underline{q}) \rangle \ \underline{n}(\underline{q})$$

where $\underline{n}(\underline{q})$ is the normal to the boundary of Λ^N at the point $\underline{q}$.

Define M to be the quotient topological space $\overline{M}/\sim$, $\pi : \overline{M} \to M$ the natural projection. We define an atlas for M in which the trajectories of the hard-sphere system have no corners.

Charts for M are either

1) Γ^0, the interior of Γ

or

2) For $\underline{x}\ \varepsilon\ \partial\,\Gamma\setminus D$:

   a) Suppose first that $x = (\underline{q},\underline{p})$ lies in a single hypersurface of $\partial\Gamma$, that is, $\underline{q}$ lies in a 3N - 1-dimensional surface in the boundary of the configuration space $\Lambda^N\setminus\{|q_i - q_j|<a:$

$1 \le i < j \le N\}$. Choose coordinates in a neighborhood of $0 \in \mathscr{R}^{3N-1}$ so that the hypersurface is given by $\underline{z} = \underline{z}(u)$ with $\underline{q} = \underline{z}(0)$. Call the unit normal field $\underline{N}(u)$. Define maps

$$F_-(u,\xi) = \underline{z}(u) - \xi\underline{N}(u) \qquad 0 \ge \xi \ge -\varepsilon$$

$$F_+(u,\xi) = \underline{z}(u) + \xi\underline{N}(u) \qquad 0 \le \xi \le \varepsilon$$

Denoting the derivative of $F_\pm$ by $DF_\pm$ and tangent vectors to $\mathscr{R}^{3N-1} \times \mathscr{R}$ by (k,η) we have, if $\eta \ne 0$

$(F_-(u,0), DF_-(k,\eta)) \sim (F_+(u,0), DF_+(k,\eta))$.

Thus for $(\underline{q},\underline{p}) \in \partial\Gamma \setminus D$ a chart in M for a neighborhood of $\pi(\underline{q},\underline{p})$ is given by

$$F(u,\xi,k,\eta) = \begin{cases} \pi(F_+(u,\xi), DF_+(k,\eta)) & \xi \ge 0,\ \eta \ne 0 \\ \pi(F_-(u,\xi), DF_-(k,\eta)) & \xi \le 0,\ \eta \ne 0 \end{cases}$$

b) If q lies in the surface formed by the intersection of k mutually orthogonal hypersurfaces, define functions

$$F_\nu(u,\xi) = \underline{z}(u) + \Sigma\ \nu_i\, \xi_i\, \underline{n}_i(u)$$

where $1 \le \nu \le 2^k$ and $\nu_i = -1 + 2.\,[i^{th}$ digit in binary expansion of $\nu]$. Again $\underline{x} \sim \underline{y}$ if and only if for some ν, $(F_\nu, DF_\nu)^{-1}(\underline{x}) = (F_\nu, DF_\nu)^{-1}(\underline{y})$ and so the F_ν's define a chart for some neighborhood of $(\underline{q},\underline{p}) \in \pi(\partial\Gamma \setminus D)$.

B. Construction of the Motion

This section is devoted to the proof of the following theorem:

Theorem II. B.1 (Existence, uniqueness of solutions for finite systems)

Let $\Lambda \subset \mathscr{R}^3$ be a bounded open set with piecewise smooth boundary satisfying the conditions of the last section, and let Γ be the phase space for N hard spheres in Λ, D the singular points of $\partial\Gamma$, and M the manifold made from $\Gamma \setminus D$ by identifying incoming and outgoing momenta at collision points.

Let $\{t_n\}$ be an increasing sequence diverging to infinity. Then for every n there is an open dense subset U_n of full measure in M such that for every $\underline{x}_0 \in U_n$ there is a mapping $\underline{x}: [-t_n, t_n] \to M$ with $\underline{x}(0) = \underline{x}_0$, enjoying the following properties:

a) $\{\underline{x}(t)\}$ is a solution of the equations of motion with initial point $\underline{x}_0$;

b) $\underline{x}(t)$ never meets D (that is, there are no triple collisions and no grazing collisions);

c) any mapping $\underline{x}': [-t_n, t_n] \to M$ satisfying a) coincides with $\underline{x}$;

d) the shift mappings $\underline{x}(0) \to \underline{x}(t)$ are measure-preserving transformations of M.

Corollary II.B.1 (Consistency) Let $m < n$ and $\underline{x}_0 \in U_m \cap U_n$, $\underline{x}_m, \underline{x}_n$ the corresponding solution mappings on $[-t_m, t_m]$, $[-t_n, t_n]$ respectively. Then $\underline{x}_n \restriction [-t_m, t_m] = \underline{x}_m$.

The above theorem immediately implies that almost all phase points have solutions through them which are defined for all time.

Theorem II.B.2 In M there is a residual subset R, whose complement is a Lebesgue null set, such that for any $x_0 \in R$ there is a unique mapping $\underline{x}: \mathscr{R} \to R$ which is a solution of the equations of motion having $\underline{x}(0) = \underline{x}_0$.

Moreover the shifts along trajectories

$$S^t \underline{x} = \underline{x}(t)$$

define a one-parameter group of measure-preserving transformations in M.

The proof of Theorem 1 is accomplished in essentially two steps. First we show that for any $t > 0$, the set of points $x \in \Gamma$ which have solutions existing throughout $[-t,t]$ is open. It will be clear from the proof that any such solution is unique. The second part of the proof proceeds by probability arguments: we show that the Lebesgue volume in phase space of the set of points which do not have solutions on $[-t,t]$, is zero.

To begin the proof, let $\underline{x}_0 \in \Gamma^0$ and let t_0 be the smallest positive time t for which $\underline{x}_0(t) = (\underline{q}_0 + t\underline{p}_0, \underline{p}_0) \in \partial\Gamma$. Assume that $\underline{x}_0(t_0) \in \partial\Gamma \backslash D$, and assume that precisely one pair of particles collides or that exactly one particle touches $\partial\Lambda$ in $\underline{x}_0(t_0)$. Then there is a neighborhood U of $\underline{x}_0$ and a time $t_1 > t_0$ such that:

i) for every $\underline{x} \in U$, there is a unique solution trajectory $\{\underline{x}(t): 0 \le t \le t_1\}$ along which there occurs exactly one collision, which involves the pair of particles or the particle touching $\partial\Lambda$ in $\underline{x}_0(t_0)$.

ii) For any t, $0 \le t \le t_1$ the mapping $\underline{x} \to \underline{x}(t)$ is a measure-preserving diffeomorphism of U.

To show the existence of such a U and t_1, note first that since $\underline{x}_0(t_0) \in \partial\Gamma \backslash D$ there is a $t_1 > t_0$ to which, by reflecting the momenta of colliding particles at t_0, we can continue the motion of $\underline{x}_0$ with no further collisions.

Next, for any pair of particles which do not collide, say q_i, q_j the function

$$d_{ij}(t) = |q_i + tp_i - (q_j + tp_j)| - a$$

is positive on the compact interval $[0,t_1]$ and thus has a positive minimum. The same goes for the function

$$d_i(t) = d(q_i(t), \partial\Lambda)$$

defined for any particle q_i which does not meet the wall during $[0,t_1]$.

Thus for any particle q_i which does not collide, define

$$r_i = \frac{1}{2}\left(\inf_{0\le t\le t_1} d_i(t) \quad \Lambda \quad \min_j \inf_{0\le t\le t_1} d_{ij}(t) \right)$$

and find a neighborhood $U_i \subset \mathscr{R}^6$ of (q_i, p_i) so that

$$\sup_{\substack{0\le t\le t_1, \\ (q,p)\varepsilon U_i}} |q_i + tp_i - (q + tp)| < r_i.$$

For a particle q_i which suffers a collision at time t_0, either t_0 is the smallest time for which

$$d(q_i + tp_i, \partial\Lambda) = 0$$

or for some particle q_j, t_0 is the smaller of the two positive roots of

$$(q_i + tp_i - (q_j + tp_j))^2 - a^2 = 0.$$

In either case, because of the smoothness of the boundary surfaces and because the collision time evidently depends smoothly on q_i, p_i, q_j, p_j a neighborhood U_i of q_i, p_i may be determined so that if $(q,p) \varepsilon U_i$:

a) the collision reached by (q_i, p_i) at time t_0 is reached by (q,p) at some time $t < t_1$ which depends smoothly on (q,p)

b) there is nonzero momentum transfer at this collision, which also depends smoothly on (q,p)

c) no further collisions are introduced.

The construction is finished: take the neighborhood $U = \prod_{i=1}^{N} U_i$.

That the shifts along the trajectories starting at points of U are measure-preserving follows from the fact that for any $(\underline{q},\underline{p}) \in U$, and for any i, the map $(q_i,p_i) \to (q_i(t), p_i(t))$ $0 \le t \le t_1$, is made up of a finite sequence of translations

$$(q_i,p_i) \mapsto (q_i + tp_i, p_i)$$

and reflections

$$(q_i,p_i) \mapsto (q_i,p_i')$$

which depend smoothly on $(q_i,p_i) \in U_i$, and all of which have Jacobian equal to one.

From these simple considerations we get immediately the fact that trajectories for any interval $[0,t]$ exist on an open set:

<u>Proposition II.B.1</u> Let $\underline{x}_0 \in \Gamma$ and assume there is a well-defined trajectory $\underline{x}(t)$ through $\underline{x}_0$ having finitely many collisions at times $t_1 < t_2 < \cdots < t_n$. Then there is a neighborhood U of $\underline{x}_0$ and a time $t_n' > t_n$ so that every $\underline{x} \in U$ has the same collision-history as $\underline{x}_0$ on $[0,t_n']$. Moreover for every $t \in [0,t_n']$ the mapping $\underline{x} \to x(t)$ is a diffeomorphism of U onto a neighborhood of $\underline{x}_0(t)$ which leaves Lebesgue measure invariant.

Proof: Apply the results above to obtain a sequence $\{t_k'\}_{k=1}^{n}$, $0 < t_1 < t_1' < t_2 < t_2' < \cdots < t_n < t_n'$ and neighborhoods U_k of $\underline{x}(t_k')$,

$1 \le k \le n$, so that every $\underline{x} \in U_k$ has the same collision history on $[0, t'_{k+1} - t'_k]$ as has $\underline{x}_0$ on $[t'_k, t'_{k+1}]$, and shifts along trajectories are measure-preserving diffeomorphisms. Put

$$U = \bigcap_{k=1}^{n} \left(\prod_{j=1}^{k-1} S(t_{j+1}-t_j)^{-1} U_k \right) \text{ where } S(t)\,\underline{x} = \underline{x}(t);$$

then this U is a neighborhood of $\underline{x}_0$ and has the desired properties.

We now know that the set of phase points having solutions up to time t is open for all t; we do not know whether it is non-empty, and we do not know whether any configurations have solutions existing for all time.

In the remainder of this section we show that the set of initial configurations which fail to have solutions for all time is contained in a set of Lebesgue measure zero.

Here we take advantage of the fact that we are working with pure hard spheres to simplify the argument: we fix $E > 0$ and consider Γ_E, the set of configurations of energy less than E. Γ_E is just the Cartesian product of the configuration space with the ball of radius $\sqrt{\frac{2E}{m}}$ in velocity space, and since energy is conserved any trajectory which starts out in Γ_E stays there. Moreover, the motion of any point $(\underline{q},\underline{p})$ in Γ can be found by looking at a corresponding point $(\underline{q}, c\cdot\underline{p}) \in \Gamma_E$ (for c small enough) and scaling the time appropriately. Thus it will suffice to show that the time-development exists almost everywhere on Γ_E.

Pursuing this observation further, we see that the set of points which fail to have global solutions is invariant under homothetic transformations in velocity space. Thus our argument will show that in any energy surface, the set of phase points which do not have solutions existing for all time has probability zero for the microcanonical distribution.

For convenience, we choose E so that the maximum velocity any particle can have is 1.

The next four lemmas contain elementary geometrical estimates which show that the flow can be put together from pieces of trajectories along which only single collisions occur.

By P is meant Lebesgue measure on Γ_E normalized to 1.

Lemma II.B.1 There is a constant C_1 depending only on Λ and N, such that for all δ, $0 < \delta < a/2$,

$$P[\text{ some particle will collide with two others within time } \delta] \le C_1\,\delta^2.$$

Proof: Here and in the lemmas to follow we suppress reference to momentum space from the notation. Integrals over momentum space contribute a fixed factor, namely the volume of the 3N-dimensional ball of radius E, to all volume integrals over phase space.

The set in question is thus contained in the set

$$\{\underline{q}\varepsilon\Lambda^N\text{: for some triple of distinct indices } i,j,k,\ a\le|q_i-q_j|\le a+2\delta \text{ and } a\le|q_i-q_k|\le a+2\delta\}$$

whose volume is bounded by

$$\binom{N}{3}\int\limits_{\substack{\underline{q}\varepsilon\Lambda^N:\ a\le|q_2-q_1|\le a+2\delta\\ a\le|q_3-q_1|\le a+2\delta}} d\underline{q} \quad\le\quad \binom{N}{3}\ |\Lambda|^{N-2}\left(\frac{28}{3}\,\pi a^3\right)^2\cdot\frac{4\delta^2}{a^2}$$

$$= a\left(1+\frac{2\delta}{a}\right)$$

where we have used the estimate of Proposition I.C.1 for the volume of the spherical shell, which is valid because $2\delta < a$.

Lemma II.B.2 There is a constant C_2, depending only on Λ and N, such that

P[some particle collides with the wall and with another particle by time δ] $\leq C_2\, \delta^2$.

Proof: The set in question is contained in the set where

i) there is a particle within δ of $\partial\Lambda$

and ii) there is a second particle within $a+2\delta$ of the first.

A bound for the volume of the latter set is

$$\binom{N}{2} \int\limits_{\substack{\underline{q}\in\Lambda^N : d(q_1,\partial\Lambda) < \delta \\ a \leq |q_1-q_2| \leq a+2\delta}} d\underline{q} \leq \binom{N}{2} C_\Lambda\, |\Lambda|^{N-4/3} \left(\frac{28}{3}\pi a^3\right) \frac{2\delta^2}{a} ,$$

in which 2) of section A has been used.

Lemma II.B.3 There are constants C_3' and C_3'' depending only on N and the domain Λ, such that

P[Some particle strikes $\partial\Lambda$ twice during time δ] $\leq C_3'\, \delta^2 + C_3''\, \delta^2$

Proof:

Case 1: Two impacts on a single surface of $\partial\Lambda$. (Figure 1)

Let S be one of the smooth surface components of $\partial\Lambda$ and let $q \in S$. The sphere σ of radius ρ_0 which is tangent to S at q lies entirely inside S; therefore, if a particle can hit q and another point of S within time δ it must be able to hit q and another point of σ within time δ.

A chord of $\mathcal{O}$ whose length is δ subtends an angle at the center of $\mathcal{O}$ which is given by

$$\rho_0^2 + \rho_0^2 - 2\rho_0\rho_0 \cos\alpha = \delta^2$$

and this chord makes an angle $\theta = (\pi-\alpha)/2$ with the radius. By elementary trigonometry compute $\cos\theta = \delta/(2\rho_0)$.

Thus if a particle is to collide with q and another point of $\mathcal{O}$ within time δ its distance from the tangent plane at q is at most $\delta\cos\theta = \frac{\delta^2}{2\rho_0}$. By the condition 2) a) of section A on the curvature of $\partial\Lambda$ it follows that there is a constant c' such that for all δ small enough such a particle is within a distance $c'\delta^2$ of $\partial\Lambda$. Again using 2) of section A we get as an estimate for the volume of such configurations

$$N|\Lambda|^{N-1} \int_{d(q,\partial\Lambda) < c'\delta^2} dq \leq NC_\Lambda |\Lambda|^{N-1/3} c'\delta^2$$

Case 2: Impact with two different surface components (Figure 2).

Let $\alpha > 0$ be the infimum of the angles at which two surfaces in $\partial\Lambda$ intersect. For sufficiently small δ, then, a particle which is within a distance δ of two surfaces must lie within a distance $\frac{4\delta}{\sin\alpha}$ of their intersection (see Figure 2). Thus, there exists a constant C_4 such that any particle which can collide with two different surfaces in time δ must lie in the union of cylinders of radius $C_4\delta$ about the intersection curves. If the total length of these curves is L, the volume in Γ_E of configurations having such a particle is less than

$$N|\Lambda|^{N-1} \sum_{i\neq j} \int_{d(q,\sin S_j) < C_4\delta} dq \leq N|\Lambda|^{N-1} \cdot \pi L (C_4\delta)^2$$

and this completes the proof.

Proposition II.B.2 Let F be the set of configurations whose next collision point belongs to D. F is a finite union of submanifolds whose codimension is at least 1.

This Proposition is proved by a series of lemmas.

Lemma II.B.4 D is a finite union of submanifolds of codimension at least two.

The proof of this is simple, and uses the fact that D is defined by constraints involving only one or two coordinates, which specify whether a particle is inside or on the boundary of Λ or whether two particles are separated or in contact.

Define a function τ on D by

$$\tau(\underline{q},\underline{p}) = \inf \{t > 0 : (\underline{q} - t\underline{p},\underline{p}) \in (\Gamma^0)^c\} .$$

Thus τ is the time elapsed since the last collision.

Lemma II.B.5 τ is lower semi-continuous.

Proof: For each pair of particles q_i, q_j define

$$\tau_{ij} (\underline{q},\underline{p}) = \inf \{t > 0: |(q_i - tp_i) - (q_j - tp_j)| = a\}$$

and for each particle q_i define

$$\tau_i(\underline{q},\underline{p}) = \inf \{t > 0 : (q_i - tp_i) \in \Lambda^c\}.$$

Each function τ_{ij}, τ_i is lower semi-continuous; therefore so is

$$\tau(\underline{x}) = \inf_i \tau_i(\underline{x}) \wedge \inf_{i,j} \tau_{ij}(x).$$

Lemma II.B.6 Let U be a manifold, τ a nonnegative lower semi-continuous function on U, $\delta > 0$. Then

$$U_\delta = \{(x,t) \in U \times \mathscr{R} \mid 0 < \tau(x) \wedge \delta\} \text{ is a manifold.}$$

Proof: It is sufficient to exhibit a neighborhood of the form $N_x \times (0,t_1)$ of a given point $(x,t) \in U_\delta$. If $(x,t) \in U_\delta$ we have $0 < t < \tau(x) \wedge \delta$ so there is a t_1 such that $t < t_1 < \tau(x) \wedge \delta$. The set $[\tau(x) > t_1]$ is open in U, so it contains a neighborhood N_x of x, and the proof is complete.

The proof of Proposition II.B.2 is completed by taking each manifold U of D, forming U_δ, and mapping U_δ into Γ_E by $(\underline{q},\underline{p},t) \to (\underline{q}-t\underline{p},\underline{p})$.

We can now construct the flow in Γ_E (and hence in Γ). Only two events can prevent a trajectory from being extended to all times: reaching D, or having infinitely many collisions in finite time. These catastrophes occur for a set of initial configurations which has measure zero.

Proposition II.B.3 The set of points which are initial points of trajectories defined for all time is of full measure in Γ_E.

Proof: Let $t_0 > 0$. For any $\varepsilon > 0$, we prove that the set of points of Γ_E which fail to have solutions throughout $[0,t_0]$ is of outer measure less than ε.

Let $C = 4 \max \{c_1, c_2, c_3', c_3''\}$, where these are the constants in Lemmas II.B 1-3.

Let M be so large that $\frac{t_0 C}{M} < \varepsilon$, $\frac{2}{M} < a$, and $\delta = \frac{1}{M}$ is small enough that Lemmas II.B.1-3 hold for δ.

Set $k \leftarrow 1$, $t \leftarrow 0$. By Lemmas II.B.1-3 and Proposition II.B.2, there is a set of measure less than $C\delta^2$, on whose complement solutions having only one collision exist from time 0 to time δ. Set $k \leftarrow k + 1$, $t \leftarrow t+\delta$. If $t \geq t_0$ we are through. If not, another time-step of size δ may be taken provided we discard another set of measure at most $C\delta^2$. (Unwind this set by T^{-t}, which preserves Lebesgue measure, and notice that this amounts to throwing away a k^{th} set of the same measure originally.)

After $t_0/\delta = Mt_0$ steps we reach t_0 on the complement of a set of measure less than

$$Mt_0 \cdot C\delta^2 = Mt_0 \frac{C}{M^2} < \varepsilon.$$

Finally, take any sequences $t_n \to \infty$ and $\varepsilon_k \to 0$ and let F_{nk} be a set of measure less than ε_k on whose complement it is possible to reach t_n. Then

$$F_n = \bigcap_k F_{nk}$$

is a closed set of measure zero on whose complement solutions are defined throughout $[0,t_n]$. Putting $U_n = F_n^c$ finishes the proof of Theorem II.B.1. The proof of Theorem II.B.2 is immediate if we set $R = \bigcap_n U_n$, for then R is a residual subset of full measure on which solutions starting at any point exist for all time.

C. Singularities

This section is devoted to the study of singularities in the trajectory of a single billiard in a two-dimensional domain. We construct examples in which infinitely many collisions with the boundary occur in finite time, and then state necessary conditions for such singularities to occur.

In our first example, the particle gets trapped between converging walls in a cul de sac. We first construct the path, lying in the unit square $[0,1] \times [0,1]$ of the plane. The particle starts at the point $(0,1)$ with velocity $(1,-2)$ and reaches a horizontal wall at $(\frac{1}{2},0)$. It travels to $(\frac{3}{4},\frac{1}{2})$, $(\frac{7}{8},\frac{1}{4})$, and so on, each time being reflected at an angle $\pi/4$ from a horizontal wall, the distance between successive collisions being halved. At time 1 the particle reaches the point $(1,\frac{1}{3})$ after infinitely many collisions (Figure 3).

The walls are constructed by joining together pieces of C^{∞} functions which have horizontal tangents at the collision points. Take Φ to be any $C^{\infty}(-\varepsilon, 1+\varepsilon)$ function such that:

$$\Phi \geq 0, \quad \Phi(x) = 0 \text{ if } x \leq 0, \quad \Phi(x) = 1 \text{ if } x \geq 1,$$

$$\Phi^{(n)}(0) = 0 = \Phi^{(n)}(1) \text{ for } n \geq 1.$$

At the n^{th} bounce, the position of the particle is to be

$$(x_n, y_n) \equiv (1-2^{-n}, 1 + 2\sum_{k=1}^{n} (-1)^k 2^{-k}) = (1-2^{-n}, \frac{1}{3} + \frac{2}{3}(-\frac{1}{2})^n).$$

The even-numbered collisions occur against the upper wall. Put a translated magnified Φ between (x_{2k}, y_{2k}) and (x_{2k+2}, y_{2k+2}):

$$g_k(x) = y_{2k} - (y_{2k}-y_{2k+2})\Phi\left(\frac{x - x_{2k}}{x_{2k+2}-x_{2k}}\right) I_{[x_{2k},\, x_{2k+2}]} \qquad (k \geq 0).$$

At the odd-numbered collisions the particle strikes the lower wall. Define functions

$$h_k(x) = y_{2k-1} + (y_{2k+1}-y_{2k-1})\,\Phi\left(\frac{x-x_{2k-1}}{x_{2k+1}-x_{2k-1}}\right) I_{[x_{2k-1}, x_{2k+1}]}(k \geq 1).$$

The upper wall is given by $g(x) = \Sigma_{k\geq 0}\, g_k(x)$, the lower wall by $h(x) = \Sigma_{k\geq 1}\, h_k(x)$; they are C^{∞} because only one summand differs from zero at any point, and successive pieces of the wall match to all orders where they meet.

The second example is of a plane region with C^∞ boundary from which a properly incident particle is reflected infinitely often in finite time.

First we construct the trajectory. Let $(x_k)_{k\geq 0}$ be a strictly increasing sequence with limit $x_\infty < \infty$; let θ_0, $(\varepsilon_k)_{k\geq 1}$ be positive numbers such that

$$\theta_0 + 2 \sum_{k=1}^{\infty} \varepsilon_k < \pi/2 . \qquad (1)$$

Let the particle travel from left to right, and be reflected first at a point above x_0, its trajectory making an angle θ_0 with the horizontal axis.

Above x_1, the particle strikes the boundary again. Here the boundary is inclined at an angle

$$\Phi_1 = \theta_0 + \varepsilon_1 \qquad (2)$$

to the horizontal, and the incident trajectory makes angle ε_1 with the boundary, so the path of the reflected particle makes an angle

$$\theta_1 = \Phi_1 + \varepsilon_1 = \theta_0 + 2\,\varepsilon_1 \qquad (3)$$

with the horizontal axis.

It should be clear how to continue. Above the point x_k the particle, whose trajectory has angle of inclination

$$\theta_{k-1} = \theta_0 + 2 \sum_{i=1}^{k-1} \varepsilon_i \qquad (4)$$

strikes the boundary with angle ε_k, since the boundary is inclined at the angle

$$\Phi_k = \theta_{k-1} + \varepsilon_k = \theta_0 + 2 \sum_{i=1}^{k-1} \varepsilon_i + \varepsilon_k. \qquad (5)$$

After reflection, the particle's trajectory makes the angle

$$\theta_k = \theta_0 + 2 \sum_{i=1}^{k} \varepsilon_i = \Phi_k + \varepsilon_k \qquad (6)$$

with the horizontal.

We now show that under the assumptions

$$\lim_{k \to \infty} \frac{\varepsilon_k + \varepsilon_{k+1}}{(x_{k+1} - x_k)^n} = 0 \quad \text{for every } n \geq 1 \qquad (7)$$

and

$$\text{the sequence } \left(\frac{\varepsilon_{k+1}}{\varepsilon_k} \right)_{k \geq 1} \text{ is bounded away from 0 and } \infty, \qquad (8)$$

we can define a function $f \in C^\infty (x_0 - \delta, x_\infty + \delta)$ so that

$$\frac{f(x_{k+1}) - f(x_k)}{x_{k+1} - x_k} = \tan \theta_k \qquad (9)$$

(that is, chords of the graph of f are segments of the trajectory)

and

$$f'(x_k) = \tan \Phi_k \qquad (10)$$

(the function has the right slope at each point of collision).

It is obvious that the values of f and f' at the points x_k are determined by the sequences (x_k), (ε_k), and the numbers θ_0 and $f(x_0)$. For brevity, we denote these values of f and f' by f_k and f_k', respectively.

If such a function f exists, it is possible to define a sequence of functions $g_k \in C^\infty [0,1]$, $k = 1,2,\cdots$, by

$$g_k(t) = \frac{1}{\varepsilon_k} \left\{ \frac{f(x_k + t(x_{k+1} - x_k)) - f_k}{x_{k+1} - x_k} - tf'_k \right\}, \quad 0 \le t \le 1 \tag{11}$$

Our object will be to reverse this procedure, constructing a sequence $\{g_k\}$ which will be used to interpolate the values of f. Simple computation shows that the functions g_k must satisfy:

$$g_k(0) = g'_k(0) = 0 \tag{12}$$

$$g_k(1) = \frac{1}{\varepsilon_k}\left(\frac{f_{k+1}-f_k}{x_{k+1}-x_k} - f'_k\right) = \frac{1}{\varepsilon_k}(\tan\theta_k - \tan\Phi_k) \equiv c_k \tag{13}$$

$$g'_k(1) = \frac{1}{\varepsilon_k}(f'_{k+1} - f'_k) = \frac{1}{\varepsilon_k}(\tan\Phi_{k+1} - \tan\Phi_k) \equiv b_k \tag{14}$$

Notice that $b_k > c_k$, and because of (8) all b_k, c_k are bounded above by some constant times $\sup_k \sec^2\Phi_k$, and are bounded away from 0.

The second and higher derivatives of the g_k's must satisfy a compatibility condition at the end points; in particular:

$$\frac{\varepsilon_k}{x_{k+1}-x_k}\, g''_k(1) = \frac{\varepsilon_{k+1}}{x_{k+2}-x_{k+1}}\, g''_{k+1}(0). \tag{15}$$

We shall construct f by defining a sequence $(g_k)_{k \ge 1}$ satisfying (12) - (16),

$$g_k^{(n)}(0) = 0 = g_k^{(n)}(1) \quad \text{for } n \ge 3, \tag{16}$$

in such a way that the $\{g_k^{(n)}\}$ are uniformly bounded in k for each $n = 0,1,2,\cdots$. Then f is defined by

$$f(x_k + t(x_{k+1} - x_k)) = f_k + (x_{k+1} - x_k)(\varepsilon_k g_k(t) + tf'_k)$$

$$(0 \leq t < 1, \; k = 1,2,\cdots) \tag{17}$$

and f will be C^∞ up to x_∞ because for every $n \geq 2$:

$$f^{(n)}(x_k + t(x_{k+1} - x_k)) = \frac{\varepsilon k}{(x_{k+1}-x_k)^{n-1}} g_k^{(n)}(t) \to 0 \text{ as } k \to \infty$$

by (7) and the uniform boundedness in k of all sequences $\{g_k^{(n)}\}_{k \geq 1}$.

It should be noted that it is easy to construct an f if we satisfy (15) by taking $g''_k(0) = g''_k(1) = 0$ for all k. Then the g''_k can be taken to be translates of a single bump function. What is of interest about our construction is that it yields a boundary whose curvature is positive on (x_0, x_∞), vanishing only at x_∞. We shall see later that it is necessary that the curvature of the boundary vanish at an accumulation point of collisions, and anyhow because of (7) we have

$$\frac{\varepsilon_k + \varepsilon_{k+1}}{x_{k+1} - x_k} = \frac{\text{arc tan } f'_{k+1} - \text{arc tan } f'_k}{x_{k+1} - x_k}$$

$$= \frac{d}{dx} \text{arc tan } f'(x)\Big|_{x_k + t(x_{k+1} - x_k)} \qquad (0 < t < 1)$$

$$= f''/(1 + f'^2)\Big|_{x_k + t(x_{k+1} - x_k)} \to 0 \text{ as } k \to \infty .$$

To begin the construction, define

$$\sigma_k = \varepsilon_{k-1}/(x_k - x_{k-1}). \tag{18}$$

Then (15) will be satisfied if we put

$$g_k''(0) = \sigma_k, \; g_k''(1) = \sigma_{k+2}. \tag{19}$$

We construct the sequence $\{g_k\}$ by defining a sequence of functions $h_k \in C^\infty(0,1)$ so that $\{h_k^{(n)}\}_{k\geq 1}$ is uniformly bounded for $n = 0,1,2,\cdots$, and

$$0 < g_k''(t) \equiv \sigma_k + b_k \int_0^t h_k(s)ds, \; 0 \leq t \leq 1, \tag{20}$$

where b_k was defined in (14). Write down the integrals for g_k' and g_k in terms of h_k, invert the order of integration, and use (12), (13), (14) and (19) to arrive after simple computations at the other requirements on the h_k:

$$\int_0^1 h_k(t)dt = (\sigma_{k+2} - \sigma_k)/b_k \tag{21}$$

$$\int_0^1 t\, h_k(t)dt = -1 + \sigma_{k+2}/b_k \tag{22}$$

$$\int_0^1 t^2\, h_k(t)dt = -2(1 - c_k/b_k) + \sigma_{k+2}/b_k. \tag{23}$$

By (5), (6), (8), (13), (14) it is easy to see that the ratios c_k/b_k are bounded away from 0 and 1; since $\sigma_k \to 0$ by (7) and (18), we can find an index k_0 and a positive number δ so that for $k \geq k_0$:

$$-1 < -1 + \sigma_{k+2}/b_k < -1 + \delta \tag{24}$$

$$-2 + 4\delta < -2\,(1 - c_k/b_k) + \sigma_{k+2}/b_k < -4\delta. \tag{25}$$

To define the h_k's, let $\rho \in C^\infty(\mathscr{R})$ with support in $(-\frac{1}{2}\delta\,, \frac{1}{2}\delta\,)$ be such that $\int \rho(t)dt = 1$ and $\rho(t) = \rho\,(-t)$. We choose parameters

$\mu_k \in (\delta/2,\ 1 - 3\ \delta/2)$ and $a_k \in (1/(2\delta),\ 2/\delta)$ so that by defining

$$h_k(x) = \left(a_k + \frac{\sigma_{k+2}}{b_k}\right) \rho(x - \mu_k) - \left(a_k + \frac{\sigma_k}{b_k}\right) \rho(x - \mu_k - \delta)$$
$$(0 \le x \le 1)$$

we get functions which satisfy (22) and (23) (it is easy to see that (20),(21) and the uniform boundedness are satisfied automatically).

The integrals $\int_0^1 x\ h_k(x)dx$ and $\int_0^1 x^2 h_k(x)dx$ are easy, if tedious, to compute explicitly. Change variables to $x - \mu_k$ or $x - \mu_k - \delta$ in the integrands and use the support and symmetry properties of ρ which imply

$$\int t\rho(t)dt = 0 \qquad (27)$$

$$\int t^2 d/\rho\ (t)dt = \frac{\delta^2}{4}\theta \quad \text{for some } 0 < \theta < 1. \qquad (28)$$

After somewhat lengthy but entirely elementary computation, one finds

$$\int_0^1 x\ h_k(x)dx = -\ a_k\delta + \frac{\sigma_{k+2} - \sigma_k}{b_k}\ \mu_k - \frac{\sigma_k}{b_k}\ \delta \qquad (29)$$

$$\int_0^1 x^2 h_k(x)dx = -\ a_k\delta(2\mu_k + \delta) + \frac{1}{b_k}\Big[(\sigma_{k+2} - \sigma_k)\ \mu^2 - 2\sigma_k\ \delta\mu_k - \sigma_k\delta^2 + (\sigma_{k+2} - \sigma_k)\ \frac{\delta^2}{4}\theta\Big] \qquad (30)$$

and it remains only to show that a_k and μ_k may be chosen to satisfy (22) and (23). For the expression (29) (resp. (30)) write $f_1(a,\mu)$ (resp. $f_2(a,\mu)$), and denote the quantity in (24) (resp. (25)) by ξ_k (resp. η_k). Then our problem is to find in the rectangle

$$F = \left\{(a,\mu) \mid 1/(2\delta) < a < 2/\delta,\ \delta/2 < \mu < 1 - 3\delta/2\right\}$$

a solution of the equations

$$f_1(a,\mu) = \xi_k \qquad (31a)$$

$$f_2(a,\mu) = \eta_k \qquad (31b)$$

for (ξ_k,η_k) in the rectangle determined by (24), (25).

From the many ways to solve this problem, we choose Newton's method, since an initial approximation immediately suggests itself: we take $a_k^{(0)} = -\xi_k/\delta, \mu_k^{(0)} = \frac{1}{2}(\eta_k/\xi_k - \delta)$, so that equations (31a-b) are satisfied up to terms of order $\sigma_k + \sigma_{k+2}$. Then the first Newton iterate $(a_k^{(1)},\mu_k^{(1)})$ satisfies

$$(a_k^{(1)},\mu_k^{(1)}) - (a_k^{(0)},\mu_k^{(0)}) < \text{const } (\sigma_k + \sigma_{k+2})$$

with a constant which is independent of k. Now $\sigma_k \longrightarrow 0$ implies that for large enough k the hypotheses of Theorem 3 of [Isaacson and Keller, p. 115] are satisfied; the initial guess and all iterates lie in F and the iterates converge to a solution of (31a-b). Alternatively, use (31a) to eliminate a from (31b) and solve the resulting quadratic equation for μ using the same $\mu_k^{(0)}$ and Problem 3 [Isaacson and Keller, p. 123].

The remainder of this section is devoted to showing that the two examples given essentially exhaust the possibilities for a single particle in a plane region: roughly speaking, the particle must be caught in a cul de sac or it must rattle up to a point of zero curvature.

<u>Proposition II.C.1</u> Let Λ be a region in the plane bounded by a piecewise C^3 curve, and let $\mathcal{O} \in \partial\Lambda$ be the unique accumulation point of collisions over a finite distance for some trajectory in Λ which is linear in Λ and obeys the law "angle of incidence at $\partial\Lambda$ equals angle of reflection."

If infinitely many collision points of the trajectory lie on each side of $\mathcal{O}$, then the left and right tangents to $\partial\Lambda$ at $\mathcal{O}$ make angle 0 with each other.

<u>Proof</u>: (Figure 4) The hypotheses imply that the set of collisions for which the next collision occurs on the opposite side of $\mathcal{O}$ is cofinal in the sequence of all collisions of the given trajectory. Notice also that when the trajectory leaves some point of the boundary, making an angle $\theta > 0$ with the tangent there, its next collision cannot be on the same side unless the tangent turns at least through an angle θ.

Assume that the left and right tangents to $\partial\Lambda$ at $\mathcal{O}$ make angle $\alpha > 0$ with each other. Let $\varepsilon < \alpha/4$.

Let P and Q be consecutive collision points on opposite sides of $\mathcal{O}$, close enough to $\mathcal{O}$ that the angle $Q\mathcal{O}P$ is greater than $\alpha - \varepsilon/2$, and the absolute curvature of $\partial\Lambda$, integrated from Q to $\mathcal{O}$ or from P to $\mathcal{O}$, is less than $\varepsilon/8$. This implies that the angle between $\mathcal{O}P$ (resp. $\mathcal{O}Q$) and the tangent to $\partial\Lambda$ at P (resp. Q) is less than $\varepsilon/4$, and that if the trajectory reaches Q with incidence angle greater than $\alpha/2$ its next collision must be on the P side.

Let R be a point on the extension of $\mathcal{O}Q$ through Q.

Then (incidence angle at Q) $> \angle PQR - \varepsilon/4$.

But $\angle PQR = \angle \mathcal{O}PQ + \angle Q\mathcal{O}P$.

Now, $\angle\, \mathcal{O}PQ >$ (incidence angle at P) $- \varepsilon/4$, and $\angle\, Q\mathcal{O}P > \alpha - \varepsilon/2$ by hypothesis.

Thus (incidence angle at Q) $>$ (incidence angle at P) $+ \alpha - \varepsilon$, and after at most $(\pi/2)/(\alpha/2)$ collisions on alternate sides of 0, and particle will be headed out of the corner.

<u>Proposition II.C.2</u> Let $\underline{x}(s)$ be a smooth (C^r, $r \geq 3$) curve in the plane parametrized by arc length, along which some trajectory has infinitely many reflections in finite time. Assume that after a certain time all collisions of this trajectory take place on one side of the accumulation point. Denote by $k(s)$ the curvature at the point $\underline{x}(s)$. Then $dk/ds = 0$ infinitely often in the neighborhood of the accumulation point, and k and all its derivatives vanish at the accumulation point.

<u>Proof</u>: We show first that $k \to 0$.

Denote the point of the j^{th} collision by $\underline{x}_j = \underline{x}(s_j)$. Let τ_j be the length of the trajectory (chord) from $\underline{x}_j$ to $\underline{x}_{j+1}$, δ_j the corresponding arc length. Write $\underline{t}$ for the unit tangent, $\underline{n}$ for the unit normal, and let Φ be the angle the incident trajectory makes with $\underline{n}(s_j)$ at $\underline{x}_j$. Then

$$\underline{x}_{j+1} = \underline{x}_j + \tau_j\,(\sin\Phi\,\underline{t} + \cos\Phi\,\underline{n})$$

$$\underline{x}_{j-1} = \underline{x}_j + \tau_{j-1}\,(-\sin\Phi\,\underline{t} + \cos\Phi\,\underline{n})$$

Expand $\underline{x}_{j+1}$ and $\underline{x}_{j-1}$ in terms of arc length about $\underline{x}_j$:

$$\underline{x}_{j+1} = \underline{x}_j + \delta_j\,\underline{t} + \frac{1}{2}k\,\delta_j^2\,\underline{n} + \mathcal{O}(\delta_j^3)$$

$$\underline{x}_{j-1} = \underline{x}_j - \delta_{j-1}\,\underline{t} + \frac{1}{2}k\,\delta_{j-1}^2\,\underline{n} + \mathcal{O}(\delta_{j-1}^3)$$

Equate tangent and normal components:

$$\tau_j \sin\Phi = \delta_j + \mathcal{O}(\delta_j^3) \qquad \tau_j \cos\Phi = \frac{1}{2} k\,\delta_j^2 + \mathcal{O}(\delta_j^3)$$

$$\tau_{j-1} \sin\Phi = \delta_{j-1} + \mathcal{O}(\delta_{j-1}^3) \qquad \tau_{j-1} \cos\Phi = \frac{1}{2} k\,\delta_{j-1}^2 + \mathcal{O}(\delta_{j-1}^3) \,. \tag{1}$$

Now suppose that beyond a certain index j_0 we have $k(s_j) \neq 0$; since we always assume $\Phi \neq 0, \frac{\pi}{2}$ we may divide the first of each pair of equations in (1) by the second to obtain:

$$\frac{\delta_j}{\delta_{j-1}} \frac{1 + \mathcal{O}(\delta_j^2)}{1 + \mathcal{O}(\delta_{j-1}^2)} = \frac{\tau_j}{\tau_{j-1}} = \frac{\delta_j^2}{\delta_{j-1}^2} \frac{1 + \frac{1}{k}\mathcal{O}(\delta_j)}{1 + \frac{1}{k}\mathcal{O}(\delta_{j-1})} \,.$$

Our assumption that $\lim_{s \to s_\infty} k(s) \neq 0$ implies that $1/k = O(1)$ as $j \to \infty$.

This implies

$$\frac{\delta_j}{\delta_{j-1}} = \frac{1 + \mathcal{O}(\delta_j^2)}{1 + \mathcal{O}(\delta_{j-1}^2)} \cdot \frac{1 + \mathcal{O}(\delta_{j-1})}{1 + \mathcal{O}(\delta_j)}$$

so there is a constant $B > 0$ so that beyond some index j_1 we have

$$\frac{\delta_j}{\delta_{j-1}} > 1 - B(\delta_j + \delta_{j-1}).$$

But since $\Sigma\delta_j < \infty$ the next lemma shows this to be impossible. The stated result is actually a corollary of a more general fact:

<u>Lemma II.C.1</u>. Let Σa_k be a convergent series of positive terms. Then $(a_{k+1} - a_k)/(a_{k+1} + a_k)^2$ is not bounded below.

Proof: Put $r_k = a_{k+1}/a_k$; then $\frac{a_{k+1} - a_k}{(a_{k+1} + a_k)^2} = \frac{1}{a_k} \cdot \frac{r_k - 1}{r_k^2 + 1}$, so the result is obvious unless $r_k \to 1$. In that case it suffices to show $(a_{k+1}-a_k)/a_k^2$ is not bounded below. If $(a_{k+1} - a_k)/a_k^2 \geq -B$ for all k, we have

$$a_k - a_{k+1} \leq Ba_k^2, \quad \text{or} \quad a_{k+1}/a_k \geq 1 - Ba_k.$$

Let k be so large that $n \geq k \implies a_n B < \frac{1}{2}$. Then

$$a_{k+2} \geq a_{k+1}(1 - Ba_{k+1}) \geq a_k(1 - Ba_k)\ (1 - Ba_{k+1}),$$

and for $p \geq 2$,

$$a_{k+p} \geq a_k \prod_{j=1}^{p-1} (1 - B\ a_{k+j}).$$

But the infinite product converges if $\prod_j (1 + Ba_{k+j})$ converges, which it does because $\sum_j Ba_{k+j}$ converges. This implies $a_{k+p} \not\to 0$, which is absurd, and the Lemma is proven.

Return to the proof of Proposition II.C.2. If $\frac{\delta_j}{\delta_{j-1}} > 1 - B(\delta_{j-1}+\delta_j)$ for $j > j_1$, repeat the argument of the Lemma and deduce from convergence of the product $\prod_{k\geq 1} [1 - B(\delta_{j_1-1+k} + \delta_{j_1+k})]$ the result $\delta_{j_1+k} \not\to 0$, which contradicts $\sum \delta_j < \infty$.

It remains to show that dk/ds has a zero in every neighborhood of the accumulation point. Then Rolle's theorem will imply that any higher derivatives of k which exist must also vanish at the accumulation point.

Consider again the j^{th} collision point, and suppose that $dk/ds < 0$ for $s_{j-1} \leq s \leq s_{j+1}$. Consider the osculating circle $\mathcal{O}$ of $\underline{x}$ at $\underline{x}_j$, i.e. the circle of center $\underline{x}_j + \frac{1}{k(s_j)}\ \underline{n}\ (s_j)$ and radius $\frac{1}{k(s_j)}$. If k and k' have no zeroes between s_{j-1} and s_{j+1}, an elementary argument [Stoker pp. 29-31] shows that the portion of the curve from $\underline{x}_{j-1}$ to $\underline{x}_j$ lies inside O, and the portion from $\underline{x}_j$ to $\underline{x}_{j+1}$ lies outside O. (In fact, under these assumptions, no two osculating circles O(s') and O(s") for $s_{j-1} \leq s' < s'' \leq s_{j+1}$ have a point in common.)

From this we deduce that the chord from $\underline{x}_{j-1}$ to $\underline{x}_j$ has length

$$\tau_{j-1} < \frac{2}{k(s_j)} \cos \Phi$$

and that

$$\tau_j > \frac{2}{k(s_j)} \cos \Phi .$$

In particular $\tau_j > \tau_{j-1}$. Evidently we must have $\tau_j \leq \tau_{j-1}$ infinitely often to obtain convergence; therefore dk/ds must vanish infinitely often in the neighborhood of the accumulation point.

III. INFINITELY MANY PARTICLES

A. The Sequence of Finite Systems

For all configurations $x \in \mathscr{X}$ and integers $R \geq 1$ define the partial flow $T_R^t(x)$ by placing an elastically reflecting wall at $|q| = R$, fixing all particles not entirely inside it, and letting the particles inside move according to the elastic reflection law.

Obviously there are initial configurations for which not all T_R can be defined for all time. That the set of all such configurations is null for every Gibbs state follows most simply from a conditional probability argument. Fix an integer $R \geq 1$, let

$$\Lambda = \{ |q| \leq R - a/2\}$$

and let

$$\mathscr{X} = \mathscr{X}_\Lambda \times \mathscr{X}_{\mathbb{R}^3 \setminus \Lambda}$$

be the familiar splitting of configurations into the part inside Λ and the part outside (note that a particle which is "inside" Λ is "entirely inside" the sphere of radius R about the origin). Let $\mathscr{A}$ be the σ-algebra generated by the coordinates of $\mathscr{X}_{\mathbb{R}^3 \setminus \Lambda}$, and B be the set of $x \in \mathscr{X}$ for which $T_R^t(x)$ does not extend to all time. It follows from the results of Chapter II that

$$\mu(B | \mathscr{A}) = 0 \text{ a.e.} \mu$$

so that $\mu B = 0$.

Hence for each R, T_R is defined for all time except on a set which is null for every Gibbs state. Taking the union over R of these null sets proves:

<u>Proposition III.A.1.</u> $\tilde{\mathscr{X}} = \{x \epsilon \mathscr{X} \mid T_R^t x$ exists for all t, for every $R = 1,2,\ldots\}$

has probability one for every Gibbs state.

Each T_R^t is evidently a measurable transformation of $\mathscr{X}$, because it affects only finitely many coordinates, and those measurably; the partial flows T_R have the further important property that every Gibbs state is <u>invariant</u> under them.

To see this, let R, Λ, $\mathscr{A}$ be as on the previous page, and let A be any measurable set in $\tilde{\mathscr{X}}$. Then

$$\mu A = \int \mu(A \mid \mathscr{A})\, d\mu$$

where $\mu(A \mid \mathscr{A})$ is the $\mathscr{A}$-Measurable function

$$\sum_n \frac{z^n}{n!} \int_{\Lambda^n} d\underline{q} \prod_{1 \leq i < j \leq n} I_{[\,|q_i - q_j| \geq a\,]} \prod_{\substack{1 \leq i \leq n \\ Y(q) \neq 0}} I_{[\,|q_i - q| \geq a\,]} \; I_A(\underline{q}, Y)$$

Now, $I_{T_R^t A}(x,Y) = I_A(T_R^{-t} x, Y)$, and it follows from Liouville's Theorem for the finite system in Λ that

$$\mu(T_R^t A|\mathscr{A}) = \mu(A|\mathscr{A}) \text{ a.e. } (\mu)$$

and therefore $\mu(T_R^t A) = \mu A$.

B. Probability Estimates for the Partial Flows.

Our goal is to construct the flow T^t on a subset $\hat{\mathscr{X}}$ of $\tilde{\mathscr{X}}$ to which the partial flows T_R converge in measure as $R \to \infty$. We do this by showing that for almost all initial configurations the motion of a given particle during a given finite interval of time is indepen-dnet of R once R is large enough.

To establish this requires some care. To see the dificulty, suppose that the motion of the particles in some configuration in Λ_R under T_R is known. In the motion of the same configuration under $T_{R'}$, where $R' > R$, say that a particle in Λ_R at $t = 0$ is influenced by the removal of the wall and the motion of the particles in $\Lambda_{R'} \setminus \Lambda_R$ if its $T_{R'}$ motion differs from its T_R motion.

A particle is influenced, then, if another particle is knocked into its path and the two suffer a collision under $T_{R'}$ which does not occur under T_R. This influence can be indirect: a particle's trajectory will be changed if one of its T_R collision-partners is knocked out of its path so that no collision takes place.

The reader can easily invent more complicated schemes. It is well known from computer simulation of hard-sphere systems that a slight disturbance of the collision history leads very soon to a dramatically different motion of the system.

The effect of the motion of the particles outside Λ_R can spread rapidly in two ways. The first occurs when many particles are lined up very close together. The chain estimate implies that very long chains occur with small probability.

The second way in which influence of a particle moves rapidly is by the high velocity motion of the particle itself. In a Maxwellian velocity distribution, arbitrary large velocities occur with positive probability. Here is an estimate of that probability.

Proposition III.B.1 (Free distance estimate)

Let Λ be a bounded measurable set in $\mathscr{R}^3$, and let T^t be a flow on $\tilde{\mathscr{X}}$ which leaves Gibbs states invariant. Let μ be a Gibbs state for $\mathscr{X}$ with inverse temperature β. Define

$$v_{max}(t) = v^{\Lambda}_{max}(t) = \sup_{q_i(t)\varepsilon\Lambda} |v_i(t)|$$

Then there is a constant M depending only on $\gamma < \frac{\beta}{2m}$ such that for any $\tau > 0$, $\lambda > 0$

$$\mu\left[\int_0^{\tau} v_{max}(t)dt > \lambda\right] < M\ |\Lambda|\ \exp\left(-\gamma\frac{\lambda^2}{\tau^2}\right)$$

Proof: For $x\varepsilon\tilde{\mathscr{X}}$ let $\psi_1(x) = \exp\left\{\gamma\left(\frac{1}{\tau}\int_0^{\tau} v_{max}(t)dt\right)^2\right\}$ for some $0 < \gamma < \frac{\beta}{2m}$.

Since $\frac{dt}{\tau}$ is a probability on $[0,\tau]$ and $\exp\{\gamma(\cdot)^2\}$ is convex, we have by Jensen's inequality

$$\psi_1(x) \leq \frac{1}{\tau}\int_0^\tau \exp\left(\gamma v_{max}^2(t)\right)dt \equiv \psi_2(x).$$

Now ψ_2 is μ-integrable, for by Tonelli's theorem, the positive function $\exp[\gamma v_{max}^2(t)](x)$ is integrable over $[0,\tau]\times\mathscr{X}$ if either iterated integral is finite. But

$$\int_{\mathscr{X}} d\mu \exp\left(\gamma v_{max}^2(t)\right) = \int_{\mathscr{X}} d\mu \exp\left(\gamma v_{max}^2(0)\right)$$

because μ is invariant under T^t, so that $v_{max}(t)$ has the same distribution as $v_{max}(0)$. The last integral is $\leq M|\Lambda|$ for constant M depending only on γ, by the basic estimates for velocities in Gibbs states.

Therefore,

$$\int \psi_1 d\mu \leq \int \psi_2 d\mu \leq M|\Lambda|.$$

Finally,

$$\left\{\int_0^\tau v_{max}(t)dt > \lambda\right\} = \left\{\exp\{\gamma(\frac{1}{\tau}\int_0^\tau v_{max}(t)dt)^2\} > \exp\left(\gamma\frac{\lambda^2}{\tau^2}\right)\right\},$$

so that from the fact that for $X \geq 0$, $\mu[X>\lambda] \leq \frac{1}{\lambda}EX$ we deduce

$$\mu\left\{\int_0^\tau v_{max}(t)dt > \lambda\right\} \leq M|\Lambda| \exp\left(-\gamma\frac{\lambda^2}{\tau^2}\right)$$

and the proof is complete.

Fix notation for the remainder of Section B:

$R \geq 2$ is an integer.

μ is a Gibbs state for $\mathscr{X}$ with inverse temperature β.

$\gamma < \frac{\beta}{2m}$, M, are constants from the free distance estimate.

C_0 is the constant in the chain estimate of Chapter I.

$\Lambda_R = \{|q| \leq R\}$ is the sphere of radius R.

Now let $\alpha > 5/2$, $c > 0$. For any such α and c we shall find a set of full measure on which global solutions of the equations of motion are defined and enjoy certain regularity properties.

If λ is a real number, the symbol $\lceil \lambda \rceil$, "ceiling of λ", denotes the least integer greater than or equal to λ.

Having fixed α and c, we define η and ω constants, and N_R and τ which depend on R, by

(1) $\eta = 3\alpha/5$

(2) $\omega \varepsilon (\alpha - \eta, \eta - \frac{1}{2})$

(3) $N_R = \left\lceil \frac{c}{2a} (\log R)^{2\alpha/5} \right\rceil$

(4) $\tau = (\log R)^{-\eta}$

It follows from this that

(5) $\eta - \frac{1}{2} > \omega > \alpha - \eta = 2\alpha/5 > 1$

(6) $2(\eta - \omega) > 1$

Finally, take R large enough that

(7) $4(\log R)^{-\omega} < a$

(8) $(\log R)^{-\omega} < \frac{c}{8} (\log R)^{2\alpha/5}$.

We are now ready to prove a series of probability estimates which not only give strong control on the T_R, but also have a more general application.

For the application, assume that S^t is a 1-parameter group of transformations of $\mathscr{X}$ leaving every Gibbs state invariant, such that for almost every $x \varepsilon \mathscr{X}$ the trajectory $\{x(t) = S^t x \mid -\infty < t < \infty\}$ is a solution of the equations of motion.

Our estimates will show that requiring S^t to be measure-preserving leads to very nice regularity properties of its trajectories.

Lemma III.B.1 For $T_R^{\ t}$ consider $x \varepsilon \tilde{\mathscr{X}}$; for S^t take any $x \varepsilon \mathscr{X}$.

Put $$v_{max}(t) = v_{max}^{(R)}(t) = \sup_{q_i(t) \varepsilon \Lambda_R} |v_i(t)|$$

Let A_R be the event that either

$$\text{a)} \int_0^\tau v_{max}(t)dt > \frac{1}{2} (\log R)^{-\omega}$$

or b) there are N_R particles $q_{i_1}, \ldots, q_{i_{N_R}} \varepsilon \Lambda_R$ with

$$|q_{i_j} - q_{i_{j+1}}| \leqslant a + 4(\log R)^{-\omega} \qquad 1 \leqslant j \leqslant N_R - 1.$$

$$\text{Then } \mu A_R \leqslant |\Lambda_R| \left\{ M \exp\left(-\frac{\gamma}{4}(\log R)^{\ 2(\eta-\omega)}\right) + N_R! \left(\frac{4C_o}{a(\log R)^\omega}\right)^{N_R-1} \right\}$$

Proof: Immediate from the free distance estimate and the chain estimate. In the free distance estimate we use $\tau = (\log R)^{-\eta}$, $\lambda = \frac{1}{2}(\log R)^{-\omega}$. In the chain estimate we have $\varepsilon_j = \dfrac{4}{a(\log R)^\omega} < 1$ by (7).

This lemma has an immediate extension. If $t_o > 0$, we let

$$K = \left\lceil t_o \; (\log R)^{3\alpha/5} \right\rceil .$$

For fixed k, $0 \leq k < K$ we define the event $B_{R,k}$ by

a) $$\int_{k\tau}^{(k+1)\tau} v_{max}(t)dt > \tfrac{1}{2}(\log R)^{-\omega}$$

or b) At time $k\tau$ there are N_R particles $q_{i_1}, \ldots, q_{i_{N_R}} \varepsilon \Lambda_R$ with

$$|q_{i_j}(k\tau) - q_{i_{j+1}}(k\tau)| \leq a + \frac{4}{(\log R)^{\omega}} .$$

Then by the invariance of μ under T_R^t or S^t, $\mu B_{R,k} = \mu A_R$. This proves

<u>Lemma III.B.2.</u> Let $B_R = \bigcup_{k=0}^{K-1} B_{R,k}$. Then $\mu B_R \leq K\mu A_R$.

Direct application of these estimates gives the desired regularity property of the trajectories. In the following Proposition, where the partial flows T_R are considered, each set B_R is defined by the motion under the corresponding T_R of the particles in Λ_R.

<u>Proposition III.B.2</u> For either the family of partial flows $\{T_R: \; R = 1,2,\ldots\}$ or any one parameter group S^t of transformations of $\mathscr{X}$ which leave all Gibbs states invariant and almost all of whose trajectories are solutions of the equations of motion, there is a measurable subset $\hat{\mathscr{X}}$ of $\mathscr{X}$ with the following properties:

a) $\mu \hat{\mathscr{X}} = 1$ for every Gibbs state μ.

b) For each $x \varepsilon \hat{\mathscr{X}}$ and t_o positive there is an $R_o = R_o(x,t_o)$ such that if $R > R_o$

i) there is <u>no</u> subinterval $I \subset [-t_o, t_o]$ of length

$\tau(R) = (\log R)^{-3\alpha/5}$

for which $\int_I v_{max}(t)dt > (\log R)^{-\omega}$

ii) At no time $t \varepsilon [-t_o, t_o]$ is there a chain of $N = N_R$ particles $q_{i_1}(t), \ldots, q_{i_{N_R}}(t) \; \varepsilon \Lambda_R$ such that

$$|q_{i_j}(t) - q_{i_{j+1}}(t)| \leqslant a + 2(\log R)^{-\omega} \qquad 1 \leqslant j < N_R.$$

Proof: Let B_R be as in the preceeding lemma, with $t_o = k$, and let $\mathscr{X}_k = [B_R \text{ i.o.}]^c$. We show $\sum_R \mu B_R < \infty$, so by the Borel-Cantelli Lemma $\mu \mathscr{X}_k = 1$.

By Lemmas III.B.1-2 write the upper bound for μB_R as the sum of two terms. The first is

$$K|\Lambda_R| \; M \exp\left(-\frac{\gamma}{4}(\log R)^{2(\eta-\omega)}\right) = \left[k(\log R)^{3\alpha/5}\right] \frac{4}{3} \pi R^3 \exp\left(-\frac{\gamma}{4}(\log R)^{2(\eta-\omega)}\right),$$

and since $2(\eta-\omega) > 1$ by equation (6) above this term is summable in R.

The second term is

$$K|\Lambda_R| \; N_R![4 \; C_o \; a^{-1}(\log R)^{-\omega}]^{N_R - 1}$$

$$= \left[k(\log R)^{3\alpha/5}\right] \frac{4}{3} \pi R^3 \; \Gamma(N_R + 1) \exp\{-\omega(N_R - 1) \log \log R + O(N_R)\}$$

Since $N_R = \left[\frac{c}{2a} (\log R)^{\alpha-\eta}\right]$, we have from Stirling's formula:

$$\Gamma(N_R + 1) = \exp\{N_R\,(\alpha-\eta)\log\log R + O(N_R)\},$$

so the term in question is

$$\left[k(\log R)^{3\alpha/5}\right] \frac{4}{5}\pi R^3 \exp\{(\alpha-\eta-\omega)\frac{c}{2a}(\log R)^{\alpha-\eta}\log\log R + O(\log R)^{\alpha-\eta}\}$$

and the exponential goes to zero more rapidly than any inverse power of R because $\alpha - \eta - \omega < 0$ and $\alpha - \eta > 1$ by (5) above.

This completes the proof that $\Sigma\,\mu B_R < \infty$.

Next, if $x \varepsilon B_R^c$, there is no interval I of length $\tau(R)$ in $[0,k]$ for which the free distance $\int_I v_{max}(t)dt$ exceeds $(\log R)^{-\omega}$. For if there were, we could choose j so that

$$\int_{j\tau}^{(j+1)\tau} v_{max}(t)dt \geqslant \int_{I\cap[j\tau,(j+1)\tau]} v_{max}(t)dt \geqslant \tfrac{1}{2}(\log R)^{-\omega}$$

which is impossible because $x\varepsilon B_R^c$.

Moreover, if at any time t, $0 \leqslant t \leqslant k$, there were a chain of N_R particles $q_{i_1}(t),\ldots, q_{i_{N_R}}(t) \; \varepsilon \; \Lambda_R$ with $|q_{i_j}(t) - q_{i_{j+1}}(t)| < a + 2(\log R)^{-\omega}$ for $1 < j < N_R - 1$, then by taking the nearest time to t of the form $n\tau$ we would derive $|q_{i_j}(n\tau) - q_{i_{j+1}}(n\tau)| \leqslant$

$$|q_{i_j}(n\tau) - q_{i_j}(t)| + |q_{i_j}(t) - q_{i_{j+1}}(t)| + |q_{i_{j+1}}(t) - q_{i_{j+1}}(n\tau)|$$

$$< (\log R)^{-\omega} + a + 2(\log R)^{-\omega} + (\log R)^{-\omega} = a + 4(\log R)^{-\omega}$$

which again is not possible since $x\varepsilon B_R^c$.

Finally, we put $\hat{\mathscr{X}} = \bigcap_k \mathscr{X}_k$. Then $\mu\hat{\mathscr{X}} = 1$ and all $x\varepsilon\hat{\mathscr{X}}$ satisfy b) i) and ii). The proof is complete.

C. Construction of the Motion for the Infinite System.

The next lemma is the crucial one for our construction. It says that deep inside Λ_R the particles for some time do not notice the difference between T_R and $T_{R'}$, if $R' > R$.

We preserve the notations of (1) - (8) in the last section.

Lemma III.C.1. Let $x\varepsilon\hat{\mathscr{X}}$, $t > 0$; number the particles of x in the order of their distance from the origin, and for q_i let $R > R_o(x,t_o)$ be so large that

$$|q_i| + c\sqrt{1 + t_o^2}\,(\log 2R)^\alpha < \tfrac{1}{2}R\,.$$

Then for $R' = R + j$, $1 \leqslant j \leqslant R$, and for all t, $0 \leqslant t \leqslant t_o$

$$q_i^{(R)}(t) = q_i^{(R')}(t)$$

$$p_i^{(R)}(t) = p_i^{(R')}(t)$$

Proof: Say that a particle is marked at the infimum of the times for which its $T_{R'}$ motion differs from its T_R motion.

Then obviously all particles in $\Lambda_{R'}\setminus\Lambda_R$ (except those for which $p = 0$) are marked at time 0.

Take any particle of x which is inside Λ_R at $t = 0$, and which is marked at some time t_1, $0 \leq t_1 \leq t_o$. Call this particle 1. We show that particle 1 cannot be too far from $\partial \Lambda_R$ by constructing a chain of particles reaching from particle 1 to $\partial \Lambda_R$.

Set $k \leftarrow 1$

(*) If particle k gets marked by reaching $\partial \Lambda_R$ the chain terminates with particle k.

If particle k is inside Λ_R at time t_k, it gets marked because it collides under either T_R or $T_{R'}$ (or possibly in both, with distinct particles) with a particle which is already marked. Choose a marked particle with which particle k collides in either T_R or $T_{R'}$ -motion at time t_k. Call this particle k+1. It was marked at time t_{k+1}, where $0 \leq t_{k+1} < t_k$.

Set $k \leftarrow k+1$ and return to (*).

In this construction, the return to (*) is possible only finitely many times because only finitely many collisions occur under $T_{R'}$ and T_R during $[0,t_o]$.

A chain of, say, N particles has now been constructed, with $|q_N(t_N)| = R$.

Suppose that $R - |q_1(t_1)| > c\sqrt{1+t_o^2}\,(\log 2R)^{\alpha}$. Notice that

$$|q_N(t_N) - q_1(t_1)| \geq R - |q_1(t_1)| \,.$$

Divide the interval $[0,t_1]$ into sub-intervals of length $\tau(2R) = (\log 2R)^{-\eta} = (\log 2R)^{-3\alpha/5}$.

During each of these sub-intervals $[k\tau,(k+1)\tau]$ $\left(0 \leq k \leq \left\lceil \frac{t_o}{\tau} \right\rceil\right)$ no particle travels a distance greater than $(\log R)^{-\omega}$ in either the

T_R or $T_{R'}$ motion; however, there must be an index k with the following property:

Denote by q_{i_k} the first particle to be marked after time $k\tau$, $q_{i_{k+1}}$ the first particle to be marked after $(k+1)\tau$. Then

$$|q_{i_k}^{(R)}(k\tau) - q_{i_{k+1}}\big((k+1)\tau\big)| > \frac{3c}{4}(\log 2R)^{2\alpha/5} .$$

This is because $q_{i_k}^{(R)}(t_{i_k}) = q_{i_k}^{(R')}(t_{i_k}),\ 0 \leq k \leq [\frac{t_o}{\tau}]$,

and $$|q_{i_k}^{(R)}(t_{i_k}) - q_{i_k}^{(R)}(k\tau)| < (\log R)^{-\omega} .$$

But if we suppose $(\log R)^{-\omega} < \frac{c}{4}(\log 2R)^{2\alpha/5}$, this shows that we must have at least $\frac{c}{2a}(\log 2R)^{2\alpha/5} > \frac{c}{2a}(\log R)^{2\alpha/5} = N_R$ particles in Λ_R with mutual distance at most $2(\log R)^{-\omega}$, which by the Proposition of the last Section is impossible.

This shows that a particle which gets marked by time t_o lies within $c\sqrt{1+t_o^2}\,(\log 2R)^{\alpha}$ of $\partial\Lambda_R$. The proof is complete.

<u>Theorem III.C.1</u> (Existence) Let $x \varepsilon \hat{\mathscr{X}}$, $t_o \varepsilon \mathscr{R}$. Then $\lim_{R\to\infty} T_R^{t_o}x$ exists in the $\mathscr{X}$-topology.

Proof: Number the particles of x in the order of their distance from the origin. For each i, take R_i to be the R of the previous lemma: repeated application of that lemma shows that if $R' > R_i$,

$$q_i^{(R')}(t) = q_i^{(R)}(t)$$

$$p_i^{(R')}(t) = p_i^{(R)}(t)$$

for $0 \leq t \leq t_o$ or $t_o \leq t \leq 0$.

Thus, for each $i \geq 1$, $\lim_{R \to \infty} q_i^{(R)}(t_o) \equiv q_i^{(\infty)}(t_o)$ and

$\lim_{R \to \infty} p_i^{(R)}(t_o) \equiv p_i^{(\infty)}(t_o)$ exist and define a configuration $x(t_o) \in \mathscr{X}$.

(At a collision point, we agree that all momenta shall be incoming.)

Let $\Sigma\phi$ be any function among those which define the $\mathscr{X}$-topology, that is, ϕ is a function on $\mathscr{R}^3 \times \mathscr{R}^3$ whose support has compact projection on the first factor, and $\Sigma\phi(x) = \sum_{x(q,p) \neq 0} \phi(q,p)$. Let $K \subset \mathscr{R}^3$ be compact such that $\phi(q,p) = 0$ if $q \not\in K$. Take $R > R(x,t_o)$ so large that all translates of K by distances less than $c\sqrt{1+t_o^2}\ (\log R)^{\alpha}$ lie inside $\Lambda_{\frac{1}{4}R}$.

Then all particles of x which could reach K by time t_o are inside $\Lambda_{\frac{3}{4}R}$, hence have the correct motion under T_R up to time t_o. Therefore, in fact $x(t_o)|_K = T_{R'}^{t_o} x|_K$ for any $R' \geq R$, so $R' \geq R$ implies $\Sigma\phi(x(t_o)) = \Sigma\phi(T_{R'}^{t_o} x)$, and this finishes the proof.

The mapping from $\mathscr{R}$ into $\mathscr{X}$ given by $t \to x(t) = \lim_{r \to \infty} T_r^t x$ is evidently a solution of the equations of motion for any $x \in \mathscr{X}$, and the trajectories enjoy an important regularity property.

To state this property explicitly, we continue to preserve the notations of (1) - (8) for the numbers α, c, ω, and for positive integers R:

$$\tau(R) = (\log R)^{-3\alpha/5}$$

$$N_R = \left\lceil \frac{c}{2a} (\log R)^{2\alpha/5} \right\rceil$$

Definition: Let $x \in \mathscr{X}$. A map $\underline{x}: \mathscr{R} \to \mathscr{X}$ is called a regular solution of the equations of motion with initial point x if

i) $\{\underline{x}(t): -\infty < t < \infty\}$ is a solution of the equations of motion and $\underline{x}(0) = x$;

ii) only finitely many collisions, each involving only two particles, occur during any interval $[-t, t]$ in any Λ_R;

iii) given any $t > 0$, there is an $R_1(x,t)$ such that if $R > R_1$ then

a) there is no subinterval I of $[-t,t]$ of length $\tau(R)$ for which $\int_I v_{max}^{(R)}(t)dt > (\log R)^{-\omega}$;

and b) at no time $s \in [-t,t]$ is there a chain of N_R particles in Λ_R with mutual distances less than $a + (\log R)^{-\omega}$.

In terms of this definition, we can reformulate the result of Proposition III.B.2:

Proposition III.C.1. Let S^t be a 1-parameter group of Gibbs-state-preserving transformations of $\mathscr{X}$ whose trajectories are solutions of the equations of motion. The set of $x \in \mathscr{X}$ whose trajectories are regular solutions has probability one for every Gibbs state.

We mentioned in the introduction examples of configurations which are initial points of more than one solution of the equations of motion. If we allow only regular solutions, however, it is possible to establish a uniqueness result:

Theorem III.C.2 (Uniqueness) For any $x \in \mathscr{X}$ there is at most one regular solution of the equations of motion with initial point x.

Proof: Let $\underline{x}'(t)$, $\underline{x}''(t)$ be any regular solutions with $\underline{x}'(0) = \underline{x}''(0) = x$. If $\underline{x}'$ is not identical to $\underline{x}''$, there is a particle q_1 and a time $t_1 > 0$ so that $t_1 = \inf\{t > 0 \mid q_1'(t) \neq q_1''(t)\}$.

Let R be any number larger than the maximum of $R_1'(x,t_1)$, $R_1''(x,t_1)$, and $|q| = |q_1(0)|$.

As in the proof of Lemma III.C.1, say that a particle q of x is <u>marked at time t</u> if either

i) $t = 0$ and $|q| > R$

or ii) $t_1 \geq t > 0$ and $t = \inf\{s \mid q'(s) \neq q''(s) \text{ or } |q'(s)| \geq R\}$

In particular, q_1 is marked at time t_1.

Now use the fact that $\underline{x}'$ and $\underline{x}''$ have only finitely many collisions in Λ_R during $[0,t_1]$ to construct a chain of particles $q_1, q_2, \ldots q_n$ and corresponding times $t_1 > t_2 > \ldots t_n \geq 0$ so that q_i is marked at time t_i, $1 \leq i \leq n$ and $|q_n(t_n)| = R$.

(If this construction did not reach the boundary we would have a particle which before its first collision moved differently for $\underline{x}'$ and $\underline{x}''$ which is impossible because both are solutions.)

Next, supposing that $R - |q_1(t_1)| > c\sqrt{1+t_1^2}\,(\log R)^\alpha$, we argue exactly as in Lemma III.C.1 that, because of the velocity bound (condition (iii)(a) for a regular solution), the chain condition (iii)(d) must be violated.

Therefore, since $\underline{x}'$ and $\underline{x}''$ are regular solutions, we must have

$$|q_1(t_1)| > R - c\sqrt{1+t_1^2}\,(\log R)^\alpha$$

or, by the velocity bound,

$$|q_1(0)| > R - c\sqrt{1+t_1^2}\,(\log R)^{\alpha} - \frac{t_1}{\iota(R)}\,(\log R)^{-\alpha}\,.$$

but $R > \max\{R_1'(x_1 t_1),\ R_1''(z,t_1),\ |q_1(0)|\}$ was arbitrary. The proof is complete.

Let $\bar{\mathscr{X}}$ be the set of $x\varepsilon\mathscr{X}$ which are initial points of regular solutions. The existence theorem shows $\bar{\mathscr{X}} \supset \hat{\mathscr{X}}$, so regular solutions exist almost surely in every Gibbs state.

The first remark to make about $\bar{\mathscr{X}}$ is that if $x\varepsilon\bar{\mathscr{X}}$ so is $x(t_o)$ for any t_o. In fact, properties i) and ii) of the definition follow immediately from the fact that $\{x(t): -\infty < t < \infty\}$ is a regular solution, and to see that the bounds in part iii) hold for any $t > 0$ it is enough to take $R_1(x(t_o),t) = R_1(x,t + |t_o|)$. This proves

Proposition III.C.2 For all $x\varepsilon\bar{\mathscr{X}}$ define the time evolution mapping T^t to be the one-parameter group of shifts along the trajectory of the regular solution through x:

$$T^t_{(x)} = x(t)$$

Then $\bar{\mathscr{X}}$ is invariant under every T^t.

A further property of T^t is that it is measure-preserving.

Proposition III.C.3. Every T^t leaves all Gibbs states invariant.

Let μ be any Gibbs state, and let f be a bounded continuous function on $\mathscr{X}$. For each $x\varepsilon\mathscr{X}$ and r finite integer put $f_r(x) = f(T_r^{-t}x)$ and define $f_\infty(x) = f(T^{-t}x)$

Since $\lim_{r\to\infty} T_r^{-t}x = T_x^{-t}$ for all $x\varepsilon\tilde{\mathscr{X}}$, $f_r \to f_\infty$ a.s. $-\mu$, and therefore f_∞ is μ- measurable.

Moreover, the f_r $1 \leq r \leq \infty$, are uniformly bounded by $\|f\|_\infty$. Thus $\int f_\infty d\mu = \lim_{r \to \infty} \int f_r d\mu = \int f d\mu$, the last equality holding because μ is invariant under every T_R^t.

It now follows from the basic facts stated in Chapter I about Borel probability measures on Polish spaces that the measures μ and $\mu' = \mu \circ T^t$ are the same, because they agree on all bounded continuous functions. The proof is complete.

Using this result and Proposition III.C.1, it is possible to reformulate the uniqueness theorem so that the regularity condition does not appear explicitly.

Theorem III.C.3. Let $\mathscr{X}'$ be a subset of $\mathscr{X}$ whose complement is null for every Gibbs state, and let S^t be a one-parameter group of transformations of $\mathscr{X}'$ into itself such that

i) every trajectory $\{S^t x: -\infty < t < \infty\}$ is a solution of the equations of motion, and

ii) S^t leaves every Gibbs state invariant.

Then for all x in the complement of a set which is null for every Gibbs state, $S^t x = T^t x$ for all t.

REFERENCES

[Feller] Feller, W., An Introduction to Probability Theory and its Applications, Vol. 2, New York: John Wiley & Sons, Second Edition 1971.

[Lanford 1968] Lanford, O. E., III, One-Dimensional Systems of Infinitely Many Particles I: An Existence Theorem, Comm. Math. Phys. 9 (1968) 169-181.

[Lanford 1969] _____, One-Dimensional Systems of Infinitely Many Particles II: Kinetic Theory, Comm. Math. Phys. 11 (1969) 257 - 292.

[Lanford 1974] _____, Time Evolution of Large Classical Systems, in Proc. Battelle Rencontres on Dynamical Systems, Lecture Notes in Physics Vol. 38, Berlin: Springer-Verlag, 1975.

[Lanford and Ruelle] Lanford, O. E., III, and Ruelle, D., Observables at Infinity and States with Short-Range Correlations in Statistical Mechanics, Comm. Math. Phys. 13 (1969) 194-215.

[Marchioro et al. 1975a] Marchioro, C., Pellegrinotti, A., and Presutti, E., Existence of Time Evolution for ν-Dimensional Statistical Mechanics, Comm. Math. Phys. 40 (1975) 175-186.

[Marchioro et al. 1975b] Marchioro, C., Pellegrinotti, A., Presutti, E., and Pulvirenti, M., On the Dynamics of Particles in a Bounded Region: A Measure-Theoretical Approach, preprint.

[Ruelle 1969] Ruelle, D., Statistical Mechanics, Rigorous Results, New York: Benjamin, 1969.

[Ruelle 1970] _____, Superstable Interactions in Classical Statistical Mechanics, Comm. Math. Phys. 18 (1970) 127-159.

[Ruelle 1971] _____, Equilibrium Statistical Mechanics of Infinite Systems, in Statistical Mechanics and Quantum Field Theory, 1970 Les Houches Lectures ed. by C. DeWitt and R. Stora, Gordon and Breach 1971.

[Schwartz] Schwartz, L., Radon Measures on Arbitrary Topological Spaces and Cylindrical Measures, Tata Institute for Fundamental Research: Oxford University Press, 1973.

[Sinai 1972] Sinai, Ya. G., Construction of the Dynamics for One-Dimensional Systems of Statistical Mechanics, Teoret. Mat. Fiz. 11 (1972) 248 - 258. English Translation: Theor. Math. Phys., February 1973, 487 - 494.

[Sinai 1974] _______, The Construction of Cluster Dynamics for Dynamical Systems of Statistical Mechanics, Vestn. Mosk. Univ. Ser. I: Mat. - Meh. 29 (1974) 152 - 159. English Translation: Mosc. Univ. Math. Bull. 29 (1974) 124 - 130.

[Stoker] Stoker, J. J., Differential Geometry, New York: Wiley-Interscience, 1969.

[Isaacson and Keller] Isaacson, E., and Keller, H. B., Analysis of Numerical Methods, New York: John Wiley & Sons, 1966.

Figure 1

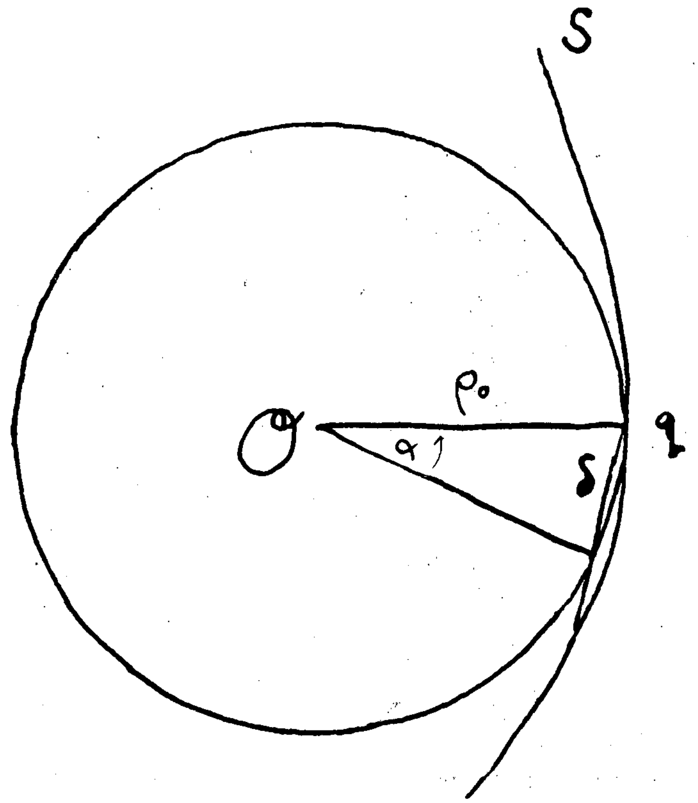


Figure 2

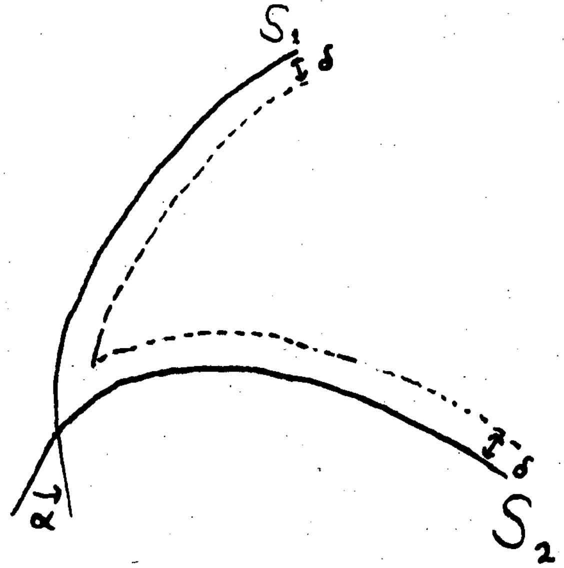


Figure 3

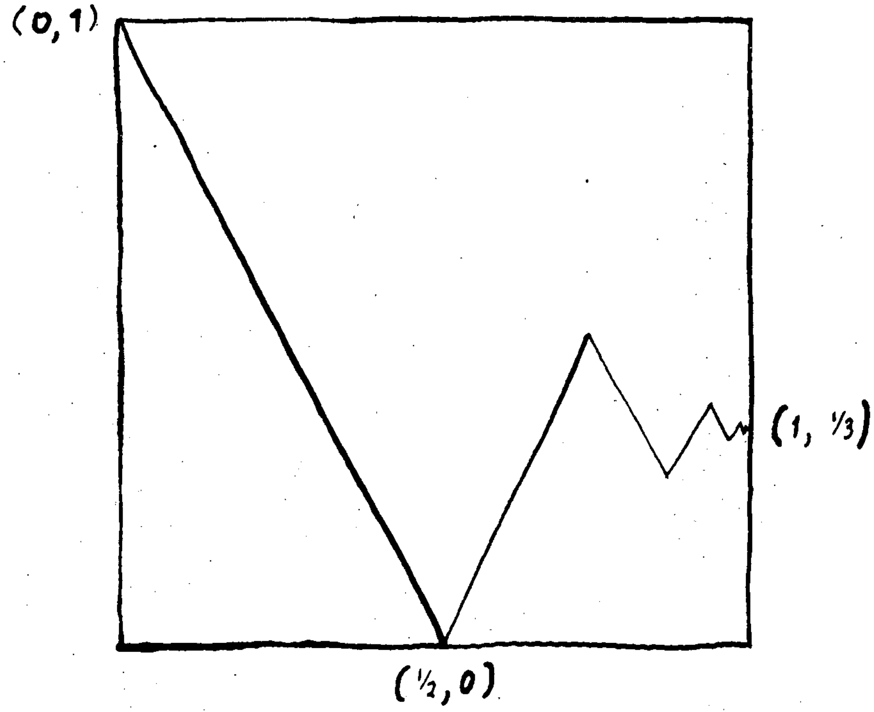
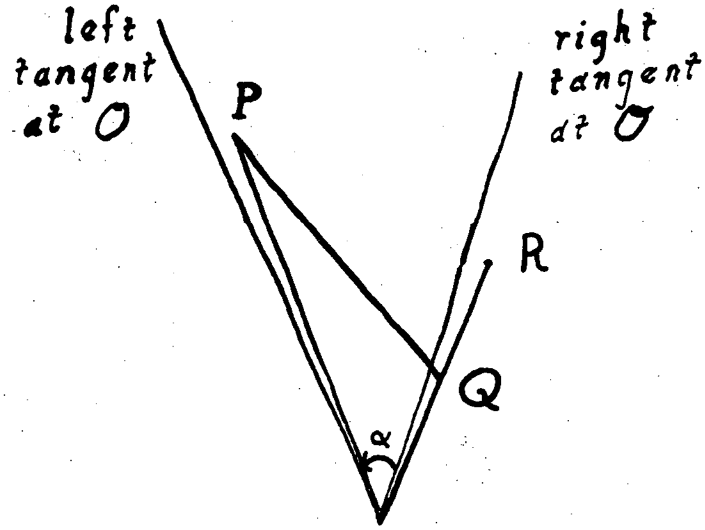


Figure 4



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