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Poincaré Recurrences*

HARRY L. FRISCH†
Department of Chemistry, University of Southern California, Los Angeles, California
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In connection with the tracing of the origin of the apparent irreversibility exhibited by a class of simple mechanical systems, namely all multiply or conditionally periodic Hamilton-Jacobi systems, estimates are obtained for the Poincaré recurrence time of such a system in terms of the preassigned limits of error of the mechanical recurrence, ϵ. By applying the theory of diophantine approximations, the asymptotic fraction of the time a system spends in such recurrences is found exactly. These results allow further deductions concerning the fraction of time a given system obeys a strict version of the second law of thermodynamics, as well as the existence and order of magnitude of the average Poincaré recurrence time of a Gibbsian ensemble of such systems whose degrees of freedom are indistinguishable.

The relation of the results obtained for this important class of mechanical systems and the resolution of the paradoxes of heat theory propounded by Zermelo, Loschmidt, etc., due to Boltzmann and von Smoluchowski, is discussed. An especially easily visualized model, the one-dimensional gas of hard spheres, is treated, in particular, in some detail.

I. INTRODUCTION

CENTRAL in the theory of heat lies the problem of reconciling the irreversible phenomenological laws governing the transport of properties and matter and the reversible laws of mechanics which are simultaneously obeyed by the molecules involved in the transport process. In particular the Poincaré cycle theorem[1] has been the starting point for a number of paradoxes showing the incompatability of statistical mechanics (based on dynamics) and macroscopic thermodynamics on the one hand and the kinetic theory of gases on the other.[2] The resolution of these paradoxes by Boltzmann,[3] von Smoluchowski,[4] and others have depended on the recognition that the period of one such Poincaré cycle is so very large that the recurrence of an initially improbable state is so highly improbable that during the times normally available for observation the chance of reversal of a spontaneous thermodynamic process is exceedingly small. Unfortunately, except for an incomplete and very rough estimate of this recurrence time for a gas by Boltzmann,[1,3] no completely satisfactory demonstration of the emergence of apparent irreversibility from a strictly mechanical system has been achieved.[5] In this connection, a number of quasi-mechanical models incorporating certain statistical assumptions, such as the urn and wind-tree model,[6] have been recently investigated.[7,8]

The purpose of the present investigation will be to elucidate certain details of the reconcilation suggested

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† Present address: Bell Telephone Laboratories, Murray Hill, New Jersey.

[1] For an excellent review of these matters see S. Chandrasekhar, Revs. Modern Phys. **15**, 1 (1943). This theorem asserts that for a system of material particles under the influence of forces which depend only on the spatial coordinates, a given initial state (given by a representative point in phase space) must, in general, recur, not exactly, but to any desired degree of accuracy, infinitely often, provided the system always remains in the finite part of the phase space.

[2] J. Loschmidt, Wien. Ber. **73**, 139 (1876); **75**, 67 (1877); E. Zermelo, Ann. Physik **57**, 485 (1896); **59**, 793 (1896).

[3] L. Boltzmann, Ann. Physik **57**, 773 (1896); **60**, 392 (1897).

[4] M. von Smoluchowski, Physik. Z. **13**, 1069 (1912); **14**, 261 (1913).

[5] This includes von Smoluchowski's theory of fluctuations in molecular concentrations[1] which has been criticized by M. Kac, Am. Math. Monthly **54**, 369 (1947).

[6] P. and T. Ehrenfest, Physik. Z. **8**, 311 (1907).

[7] B. Friedmann, Comm. Pure and Appl. Math. **2**, 59 (1949).

[8] D. ter Haar and C. D. Green, Proc. Phys. Soc. (London) **A66**, 153 (1953); Proc. Cambridge Phil. Soc. **51**, 141 (1955); Physica **21**, 63 (1955).

by Boltzmann, von Smoluchowski, etc. for a class of simple mechanical systems. In particular this will involve finding estimates of the Poincaré recurrence time of conditionally or multiply periodic mechanical systems derivable from a time-independent Hamiltonian function. More to the point, we will describe exactly the asymptotic distribution of recurrences up to a given time of observation in terms of the preassigned limits of error of the mechanical recurrence. For simplicity we shall carry out the discussion in terms of the least complicated mechanical model system of the general type described, namely a one-dimensional gas of identical rigid spheres. The ease with which details of the statistical behavior of this model can be grasped suggest further pedagogical resons for the procedure we shall follow below.

II. VELOCITY DISTRIBUTION OF THE ONE-DIMENSIONAL GAS OF RIGID SPHERES

Consider a one-dimensional gas composed of $N-1$ identical perfectly elastic spheres contained between two perfectly reflecting (elastic) walls. Without loss in generality, we can represent the walls as another perfectly elastic sphere and think of all N spheres now as being distributed along the circumference of a circle of unit radius. Let the mass, (angular) position, and (angular) velocity of the spherical gas molecules be m, θ_i, ω_i, respectively, with $i=1, 2, \cdots, N$. Since the molecules must collide head-on and the molecules are elastic, we have on collision to satisfy the two conservation conditions:

$$\omega_i+\omega_{i+1}=\omega_i'+\omega_{i+1}',$$
$$\omega_i^2+\omega_{i+1}^2=\omega_i'^2+\omega_{i+1}'^2,$$

where the primed quantities refer to the molecules before the collision and the unprimed quantities to the molecules after collision. The solution

$$\omega_i=\omega_{i+1}', \quad \omega_{i+1}=\omega_i',$$

shows that the velocities are only permuted among the different particles. Furthermore, a collision involving more than two particles can always be factored into a product of two-particle collisions. Since the molecules are indistinguishable, we can think of a collision as not only exchanging momentum but also the assigned numbers by which the particles had originally been distinguished. The particle with a given assigned number moves as if it passed clear through another particle without collision.

If $\mu=\mu(\theta_1,\cdots,\theta_N;\omega_1,\cdots,\omega_N;t)$ denotes the density in phase space of a Gibbsian ensemble of such systems, then the (N-particle) molecular velocity distribution (M.V.D.) $\phi(\omega_1,\cdots,\omega_N;t)$ is given by

$$\phi(\omega_1,\cdots,\omega_N;t)$$
$$=\int\cdots\int_{(N)}\mu(\theta_1,\cdots,\theta_N;\omega_1,\cdots,\omega_N;t)d\theta_1\cdots d\theta_N,$$

with the normalization condition

$$\int_{-\infty}^{\infty}\cdots\int\phi(\omega_1,\cdots,\omega_N;t)d\omega_1\cdots d\omega_N=1.$$

Let $\phi(\omega_1,\cdots,\omega_N;t=0)=\phi(\omega_1,\cdots,\omega_N)=\phi$ be the initial M.V.D. If the particles are indistinguishable, ϕ must be a symmetric function of its arguments. Since we have shown that collisions in the system only permute the ω_i and since a symmetric function remains invariant under the permutation of its arguments, it follows that for all times

$$\phi(\omega_1,\cdots,\omega_N;t)=\phi(\omega_1,\cdots,\omega_N). \tag{1}$$

Thus our M.V.D. is determined if the initial symmetric distribution is given. We can say something about the physically unrealistic case where ϕ is initially *not* symmetric for, by the above argument, ϕ can never become symmetric and hence can never represent indistinguishable particles.

An immediate consequence of Eq. (1) is the vanishing of the time derivative of the average over phase of any time-independent function F of the velocities ω_i, i.e.,

$$d\langle F(\omega_1,\cdots,\omega_N)\rangle/dt=0, \tag{2}$$

where

$$\langle F\rangle=\int\cdots\int F(\omega_1,\cdots,\omega_N)\mu(\theta_1,\cdots,\omega_N;t)d\theta_1\cdots d\omega_N$$
$$=\int_{-\infty}^{\infty}\cdots\int F(\omega_1,\cdots,\omega_N)\phi(\omega_1,\cdots,\omega_N)d\omega_1\cdots d\omega_N.$$

III. DENSITY DISTRIBUTION IN A ONE-DIMENSIONAL GAS OF RIGID SPHERES

While the above system is highly "nonergodic" as regards its velocity distribution, it behaves in a manner expected insofar as the distribution in the positions of the N molecules is concerned; exhibiting the expected "diffusion" of molecules from regions of high density to regions of low density in molecules. Thus if initially the molecules are uniformly distributed everywhere except in a circular sector of θ radians and the velocities are bounded from above, then the probability of finding m particles in the sector of θ radians at any later time t is given by a Bernoulli distribution $\{[N!/m!(N-m)!]\times p^m(t)[1-p(t)]^{N-m}\}$ with the parameter $p(t)$ dependent on the time, which can be explicitly obtained by induction on N, the total number of particles. For large N, this distribution becomes more and more peaked and in the limit approaches a Gaussian distribution. The latter is centered about the mean $\langle m\rangle$ which incidentally rapidly approaches,[9] in an oscillating fashion, $\langle m\rangle_{t\to\infty}=(\theta/2\pi)N$. Thus the sort of diffusion

[9] This and similar results were also obtained by E. Teramoto and C. Suzuki, Progr. Theoret. Phys. (Japan) 14, 411 (1955), whose discussion of these points is quite explicit.

of molecules predicted by a Second Law consideration actually occurs.

IV. POINCARÉ RECURRENCE TIME

How can one reconcile then this apparent "irreversible" behavior with the approximate recurrence of any initial state in time according to the theorem of Poincaré? To answer this, we will first clarify the meaning of such a recurrence and then estimate its duration. By a Poincaré recurrence of such a mechanical system, we will mean a recurrence of a given initial pattern of positions and velocities, the former specified to within an error of $2\pi\epsilon$ radians, $0\leqq\epsilon<1$, independently of any permutation in the numbering of the gas molecules. The Poincaré recurrence time is then the time of the first recurrence of such a pattern, $\bar{t}=\bar{t}(\nu_1,\cdots,\nu_N;\epsilon)$ where $\nu_i=\omega_i/2\pi$ are the angular frequencies. The remarkable thing is that $\bar{t}$ depends only on the frequencies and ϵ. Precise recurrence (i.e., $\epsilon=0$) occurs only if the ν_i are rationally dependent, i.e. there exist integers $m_1,\cdots,m_N$ such that $\sum_i m_i\nu_i=0$. Otherwise $\bar{t}$ is the least real number such that, given $N+1$ arbitrary real numbers $\nu_i(i=1,\cdots,N)$ and ϵ, $\epsilon>0$, the N inequalities

$$|\bar{t}\nu_i-n_i|<\epsilon \tag{3}$$

are simultaneously satisfied for suitable integers n_i.

Before proceeding with the development of Eq. (3), we would like to show the almost complete analogy in the dynamical behavior between the one-dimensional gas of rigid spheres and a multiply periodic mechanical system with a time-independent Hamiltonian function. Let the generalized coordinates and momenta of the latter system be $q_1,\cdots,q_N$ and $p_1,\cdots,p_N$ and the total energy E. Making use now of well-known results from the Hamilton-Jacobi theory,[10] we can introduce action and angle variables $J_1,\cdots,J_N$ and $w_1,\cdots,w_N$ in terms of Hamilton's principal function S and the characteristic function W satisfying

$$S=-Et+W,$$

$$p_i=\partial S/\partial q_i=\partial W/\partial q_i,$$

$$J_i=\oint p_i dq_i=\oint \frac{\partial S}{\partial q_i}dq_i=\oint \frac{\partial W}{\partial q_i}dq_i,$$

$$w_i=2\pi\partial W/\partial J_i=2\pi(\nu_i t+\delta_i)\,;\ \delta_i=\partial S/\partial J_i.$$

In terms of these variables, E is a function of the J's alone and

$$\partial E/\partial J_i=\nu_i \tag{4}$$

yields the constant angular frequencies ν_i. A multiply periodic system is further, by hypothesis,[10,11] a system for which the characteristic function W is separable in at least one set of canonical variables q_i, $p_i(i=1,\cdots,N)$. For these systems the recurrence behavior is completely determined by the set of frequencies $\nu_1,\cdots,\nu_N$ since all coordinates can be represented as a Fourier series:

$$q_k=\sum_{n_k=-\infty}^{\infty} c_{n_k}e^{2\pi i n_k\nu_k t}.$$

It can be shown[12] that the motion of any such system is completely specified in any cube of w space of length 2π. The locus of the motion of the system in this space is a straight line whose direction cosines γ_k with the axes stand in the relation

$$\gamma_1:\gamma_2:\cdots:\gamma_N=\dot{w}_1:\dot{w}_2:\cdots:\dot{w}_N=\nu_1:\nu_2:\cdots:\nu_N,$$

in complete analogy with the behavior of our model gas. The Poincaré recurrence time is again given by Eq. (3) with the constant frequencies ν_i [see Eq. (4)] and $2\pi\epsilon$ the error in w_i. Henceforth, in treating the mechanical recurrence properties of this class of systems, it suffices to examine the analogous property of a one-dimensional gas of rigid spheres. If furthermore we specialize to the class of multiply periodic mechanical systems whose degrees of freedom are indistinguishable, then the analogy is complete and the statistical mechanics of this subclass and our model are identical; e.g., Eq. (1) applies.

Returning now to Eq. (3), the item of greatest physical interest concerning $\bar{t}$ is its behavior as $\epsilon\to 0$ for fixed N. In order to deal with dimensionless parameters, let $\nu=\max\nu_i(i=1,\cdots,N)$, $\tau=\nu^{-1}$, $\bar{t}=\nu\zeta$, and $\xi_i=\nu_i/\nu$; then Eq. (3) becomes

$$|\zeta\xi_i-n_i|<\epsilon. \tag{5}$$

An upper bound for ζ is immediately obtained by virtue of the following theorem[13]: N real numbers $\xi_1,\cdots,\xi_N$ are to be approximated by rational fractions with denominator q such that the error

$$\left|\xi_i-\frac{n_i}{q}\right|<\frac{1}{q^{1+1/n}}.$$

If at least one of ξ_i is irrational, then there exist an infinite number of systems of N fractions of this type. Thus, with given ϵ, choose the least q such that $\epsilon>q^{1/N}$; then we certainly have [see Eq. (5)]

$$\zeta\leqq\epsilon^{-N},$$

which can by a theorem due to Minkowski[14] be improved

[10] H. Goldstein, *Classical Mechanics* (Addison-Wesley Press, Inc., Cambridge, 1950), Chap. 9.

[11] A thorough discussion of the existence theorems involved here is given by M. Born, *The Mechanics of the Atom*, translated by J. W. Fisher (G. Bell and Sons, London, 1927).

[12] See, e.g., W. Weizel, *Lehrbuch der Theoretischen Physik* (Springer-Verlag, Berlin, 1949), pp. 121–125.

[13] O. Perron, *Irrationale Zahlen* (Chelsea Publishing Company, New York, 1948), second edition, p. 132 (Th. 54).

[14] J. F. Koksma, *Diophantische Approximationen* (Chelsea Publishing Company, New York, 1936), pp. 70–86.

to

$$\zeta \leqslant \left[\frac{(N+1)\epsilon}{N}\right]^{-N}$$

or

$$0 \leqslant \bar{t} \leqslant \tau\left[\frac{(N+1)\epsilon}{N}\right]^{-N}. \tag{6}$$

The fact that $\bar{t} \sim \tau \bar{C}_N \epsilon^{-N}$, with

$$1+1/N < \bar{C}_N \leqslant [2(N+1)]^{\frac{1}{2}}[N+1]^{\frac{1}{2}N},$$

is suggested by the further result due to Furtwängler[14] that there exist many sets of N real numbers $\xi_1, \cdots, \xi_N$ such that there exist at most a finite number of fractions with common denominator q for which

$$\left|\xi_i - \frac{n_i}{q}\right| < 1/C_N q^{1+1/N}$$

and $C_N \leqslant [2(N+1)]^{\frac{1}{2}}[N+1]^{1/2N}$.

$\bar{t}$ rises very sharply as expected with decreasing ϵ. This result still applies if the mechanical system is m-fold degenerate ($m<N$); i.e., there exist integers j_i such that $\sum_{i=1}^{m} j_i \nu_i = 0$. An extension[15] of a previously cited theorem allows us to conclude that $\bar{t} \leqslant \tau \epsilon^{-(N-m)}$.

A further question concerns itself with whether there exists an average recurrence time for these systems where the averaging is carried out over the Gibbsian ensemble of systems. Assuming that Eq. (1) holds, we can write for the average recurrence time $T(\epsilon)$:

$$T(\epsilon) = \int_{-\infty}^{\infty} \cdots \int \bar{t}(\nu_1, \cdots, \nu_N; \epsilon)\phi(\omega_1, \cdots, \omega_N) d\omega_1 \cdots d\omega_N.$$

From Eq. (6), we can conclude that

$$T(\epsilon) \leqslant \left[\frac{(N+1)\epsilon}{N}\right]^{-N} \langle \tau \rangle,$$

$$\langle \tau \rangle = \int_{-\infty}^{\infty} \cdots \int \frac{2\pi}{\omega_1} \phi(\omega_1, \cdots, \omega_N) d\omega_1 \cdots d\omega_N.$$

Hence for M.V.D.'s for which $\langle \tau \rangle$ is finite, $T(\epsilon)$ certainly exists. It is this time which von Smoluchowski[4] chooses as a scale for the apparent irreversibility of a process. Thus, a process appears irreversible (or reversible) according as whether the initial state is characterized by a long (or short) average time of recurrence compared to the times during which the system is under observation.[1]

V. ASYMPTOTIC DISTRIBUTION OF RECURRENCES

While the previously given estimates of the Poincaré recurrence times support strongly the central intention of this paper, they do not by themselves suffice to satisfy our curiosity as to the recurrence of an initially improbable state. The type of question we should like to ask is not, given that we start from some arbitrary initial state in phase space, what is the average length of time before we return to an ϵ neighborhood of that state; but rather, assuming that we perform a large number of observations on our system, what fraction of the time does the system actually spend in states within an ϵ neighborhood of our initial one?

An answer to the above question is obtained by a modification of a theorem due to Weyl[14,16]: If to a system of whole numbers $n_1, \cdots, n_N$ ($N>1$) there belong $N+1$ real numbers, $\nu_1, \cdots, \nu_N$ and y, such that

$$\eta_i < \nu_i y - n_i < \eta_i + \alpha_i; \quad \alpha_i < 1, \tag{7}$$

then there exist an infinite number of such y and these form an open interval. Because $\alpha_i<1$, no y can belong simultaneously to two different systems $n_1, \cdots, n_N$. If t denotes any positive number, then there exist only a finite number of systems to which belongs a y in the interval $0<y<t$, since the n_i are bounded. Those numbers y in the interval $0<y<t$ for which Eq. (7) holds for suitable integers $n_1, \cdots, n_N$ form a finite number of open intervals. Their total length is henceforth denoted by $N_1(\eta_i; \alpha_i; t)$. If the numbers $\nu_1, \cdots, \nu_N$ are rationally independent and if $t_1, t_2, \cdots, t_k, \cdots$ denotes any sequence for which

$$\lim_{k\to\infty} t_k = \infty,$$

then

$$\lim_{k\to\infty} \frac{N_1(\eta_i; \alpha_i; t_k)}{t_k} = \prod_{i=1}^{N} \alpha_i. \tag{8}$$

Identifying the t_k's with the end points of the observation time intervals and choosing $\eta_i=0$ and $\alpha_i=\epsilon$, then applying Eq. (8) we find for the desired fraction F

$$F = \lim_{k\to\infty} \frac{N_1(0; \epsilon; t_k)}{t_k} = \epsilon^N. \tag{9}$$

If the error bounds on the w_i are different, then Eq. (9) becomes

$$F = \prod_{i=1}^{N} \epsilon_i; \quad 0 < \epsilon_i < 1.$$

Thus, the larger the number of molecules (degrees of freedom) of the gas (system), the smaller is the fraction of the time spent near any initial state.

Consider now some initial state of the system specified to within limits of error determined by ϵ, S_i. As the system evolves in time, it may pass through a succession of different states, each, say, specified to within the same limits of error as S_i. Assuming that a suitable system entropy can be defined,[17] we can classify all successive states to S_i according as the

[15] Reference 13, pp. 137–138 (Th. 57)

[16] Reference 13, pp. 168–169 (Th. 67).

[17] See, e.g., F. Lurcat, Compt. rend. 242, 1686 (1956).

entropy difference with respect to S_i is positive, zero, or negative. Denote the fraction of all accessible states of the system from S_i in an arbitrarily large time which are characterized by a negative entropy difference by $\Omega^{(-)}(S_i,\infty)$. Since the principal negative contributions come from the vicinity of the recurrent state, Eq. (9) suggests that the fraction of the time for which the Second Law[18] fails for this system is of the order of $\Omega^{(-)}(S_i,\infty)\cdot\epsilon^N\leqslant\epsilon^N$. Thus for these systems we can conclude in a restricted sense that the larger the number of molecules (degrees of freedom), the greater can be our belief in the applicability of the laws of thermodynamics.

VI. CONCLUDING REMARKS

While the Poincaré recurrence time certainly ranks as one of the important parameters characterizing the temporal unfolding of a mechanical system, it is not the only such parameter. Particularly important in the description of transport processes are various very much shorter relaxation times. Among the latter might be classed a time such as the one required on the average for the smoothing out of some initial inhomogeneity in the density of molecules of, say, our model gas. If L denotes the length of the circumference of our circle, then this time is of the order of $L/(2E/m)^{\frac{1}{2}}$.[9] A particularly challenging question arises if we consider the various interrelations between these times, since these determine the choice of the best approximate irreversible transport theory for the description of the reversible mechanical system. In view of the simplicity of this model, the study of both exact and approximate transport theory appears feasible, particularly in view of relations such as Eqs. (1) and (2).

What is very characteristic of both the Poincaré recurrence times and their distributions for the class of mechanical systems under consideration is their independence of the location in configuration space of the recurring initial state. Hence one is little surprised to find that these systems are quasi-ergodic.[10,12]

One should note that ϕ satisfying Eq. (1) can always be expressed in terms of the elementary symmetric functions $\sigma_1,\cdots,\sigma_N$, where

$$\sigma_i=\sum_{\text{all permutations}}\omega_1\omega_2\cdots\omega_i,$$

as

$$\phi(\omega_1,\cdots,\omega_N)=\psi(\sigma_1,\cdots,\sigma_N),$$

where both ϕ and ψ obviously satisfy the integral equations

$$\phi(\omega_1,\cdots,\omega_N)=\int_{-\infty}^{\infty}\cdots\int\prod_{i=1}^{N}\delta(\omega_i-\omega_i')\times\phi(\omega_1',\cdots,\omega_N')d\omega_1'\cdots d\omega_N',$$

$$\psi(\sigma_1,\cdots,\sigma_N)=\int_{(N)}\cdots\int\prod_{i=1}^{N}\delta(\sigma_i-\sigma_i')\times\psi(\sigma_1',\cdots,\sigma_N')d\sigma_1'\cdots d\sigma_N'.$$

This relationship is a direct consequence of the fact that the vector of the velocities after collision, $\boldsymbol{\omega}=\boldsymbol{\omega}(\omega_1,\cdots,\omega_N)$, is obtained from the vector of velocities before collision, $\boldsymbol{\omega}'=\boldsymbol{\omega}'(\omega_1',\cdots,\omega_N')$ by a suitable rotation of a sphere of radius $(2E/m)^{\frac{1}{2}}$ on which both $\boldsymbol{\omega}$ and $\boldsymbol{\omega}'$ lie. Since this is also true of two-, three-, etc., dimensional gases of rigid spheres, we can expect that the analog of the integral equations (10) exists for a suitable kernel function $K(\boldsymbol{\omega},\boldsymbol{\omega}')$. We shall not pursue this question further here.

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[18] By the Second Law we mean here the strong statement that the (system) entropy of an isolated system (of constant energy) never decreases.