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Ya. G. SINAI

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Abstract

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Ya. G. SINAI

ON THE JUSTIFICATION OF THE ERGODIC HYPOTHESIS FOR A DYNAMICAL SYSTEM OF STATISTICAL MECHANICS

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In the book ([1]) N. S. Krylov, apparently, was the first to emphasize the necessity of mixing in systems of statistical mechanics for explaining phenomena of the type of irreversibility and relaxation. The calculation he carried out for a system of hard balls in a box with elastic collisions showed that the trajectories of this system possess the so-called property of exponential divergence. As is known, the investigations of E. Hopf ([6], [7]) of geodesic flows on surfaces of constant negative curvature, in which the mixing property was first noted, were based on this property. For N. S. Krylov, as a physicist, such a comparison was quite sufficient to confirm his views. However, if one approaches the matter formally, then a reference to Hopf' s work cannot be considered convincing for at least the following two reasons: first, Hopf' s considerations concerned only systems with two degrees of freedom, and, second, Hopf' s requirements on the exponential character of mixing were of a somewhat different nature than those observed by Krylov. For example, from E. Hopf' s conditions there follows the absence of conjugate points, which is by no means the case for the system considered by Krylov. The later interesting results of D. V. Anosov ([8]) are also inapplicable to this system.

The principal result of the present work should be considered the theorem on the ergodicity of a system of hard balls in a rectangular box. The proof of this theorem is based on a method founded on the concepts of entropy and of a K-system, introduced by A. N. Kolmogorov ([2]). As has been emphasized more than once, in the case of classical systems the positivity of entropy and the property of being a K-system are connected with the existence of so-called bundles of asymptotic trajectories, i.e., trajectories approaching one another with exponential speed (for details see ([3], [4])). It turns out that such bundles exist for the indicated system of hard balls. There is every reason to expect that this system is a K-system, but for the present this question remains open*.

§ 1. **A sufficient condition for the positivity of entropy.** It is well known that a classical dynamical system with m degrees of freedom, in which the coordinates $(q^1 \dots q^m)$ range over some smooth manifold Q (possibly with boundary), while the momentum vectors $p = (p_1, \dots, p_n)$ are covariant tangent vectors to Q and the Hamiltonian function has the form $H = \sum a^{ij}(q)p_i p_j + V(q)$, can, for fixed H, be realized as a geodesic flow in the space M of unit contravariant tangent vectors to Q, endowed with the Riemannian metric $ds^2 = (H - V(q)) \sum a_{ij}\, dq^i dq^j$. Assuming that such a reduction has already been made, let us consider the geodesic flow $\{S_t\}$ in the space M of unit tangent vectors to Q. In the case of a manifold with boundary we consider only such systems whose trajectories, represented as geodesics, upon reaching the boundary are reflected from it

* *Note added in proof.* At present this question has been resolved positively.

according to the law "the angle of incidence is equal to the angle of reflection," i.e., the geodesics undergo refraction at a boundary point, under which the tangential component of the tangent vector to the boundary is preserved, while the normal component changes sign. We denote the invariant measure for the group $\{S_t\}$ by μ ([6]). We denote the natural mapping $M \to Q$ by π. For each $q \in Q$ set $R_t(q) = S_t(R_0(q))$, $\widetilde{R}_t(q) = \pi(R_t(q))$, where $R_0(q) = \{x : \pi(x) = q\}$. For all t, $\widetilde{R}_t(q)$ is a piecewise-smooth manifold lying in Q. If $\pi(x) = q$ and $\pi(S_t x) = q' \in \widetilde{R}_t(q)$, then by $d\sigma_t(x)$ we denote the volume element on the manifold $\widetilde{R}_t(q)$ at the point q', induced by the invariant metric in Q (of course, under the assumption that q' is a regular point of $\widetilde{R}_t(q)$). Let $d\omega$ be the invariant volume on the $(n-1)$-dimensional sphere $R_0(q)$. With the aid of the geodesic flow it is transported from $R_0(q)$ to $R_t(q)$. We denote this transported volume on $\widetilde{R}_t(q)$ by $d\omega_t(x)$, $x \in R_0(q)$. Put $a_t(x) = d\sigma_t(x)/d\omega_t(x)$.

Theorem 1. *If the following three conditions A, B, C are fulfilled, the geodesic flow $\{S_t\}$ has positive entropy.*

A. For all $q \in Q_0$, where Q_0 has positive volume,

$$\liminf_{t\to\infty} \frac{1}{t} \int_{\widetilde{R}_t(t)} \log a_t(x)\, d\omega_t(x) > 0.$$

B. There exists a countable partition ξ of the space M with finite entropy into sets $C_1, C_2, ...$, such that for some constant a, for any connected component Γ of the intersection $R_t(q) \cap C_i$,

$$\int_{\pi(\Gamma)} d\sigma_t(x) < a.$$

C. Under the conditions of B, for some $\tau > 0$ the intersections $S_\tau \Gamma \cap C_i$, $i = 1, 2, ...$, are connected.

Concerning these conditions we note that condition A is apparently close to being necessary. Conditions B and C contain certain requirements on the regularity of the spheres $\widetilde{R}_t(q)$.

§ 2. **Application to some systems with two and four degrees of freedom.** Take in the plane (q_1, q_2) the unit square E^2. Let $V(r)$ be a monotonically decreasing function, $V(r) = 0$ for $r \geq r_0$, where $r_0 < 1/2$. Consider the motion of a material point of mass m, occurring inside E^2 under the action of forces having potential $U(q_1, q_2) = V(r)$, where

$$r = \sqrt{(q_1 - 1/2)^2 + (q_2 - 1/2)^2}.$$

As for the boundary of the square, the considerations of this paragraph are valid under any of the following three assumptions: 1) the moving point is reflected from the boundary of the square according to the law "the angle of incidence is equal to the angle of reflection" ; 2) the sides of the square are identified with one another so that a two-dimensional torus is obtained; 3) the sides of the square are identified with one another so that the projective plane is obtained. The law of conservation of energy has the form $H = \frac{m}{2}(\dot{q}_1^2 + \dot{q}_2^2) + U(q_1, q_2)$. For fixed H, the configuration space of the system is the region inside E^2 singled out by the inequality $r \geq r_1$, where r_1 is the unique solution of the equation $H = V(r_1)$ (naturally, here it is assumed that $H < V(0)$). The fact that $V(r)$ is a monotonically decreasing function indicates the character of the forces acting on the point: these forces are repulsive forces from the center of the square $(1/2, 1/2)$. A special case of such a system was considered in ([5]).

Theorem 2. *For fixed H there exist constants b_1, b_2 such that if $|V'(r)| > b_1$, $|V''(r)| < b_2$, then the dynamical system described above has positive entropy.*

Let us now consider on the torus T^2 obtained from the square E^2 naturally—

* We note that in these inequalities, for $r = r_0$ the left derivative is meant, and for $r = r_1$ the right derivative

with the natural identification of sides, the motion of two material points of masses m_1 and m_2, the interaction between which occurs with forces having potential $V(r)$, where r is the distance on the torus between the moving points.

Theorem 3. *Under the same assumptions as in Theorem 2, the system of two material points has positive entropy.*

§ 3. **A system of hard balls with elastic collisions.** Consider, inside the unit three-dimensional cube E^3, n weightless hard round balls, each of which has the same diameter d and mass m^*. Suppose that, possessing a certain supply of kinetic energy H, these balls move inside the cube E^3, colliding with one another and with the walls of the cube according to the laws of elastic impact. The coordinate space Q of our system is the closed domain of points

$$q = \left(q_1^{(1)}, q_2^{(1)}, q_3^{(1)}, \dots, q_1^{(n)}, q_2^{(n)}, q_3^{(n)}\right)$$

inside the $3n$-dimensional unit cube E^{3n}, defined by the inequalities

$$\left(q_1^{(i)} - q_1^{(j)}\right)^2 + \left(q_2^{(i)} - q_2^{(j)}\right)^2 + \left(q_3^{(i)} - q_3^{(j)}\right)^2 \geq d^2 \tag{1}$$

for all i, j. Here $\left(q_1^{(i)}, q_2^{(i)}, q_3^{(i)}\right)$ are the coordinates of the center of the i-th molecule. We note that, for large d, this domain may be disconnected. In what follows, only such d are considered for which it is connected. The trajectories of our system in the space Q look like polygonal lines which are reflected from the boundary of Q according to the law "the angle of incidence is equal to the angle of reflection," as a consequence of the laws of elastic collisions. The manifold M of constant energy consists of line elements to the manifold Q, whose lengths are equal to $\sqrt{2H/m}$. The invariant measure μ in M is written in the form

$$d\mu = \prod_{k=1}^{n} \prod_{i=1}^{3} dq_i^{(k)} \, d\omega_{3n-1},$$

where $d\omega_{3n-1}$ is the invariant measure on the $(3n-1)$-dimensional sphere of line elements $R_0(q)$. The one-parameter group of shifts $\{S_t\}$ along trajectories preserves this measure μ.

Theorem 4. *The system $\{S_t\}$ has positive entropy.*

The proof, of course, reduces to checking that the conditions of Theorem 1 are satisfied. The essential condition is condition A. Consider, for a fixed point q, the manifold $\widetilde{R}_t(q)$. This is a $(3n-1)$-dimensional piecewise-smooth manifold lying in Q. Let q' be a regular point of $\widetilde{R}_t(q)$. We shall call $\widetilde{R}_t(q)$ **convex at the point** q' if the operator of the second quadratic form of this manifold, acting in the space of tangent vectors to $R_t(q)$, is nonnegative definite. If $\widetilde{R}_t(q)$ was convex at the point q, then it is clear that, under motion inside Q, it will remain convex. It turns out that in our case this manifold will remain convex also after reflection from the manifolds (1). This assertion follows from the following general formula: let q' belong to exactly one of the manifolds (1) or to a side of the cube E^{3n}; then

$$A^+ = U_1^* A^- U_1 + 2\cos\varphi \, U_2^* B U_2,$$

where A^- (A^+) is the operator of the second quadratic form of $\widetilde{R}_t(q)$ before the collision (after the collision) at the point q'; B is the operator of the second quadratic form of the reflecting manifold at the reflection point q'; φ is the angle of incidence. To explain the meaning of this formula, we note that A^+ acts in the tangent plane to $\widetilde{R}_t(q)$ after reflection, A^- before reflection, and B in the tangent plane to the reflecting manifold. The operator U_1 (U_2) defines the natural mapping, by means of infinitely close trajectories, of the domain of definition of the operator A^- (B) onto the domain of definition of the operator A^+.

* The assumption that the balls are enclosed in the unit cube E^3 and have the same dimensions is inessential and is made for simplicity. One may consider balls of arbitrary radii in an arbitrary parallelepiped.

It follows from this that the convexity property of the manifold $R_t(q)$ is preserved after reflection and

$$a_t(x) \geq \prod_{i=1}^{r} (1 + \tau_i \| U_2^* B_{iU} 2 \|) \,,$$

where τ_i is the time interval between the $(i-1)$-st and i-th reflections; r is the number of reflections up to the moment t; $U_2^* B_{iU} 2$ is the operator of the second quadratic form of the reflecting manifold at the i-th reflection in the projection onto the tangent plane to $\widetilde{R}_\tau(q)$. From this inequality it is evident that

$$\lim_{t\to\infty} \frac{\log a_t(x)}{t} > 0$$

almost everywhere. Verification of the fulfillment of conditions B and C is simpler, and we shall not give it here.

§ 4. **Transversal fields and ergodicity.** In the case of geodesic flows on manifolds of negative curvature, the existence and properties of horosphere fields, i.e., fields of manifolds orthogonal to a pencil of asymptotic trajectories, are of great importance. It turns out that in the case of the dynamical systems of §§ 2 and 3 there also exist pencils of asymptotic trajectories and manifolds orthogonal to them. We shall construct them by analogy with the geodesic flow. For $x \in M$ take $q = \pi(x)$ and put $q_t = \pi(S_{-t}x)$. The manifolds $\widetilde{R}_t(q_t)$ pass through the point q for every t. It turns out that for almost every x one can specify such a neighborhood U of the point q that the connected components of the intersection $\widetilde{R}_t(q_t) \cap U$ containing the point q will, in the natural sense, tend as $t \to \infty$ to certain limits $\widetilde{R}(q)$. This limit is the analogue of the horosphere. The linear elements perpendicular to $\widetilde{R}(q)$ and directed in the same direction as x will be denoted by $R(x)$.

Let us note some properties of $\widetilde{R}(q)$ and $R(x)$: 1) $\widetilde{R}(q)$ is a smooth manifold of class C^2 in U; 2) $S_{tR}(x) \subset R(S_{tx})$ for $t > 0$; 3) if $x' \in R(x)$, then for some neighborhood U' of the point $q' = \pi(x')$,

$$\widetilde{R}(q') \cap U' = \widetilde{R}(q) \cap U'.$$

We shall call two points x and x' equivalent if, for some $t_0 > 0$ (and therefore for all $t > t_0$),

$$\widetilde{R}(S_{t_0}x) = \widetilde{R}(S_{t_0}x').$$

The class of equivalent points will be called a direct transversal layer, and the partition into direct transversal layers will be denoted by Z. By $\mathfrak{S}(Z)$ we shall denote the σ-algebra of measurable sets consisting mod 0 of direct transversal layers. Letting $t \to -\infty$ in the constructions described above, we obtain inverse transversal layers. The partition into inverse transversal layers will be denoted by Z', and the corresponding σ-algebra by $\mathfrak{S}(Z')$.

Theorem 5. *The dynamical systems of § 3 and the first system of § 2 are ergodic.*

The proof of this theorem is carried out by Hopf' s method ([6]), according to which the σ-algebra of sets $\mathfrak{N}$ invariant with respect to $\{S_t\}$ satisfies the relation

$$\mathfrak{S}(Z) \wedge \mathfrak{S}(Z') = \mathfrak{N}.$$

The fact that $\mathfrak{S}(Z) \wedge \mathfrak{S}(Z')$ is the trivial σ-algebra is based on certain properties of absolute continuity of the transversal layers, which we do not give here ([8]).

Moscow State University
named after M. V. Lomonosov

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Note: Figure translations are in progress. See original paper for figures.