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THE FOUNDATIONAL ROLE OF ERGODIC THEORY

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Abstract

The foundation of statistical mechanics and the explanation of the success of its methods rest on the fact that the theoretical values of physical quantities (phase averages) may be compared with the results of experimental measurements (infinite time averages). In the Thirties, this problem, called the ergodic problem, was dealt with by an ergodic theory that tried to resolve the problem by making reference above all to considerations of a dynamic nature. In the present paper, this solution will be analyzed first, highlighting the fact that its very general nature does not duly consider the specificities of the systems of statistical mechanics. Second, A.I. Khinchin's approach will be presented, that starting with the more specific assumptions about the nature of systems, achieves an asymptotic version of the result obtained with ergodic theory. Third, the statistical meaning of Khinchin's approach will be analyzed and a comparison between this and the point of view of ergodic theory is proposed. It will be demonstrated that the difference consists principally of two different perspectives on the ergodic problem: that of the ergodic theory puts the state of equilibrium at the center, while Khinchin's attempts to generalize the result to non-equilibrium states.

Key Words: ergodic theory, ergodic problem, statistical mechanics, Khinchin.

Biographical Sketch

Massimiliano Badino obtained his Ph.D. with a thesis on the historical and philosophical problems of statistical mechanics. He works in the Department of Philosophy at the University of Genoa and collaborates with the Research Group for the History of Physics of the Physics Department. His research interests are in the History of Physics (especially Statistical Mechanics, Relativity and Early Quantum Theory), theory of explanation, information theory, logic of statistical inference, theory of knowledge and problems concerning progress in science. Among his publications, the most relevant are: M. Badino: 2000, L'epistemologia di Planck nel suo contesto storico. ESI, Napoli, M. Badino and N. Robotti: 2001, Max Planck and the Constants of Nature, Annals of Science 58: 137–162; and M. Badino: 2004, An Application of the Information Theory to the Problem of Scientific Experiment, Synthese 140: 355-389.

THE FOUNDATIONAL ROLE OF ERGODIC THEORY

1. INTRODUCTION.

From his very first papers about the kinetic theory of gases, L. Boltzmann used a special hypothesis according to which leaving a system in free evolution and waiting for a sufficiently long time, the system will pass through all the states consistent with its general conditions, namely with the given value of the total energy. This hypothesis, later known as the *ergodic hypothesis*, can be found more or less explicitly in all of Boltzmann's work on this subject, but it seems that he did not assign it the same meaning and perhaps even the same importance as we do today.[1] Actually, the ergodic hypothesis assumed a central role, above all due to J. Willard Gibbs' work in 1902 and to the use of the method of statistical ensembles. Indeed, it allowed us to connect in an extremely simple and natural way a set theoretical quantity, such as the phase average of a function, with a quantity defined on the system, that is, the infinite time average of a physical quantity. Therefore, the ergodic hypothesis provides an immediate way to give justification and physical meaning to the statistical ensembles method. Furthermore, from the ergodic hypothesis, some notable consequences can be derived, the most important of which are: 1) that the average time a system spends in a phase region is proportional to the measure of the region itself and 2) that one and only one probability distribution exists that is invariant with regard to the transformations taking place on the system. With Gibbs' work and the subsequent arrangement by P. and T. Ehrenfest, the ergodic hypothesis acquired a central position in statistical mechanics. But such centrality was not destined to last. In 1913, through independent means, M. Plancherel and A. Rosenthal proved that a trajectory obeying the ergodic hypothesis and occupying in the long run all the phase space, namely passing through *any* phase point, cannot be a mechanical trajectory. A first attempt in order to avoid the problem was to substitute the 'strong' ergodic hypothesis mentioned above with a weakened version, the so–called *quasi–ergodic hypothesis*: in the long run, a system trajectory will pass as near as is wanted to any point of the phase space, namely the trajectory will be *dense* in the phase space. But this attempt proved useless for two main reasons (Sklar 1993, p. 161):

> First there was the difficulty of proving of a given system that it was quasi–ergodic, a problem that proved intractable. Second, it later became apparent, in the light of results obtained through the ultimately successful approach to ergodic theory, that quasi–ergodicity even if provable would be insufficient to gain the result one wanted. It could be shown, for example, that there were quasi–ergodic systems that failed to demonstrate the equality of time average with phase average that followed from the ergodic hypothesis and that grounded the other desirable for which the hypothesis was first conjectured.

Thus, for a long time there was widespread skepticism about the ergodic hypothesis and the possibility of statistical mechanics relying on it. At the beginning of the 1930s, a completely new and original way was attempted by G. D. Birkhoff, B. Koopman and J. von Neumann. They proposed the idea of proving the results mentioned above (especially the equality of phase average with infinite time average, from which the others derive) without using the ergodic hypothesis. The theory trying to

[1] A good reconstruction of the role of the ergodic hypothesis in Boltzmann's and Maxwell's work can be found in Brush (1986, pp. 363–377) and in von Plato (1994, pp. 93–106). A very interesting thesis about the original meaning and about the etymology of the term 'ergodic' is presented in Gallavotti 1982 and Gallavotti 1999 (pp. 37–44).

derive the equality of phase averages and infinite time averages using only the dynamical properties of the system and some statistical assumptions is called *ergodic theory*. Thus, the ergodic theory has little to do with the ergodic hypothesis.[2] On the contrary, it intends to characterize the ergodicity of a physical system by purely dynamical means, without directly assuming the ergodic hypothesis. With the passage of time, the ergodic theory was developed more explicitly as an abstract mathematical theory and part of general dynamics, rather than as a strictly physical theory.

2. THE ERGODIC THEORY.

2.1 The ergodic problem and its solution.

A physical system may be represented as a set of physical states. Such a set is called *phase space*. Knowingly statistical mechanics deals with systems constituted by a very large number n of components (particles, molecules etc.), that is, with a high number of degrees of freedom. The state of such a system is definable by means of $(q_1, \ldots, q_n)$ generalized coordinates and $(p_1, \ldots, p_n)$ conjugated momenta. These phase coordinates define a $2n$–dimensional phase space Γ, in which a point $P(q_1, \ldots, q_n, p_1, \ldots, p_n)$ is said to be a *representative point* of the system and defines its state at a particular time. The representative point evolves through a transformation of the coordinates (usually Hamilton's equations) describing a phase trajectory in the phase space. However, since statistical mechanics usually deals with constant energy systems (so that a degree of freedom is fixed) a $(2n\text{-}1)$-dimensional constant energy hyper-surface is commonly used. In the following, we will use the hyper-surface Σ as a basic reference space for any physical interpretation.

A physical quantity linked to the system may be expressed as a function of the phase coordinates of the system. Consequently, for every empirically measured value of a physical quantity should correspond an analogous value for an opportune phase function on Σ. Statistical mechanics is a well-founded theory only (and to the extent that) this correspondence exists and is empirically verifiable.

Nevertheless, it is clear that it is not possible to check an exact correspondence. In fact, to compare the value of a physical quantity in a specific state with the value of the corresponding phase function, we should calculate the value of the latter in a phase point and this would require knowing all the phase coordinates (the values of the positions and momenta for all the molecules of the gas). For this reason it is supposed that the result of a physical measurement is not the exact value of the phase function, but rather its average time value. This supposition is justified by the argument according to which the temporal scale of a measurement is large with respect to the temporal scale in which molecular changes take place.

But another problem arises. At first glance, it could happen that the average time value of a phase function does not converge but assumes various values in different points of the trajectory. This problem was overcome when Birkhoff showed that the infinite limit of the time average of a phase function converges almost everywhere to a constant value, where 'almost everywhere' means that the convergence is not valid only for a set of points that have a set-theoretical measure equal to zero.

We have not gained much yet with this, since the calculation of the infinite time average of a phase function presupposes knowledge of the entire trajectory of the

[2] For a brief historical account about ergodic theory, see von Plato (1987, pp. 389–394).

representative point and therefore the integration of the phase coordinates. Since this task is clearly out of our reach, an alternative calculation becomes necessary. In particular, contrary to the infinite time average, the phase average (that is the average value assumed by the function in the space Σ) is much easier to calculate. If therefore the infinite time average of whatever function could be replaced by its phase average, statistical mechanics would be completely founded. The ergodic problem consists precisely of the justification of this replacement. It is clear that a solution to the ergodic problem would be the demonstration that the constant value whose infinite time averages converge is exactly the phase average. This is possible adding to Birkhoff's theorem the so-called *hypothesis of metric transitivity* (or *indecomposability*) (MT).

A set is said to be metrically transitive if it is not possible to decompose it into two positive measure invariant subsets. A set is invariant if and only if it contains a complete phase trajectory. Thus, the MT is the same as stating that it is not possible to divide the set in subsets having positive measure, such as a trajectory that starts in one of them remains there,[3] or that the phase space is the smallest set containing the complete phase trajectory of the system. It may be demonstrated that if the transformation that the system undergoes preserves the Lebesgue measure, the MT is a necessary and sufficient condition for equality between infinite time averages and phase averages thus this is equivalent to the old ergodic hypothesis. This equivalence implies that the MT essentially is a dynamical hypothesis (Sklar 1993, p. 166):

> Notice also the way in which the Birkhoff result [..] avoids the necessity for anything like the ergodic or quasi–ergodic hypothesis. It is now metric indecomposability that is the necessary and sufficient condition for the equality 'almost everywhere' […] of the infinite time average and the phase average. There is a condition equivalent to metric indecomposability, though, that replaces the old ergodic and quasi–ergodic hypotheses, for metric indecomposability is equivalent to the condition that given any set of positive measure in the phase space, the trajectories from all but perhaps a set of measure zero of phase points intersect that set.

For this reason, the MT is also known as 'ergodicity'. This concept can be clarified relying on the distinction between *global* and *local* integrals of motion. Generally speaking, an integral of motion is a phase function whose value does not change along the phase path. Let us consider a system with n degrees of freedom described by a hyper-surface Σ of constant energy: then we have $2n - 1$ integrals of motion. A certain integral I is called *global* if and only if it is constant all the time on a given trajectory, while it is called *local* if and only if it is constant for a limited period of time. Obviously, the energy is a global integral on Σ. Thus it can be said that MT is equivalent to state that *another global integral of motion does not exist on the system, namely another phase function constant almost everywhere on the trajectory does not exist* (GIM). Let us prove that MT is equivalent to GIM.

a) If GIM then MT: let us assume *ab absurdo* that MT does not hold, then let us prove that another phase function which has positive measure and is constant on the set can be defined. Indeed, if MT does not hold, a decomposition of the space in two positive measure sets V_1 and V_2 that are invariant can be found. Therefore, using the indicator function, a new integral such as $h(P) = 0$ on V_1 and $h(P) = 1$ on V_2 can be obtained thereby contradicting GIM.

b) If MT then GIM: let us suppose that a new global integral of motion $g(P)$ exists that assumes on the trajectories a value included within the continuous interval [a,

[3] Cf. Sklar (1993, pp. 164–165); this sense justifies the term 'metric indecomposability'.

b]. Thus it can be proved[4] that a number $\alpha \in [a, b]$ exists such as makes it possible to divide the space into two invariant portions, thus obtaining a contradiction with the MT hypothesis.[5]

Thus, the validity of MT on the hyper-surface implies that the energy is the only constant global integral on Σ, "so the condition of metric indecomposability is essentially equivalent to the condition of there not being any neglected global constant of motion that differs in its value on sets of trajectories of non–zero probability".[6]

2.2 Troubles with ergodic theory.

Ergodic theory justifies the replacement of the infinite time averages with the phase averages relying on the geometric properties of the phase space (invariance), on the properties of transformations defined therein (measuring-preserving transformation) and on a particular hypothesis (MT). In this way, this resolves the ergodic problem and founds the correspondence between particular values of phase functions and the experimental measurements of physical quantity. Before concentrating on specific criticism of ergodic theory, it is opportune to point out some considerations on the general meaning of the ergodic problem. As we have seen, this presupposes that the outcomes of measurements may be compared to infinite time averages and that convergence almost everywhere is an acceptable criterion, namely, in other words, that zero measure sets are negligible. Criticism has been made about both of these suppositions[7].

As we have seen, the first supposition relies on the following argument: the single act of measurement requires a certain time, which generally is very long in comparison to the temporal scale of microscopic events. Therefore we can assume that the result of a measurement of a quantity represents the average value of the quantity itself over such a long time as to be considered infinite. However, some observations speak against the plausibility of this argument.[8]

(1) There are cases in which the microscopic and macroscopic time scales are not very different, for example when we evaluate the effect of the interaction among the gas molecules and the walls of the container.

(2) If the measurement results really were infinite time averages, then we could obtain results concerning quantities in equilibrium only. This means that we could not measure either the change of quantities moving from a value of non-equilibrium to equilibrium, or, for example, the fluctuation in the equilibrium position we find in many physical phenomena, first among them in Brownian motion.

(3) If the conditions of the ergodic theory are accepted, 'calibrating' the initially deviate measurements, as is usually done in physics, would become impossible.[9]

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[4] Cf. Khinchin (1949, pp. 29–30).

[5] This is intuitively clear if it is considered that any global integral reduces the space accessible to the trajectories by one dimension; since the MT is the assumption according to which the hyper-surface cannot be further reduced dimensionally, consequently there cannot be global integrals of motion different from energy.

[6] Cf. Sklar (1993, p. 166).

[7] A summary of the critiques about these supposition and about the assumption that the real systems are MT-ergodic can be found in Sklar (1993, pp. 175-188).

[8] Cf. Sklar (1993, pp. 176–177) and Guttmann (1999, pp. 84–86); see also van Lith (2001).

[9] Hopf tried to avoid some of these problems suggesting that even though measurement provides time average values, in the ergodic theory identity is between phase average and average value deriving from infinite single measures. However, even if this distinction is done, the result does not change, because infinite single measures provide an infinite time average anyway.

The second supposition means that zero measure sets have zero probability, but this runs counter to the following considerations: the zero measure sets are not necessarily empty. If we consider a space of dimension n, *any* of its subsets with dimensions of less than n will have a zero measure relative to the defined measure function on the initial space. Such a fact is quite notable for statistical mechanics, where hyper-surfaces of constant energy that are spaces with minor dimensions of classical phase space, are considered. In this sense, to give zero measure and hence zero probability does not necessarily mean giving *impossibility* to certain sets.[10]

One argument that is often advanced in favor of the possibility of neglecting zero measure sets is based on the realization that these do not seem to have any 'interior' points. This would make us think that zero measure sets are in some way 'unstable', namely a phase point passing by them would not stop long within them.[11] Unfortunately, this topic has faced the opposition of Malament and Zabell, who said we could construct sets without interior points, but to which we would prefer to give higher probability than zero.[12] An alternative was suggested by Malament and Zabell themselves who proposed accepting a rather blurred property of continuity for probability. According to this property, if set A is obtained from set B *via* a small change, then the probabilities associated with the two sets will be almost equal. A consequence of this property is actually neglecting the zero measure sets. However, even by following Malament and Zabell's indications, it is possible to build sets to which zero probability would not be willingly given. Meanwhile, the chance of neglecting the zero measure sets remains an assumption that depends on our definition of the measure function.[13]

This criticism exhibits a common characteristic. The former maintain that the equivalency between measurements and infinite time averages is problematic for systems that find themselves in a state of non-equilibrium, the latter show that zero measure sets are surely negligible only for stationary measures. The general thesis supported is therefore that the foundation of statistical mechanics *via* the ergodic problem is rigorously possible only for systems in a state of equilibrium. Now, since equilibrium is a limit state of the evolution of systems, even a truly general solution to the ergodic problem should exhibit the same 'asymptotic' characteristic by becoming more and more rigorous as the system approaches equilibrium. It is clear that the ergodic theory lacks this characteristic. In fact, the ergodic theory resolves the ergodic problem basing itself on properties like the MT that are strictly true only for phase spaces that represent systems in equilibrium. The conclusions of the ergodic theory are not therefore subject to any asymptotic condition expressing that their plausibility increases the more we are far from non-equilibrium state. This situation changes radically with Khinchin's approach to the ergodic problem.

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[10] Note that the second presupposition means also that to the Lebesgue measure function, usually adopted in statistical mechanics, a privileged role should be assigned. Haar (cf. Haar, 1933) showed how, at least under some conditions, the Lebesgue measure is effectively the only invariant (cf. Guttmann 1999, pp. 134–150), but these conditions are far from representing all the physically interesting cases.

[11] Such a conclusion relies on isomorphism that can be found between zero measure sets and first category sets, a concept coming from topology, which are sets equivalent to a countable union of sets lacking interior points. The idea is that if a set does not have interior points, then every state can be approximate to the external neighborhood of the same set (cf. Guttmann 1999, p. 168 and Oxtoby 1980, pp. 39–41).

[12] Cf. Malament and Zabell (1980).

[13] A further method consists of replacing zero measure sets, with first category sets, taking advantage of the Erdös–Sierpinsky theorem and developing statistical mechanics from this on a merely topological basis (cf. Guttmann 1999, pp. 151–189, Oxtoby 1980, pp. 74–81).

3. KHINCHIN'S APPROACH TO THE ERGODIC PROBLEM.

3.1 Critiques to ergodic theory

In 1949 A. I. Khinchin proposed a new approach to the ergodic problem. His point of view was explicitly critical of the ergodic theory and may be summed up as follows: ergodic theory is too abstract and too general to treat systems of statistical mechanics in a complete way and above all, has the typical set up of theories of equilibrium. Let us see his critical remarks in detail.

First, ergodic theory was developed as a part of 'general dynamics' and thus is applied to all dynamic systems, but does not contain anything specific for systems of statistical mechanics: "in particular all these results pertain equally to the systems with only few degrees of freedom as well as to the systems with a very large number of degrees of freedom."[14] The great complexity of systems of statistical mechanics thus does not play any role in the solution to the ergodic problem that, to the contrary, is really typical of such systems.

Second, it is hard to know if for a system the MT is valid, consequently also the practical calculation of phase averages will be complex. Khinchin maintains that furnishing an approximate method for evaluating phase averages is part of the solution to the ergodic problem.[15]

Third, the hypothesis of MT seems to be a foreign body in the overall ergodic theory. The ergodic theory without MT is substantially a dynamic of the phase space: it expresses the general transformation properties of a dynamical system. The entire statistical weight is therefore supported by this hypothesis introduced without any argument in a way that is completely analogous to the ergodic hypothesis. Moreover, considered in a general sense, this is also in contradiction with the theory of dynamical systems, as Khinchin's following argument demonstrates.

Let us say actually that I is an integral not depending on energy. Then it follows that:

a) I cannot be constant on every hyper-surface, otherwise it would be determined by the energy thereby contradicting the assumption of independence; also,

b) I must be a constant or otherwise a real number a exists such as we can define, against the MT, two subsets of finite measure Σ in which $I \leq a$ and $I > a$.[16]

To get around this argument requires the consideration of a preliminary question: do we have any reason to consider energy the unique global integral of motion, namely what is the status of the other integrals? As stated, once the number n of degrees of freedom is fixed, the Hamiltonian equations defines $2n$-1 integrals of motion for the system. The point is that the evolution of the system does not depend directly on all these integrals, as even experience suggests. Actually, most integrals do not make

[14] Khinchin (1949, p. 62).
[15] Khinchin (1949, p. 47).
[16] Khinchin (1949, pp. 55–62).

physical sense. An in–depth study of the problem needs a clear specification of a condition of physical significance. To determine this condition, the following consideration will be our starting point (Khinchin 1949, pp. 56–57):

> So far it was always self–evident, although not stated explicitly, that two distinct points of the phase space represent two distinct states of our mechanical system. Actually, however, in many cases, to distinct points of the [phase] space may correspond identical states of the mechanical system. Let us explain this. In many cases we are forced to characterize the same physical state of the system not by one, but by several sets (sometimes even by infinitely many) of values of its dynamic coordinates. Thus for a point which moves uniformly along a circumference, if we determine its position by the central angle counted form a fixed radius, we must consider as identical the states for which the values of this angle differ by a multiple of 2π.

To give the conditions for physical significance, let's say that the phase function must have the same value for phase points which correspond to the same physical state. If this condition is satisfied by a phase function, then it will represent a physical quantity, and if this is satisfied by an integral of motion, then it is said to be *uniform*.[17] Actually, it can be proved that this condition is generally sufficient for a number k of integrals that, due to the fact that they correspond to a physical quantity, are called *controllable*[18]. Thereby a new invariant subset I_k can be defined, having the dimension $2n - k$, and likewise it makes sense to introduce a new invariant measure function in order to develop a new general ergodic theory. In general, however, in statistical mechanics, systems for which it makes sense to place energy as the only integral are considered in order to obtain the hyper-surface Σ, and on it all the integrals converge almost everywhere, in which case they can be considered free.[19]

Now, let us say that it is impossible to divide the set into two subsets of positive measure inasmuch as the corresponding points at the same physical phase belong to the same subset. Such a division is called *normal*, and the impossibility that this can be brought about is the hypothesis of metric transitivity *in the physical sense* (MTP).[20] Introducing this new concept, it is possible to partially avoid the above argument. Let us take an integral I; if it is uniform (or normal) the previous argument is conclusive anyway. On the other hand, if I is not a normal integral, the division of the hyper-surface into two invariant subsets of a positive measure is incompatible with the fact that the subsets must contain points of the same physical phase (Khinchin 1949, p. 58):

> If our integral I is not normal, then, in determining the sets M_1 and M_2 we cannot start by arbitrarily subdividing the set of all values assumed by the integral I in two parts. If we want the subdivision (M_1, M_2) of the surface Σ_x to be normal, we must see to it that the values assumed by I at any two physically equivalent points are always placed in the same part. This requirement […] may turn out to be incompatible with the requirement that M_1 and M_2 be invariant sets of positive measure. In such a case our argument becomes invalid, and the question of possibility of metric indecomposability in the extended sense remains open.

Consequently, it is required that the system not have other normal integrals apart from energy, and so the MTP would remain a hypothesis as long as the empirical and analytical methods are not available, in order to discover in advance the integrals of

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[17] Or *normal* according to Khinchin's terminology; by assuming the function is continuous, this reasoning holds for an arbitrary neighborhood.

[18] In order to distinguish them from the remaining called *free*.

[19] Cf. Jancel (1963, p. 325); this is due to the type of systems which are dealt with in statistical mechanics, namely isolated systems closed in a vessel.

[20] Or, in Khinchin's terminology, metric transitivity *in extended sense*.

motion. Therefore, even if basically it is possible to avoid the more obvious contradictions using the principles of mechanics, the MT remains an extremely problematic hypothesis, and especially lacking in real and proper points in its favor. Moreover, as has been seen, the contradictions deriving from the MT may be overcome only considering more closely the states of the system that have physical meaning and this requires an in-depth consideration of the specific characteristics of the system itself.

What follows, according to Khinchin, is that the general point of view assumed by ergodic theory does not lead to a satisfactory foundation of statistical mechanics, since the authentic statistical meaning of the ergodic problem is not linked either to the physical characteristics of the systems of statistical mechanics nor to physical processes effectively operating in nature (Khinchin 1949, pp. 53-54):

> All this story of the ergodic problem appears to us instructive since it makes the efficacy of introducing various hypotheses which are not supported by any argument very doubtful. As is usual in such cases, when we are not able to submit really convincing arguments in favour of replacing the time averages by the phase averages, it is preferable, and also simpler, to attempt as the 'ergodic hypothesis' the very possibility of such a replacement, and then to judge the theory constructed on the basis of this hypothesis, by its practical success or failure. This, of course, does not mean that the theoretical justification of the accepted hypothesis is to be forgotten. On the contrary, this question remains one of the most fundamental in the statistical mechanics. We wish only to say that the reduction of this hypothesis to others is little justified and does not appear to us to be very efficient.

The real foundation of statistical mechanics consists therefore in linking the solution of the ergodic problem to the essential characteristics of physical systems: their statistical nature and the large number of degrees of freedom.

3.2 The asymptotic ergodic theorem.

Khinchin's approach to the ergodic problem is based on two crucial assumptions: 1) the systems effectively studied in statistical mechanics possess a large number of degrees of freedom, namely they are comprised of many components (molecules, particles and so on); 2) the phase functions of thermodynamic interest are sum-functions, that is they may be written as the sum of phase functions calculated on single components. In other words, a phase function f is:

$$f = \sum_{i=1}^{n} f_i \ ,$$

where the f_i are the corresponding phase functions for each of the components n of the system.

Both of these assumptions regard the particularities of systems of statistical mechanics and therefore specify those conditions that the ergodic theory leaves general. The result is a weaker version of the ergodic theorem. The key passage of Khinchin's theorem is the following property: the sum-functions have a small dispersion, of the order of n. In other words, call $\bar{f}$ the phase average of the function f defined on the hyper-surface of constant energy Σ, we have:[21]

[21] Khinchin's original argument (Khinchin 1949, pp. 62–69) is not always clear. Initially he calculated dispersion with respect to whatever function A, therefore making $A = 0$ to simplify calculations and in the end, making A equal to the phase average. Obviously, this last passage only regards the definition of

$$S = \int_{\Sigma} \left| f - \bar{f} \right|^2 d\Sigma = O(n) .$$

In this way, the size of the dispersion of the sum-functions is linked to the number of degrees of freedom. Now let us define the quantity:

$$S' = \int_{\Sigma} \left| f - \bar{f} \right| d\Sigma = O(n^{1/2}) = S^{1/2} .$$

From Schwartz's inequality we have:

$$S' \leq S^{1/2} = O(n^{1/2}) .$$

The ergodic theorem concerns the distance that exists between the infinite time average and the phase average. Let us define the following averages:

$$\hat{f}_T = \frac{1}{T} \int_0^T f dt ,$$
$$\hat{f} = \lim_{T \to \infty} \hat{f}_T .$$

The first represents the time average f between the instants 0 and T, while the second represents the infinite time average, that is, the quantity that we identify with the value of empirical measurements on the system. We must now evaluate the set of phase points for which the difference between the time average and the phase average is greater than a certain value $a > 0$. Let us define the two sets:

$$M_1 = \left\{ P \in \Sigma : \left| \hat{f} - \bar{f} \right| > a \right\},$$
$$M_2 = \left\{ P \in \Sigma : \left| \hat{f}_T - \bar{f} \right| > a / 2 \right\}.$$

Birkhoff's theorem assures us that the infinite time average of f exists, therefore for T _ ∞ the following relationship between measurements of the two sets is obtained:

$$\mu(M_2) > \frac{\mu(M_1)}{2} ,$$

where μ is the measure function defined on the hyper-surface Σ. Khinchin's aim, at this point, is to show that the measure M_1 tends to diminish with the number of degrees of freedom. With some calculations we may obtain:

dispersion (or variance) and may be performed from the beginning (cf. Jancel 1963, pp. 21–27 and Truesdell 1961, pp. 45–51).

$$\frac{a\mu(M_1)}{4} < \int_{M_2} \left|\hat{f}_T - \bar{f}\right| dM_2$$
$$\leq \mu(\Sigma) \int_{\Sigma} \left|f - \bar{f}\right| d\Sigma = S' m(\Sigma),$$

from which it follows that the relative measure of M_1:

$$\frac{\mu(M_1)}{\mu(\Sigma)} < \frac{4S'}{a}.$$

If now $a = S'^{3/2}$, we have for the relative measure of the set:

$$M_1 = \left\{ \in \Sigma : \left|\hat{f} - \bar{f}\right| > kn^{3/4} \right\},$$

the following inequality is valid:

$$\frac{\mu(M_1)}{\mu(\Sigma)} \leq O\left(n^{-1/4}\right).$$

In other words, the relative measure of the set of points for which the phase average differs from the time average by a factor that decreases with the number of degrees of freedom diminishes even more rapidly with the number of degrees of freedom. Accordingly, the large number of degrees of freedom assures that the phase average will always be maintained very close to the infinite time average.

If we pass from the measure of sets to probability and we apply Tchebichev's theorem, we may express Khinchin's result in the following terms:

$$\mathbf{P}\left\{ \left|\hat{f} - \bar{f}\right| \geq K \sqrt[4]{\overline{\left(f - \bar{f}\right)^2}} \right\} \leq \frac{1}{K^2} \sqrt{\overline{\left(f - \bar{f}\right)^2}}.$$

In this way, the probabilistic meaning of Khinchin's theorem finds expression (Truesdell 1961, p. 48):

> This inequality shows that the probability of a trajectory of which [the infinite time average] differs from [the phase average] by more than a multiple of the fourth root of the phase dispersion is itself less than a multiple of the square root of that dispersion. In other words, a nearly constant function is very probably a nearly ergodic function. It is simple ergodic estimates of this kind that render possible Khinchin's solution of the ergodic problem

3.3 Remarks about Khinchin's theorem

Khinchin's theorem shows that the measure of the set of phase points for which the infinite time average of whatever function differs from the phase average more than a number small as we please, tends to zero.

First, Khinchin's theorem is a solution of the ergodic problem if zero measure implies zero probability. In formal terms, we have to assume that the measure defined on Σ is ‘absolutely continuous’ with the measure of probability.[22] Obviously, this supposition inherits the problem of zero measure sets, but as has been seen, this question is implicit in the definition of the ergodic problem that Khinchin accepts as his own starting point.

Second, Khinchin’s approach is asymptotic in two different ways. The first way is evident: the theorem tends to an exact solution of the ergodic problem if n _ ∞, therefore this is asymptotically exact for systems with a number of components that tends to the infinite. The second way, which is more obscure, regards the fundamental assumption that considers the phase functions as sum-functions. From this derives the property that is the true core of the theorem: phase functions have small dispersions.[23] To obtain this property,[24] Khinchin must perform an essential move: consider a generic phase function as a random variable sum of n individual random variables.

Khinchin’s argument is the following. The various components of the systems are considered as stochastically independent, thus the phase functions associated with them are also random variables. Accordingly, the phase function of the entire system is the random variable sum of individual random variables. This allows Khinchin to apply the central limit theorem and conclude that the comprehensive system will have a Gaussian probability density. Now, under these hypotheses, the dispersion of a sum-function is:

$$\begin{aligned} Df &= \overline{\left\{\left(f-\bar{f}\right)^2\right\}} = \overline{\left[\left\{\sum_{i=1}^{n}\left(f-\bar{f}_i\right)\right\}^2\right]} \\ &= \sum_{i=1}^{n} Df_i + \sum_{i\neq k}\left(Df_i Df_k\right)^{1/2} R\left(f_i, f_k\right), \end{aligned}$$

where $R(f_i, f_k)$ represents the coefficient of correlation between the phase functions corresponding to the components i and k. Exploiting the central limit theorem and the properties of correlation that we will examine shortly, Khinchin is able to show that:

$$Df = \sum_{i=1}^{n} Df_i + \frac{1}{B}\sum_{i\neq k}\left(b_i b_k Df_i Df_k\right)^{1/2} R\left(e_i, f_i\right) R\left(e_k, f_k\right) + O\left(n^{1/2}\right),$$

where B, b_i, b_k are respectively the variances of the system’s and of component i and k’s probability density, while e_i and e_k are the energies of the two components. Since the second sum on the right side is on the order of n^2, Khinchin may conclude that $Df = O(n)$: “this fact establishes the ‘representability’ of the mean values of the sum-functions and permit us to identify them with the time averages which represent the direct results of any physical measurement.”[25]

The true meaning of the assumption of phase functions as sum-functions is therefore that we must consider the single components of the system as dynamically

[22] Khinchin (1949, p. 66).

[23] It is clear that Khinchin’s theorem consists of essentially this statement because, if the phase functions are almost everywhere equal to their phase average, then even their infinite time average will be equal to the phase average. Having established this fundamental fact, the rest of Khinchin’s argument serves to link the measure of the sets for which convergence with the number of degrees of freedom does not occur.

[24] Khinchin (1949, pp. 156–165).

[25] Khinchin (1949, p. 157).

uncorrelated. In other words, the values of whatever individual phase function calculated in subsequent times will be stochastically independent. Khinchin shows in fact that, if:[26]

$$R(s) = \frac{1}{Df}\overline{\big(f(t)f(t+s)\big)},$$

is the coefficient of correlation between the function f calculated over time t and the same function calculated over time $t + s$, then the phase average and the infinite time average of f will coincide if $R(s)$ _ 0 when s _ ∞. Herein is the second element of asymptoticity in Khinchin's theorem.

It is helpful to examine this element in greater detail. The ergodic behavior of systems of statistical mechanics since the time of Boltzmann's studies has been traced to the energetic interaction between components of the system. If we assume, as Khinchin does, that the components are stochastically independent and that the phase functions may be written as the sum of individual functions, we obtain a paradox (Khinchin 1949, p. 42):

> If we take the particles constituting the given physical system to be the components in the above defined sense, we are excluding the possibility of any energetical interaction between them. Indeed, if the Hamiltonian function, which expresses the energy of our system, is a sum of functions each depending only on the dynamical coordinates of a single particle (and representing the Hamiltonian function of this particle) then, clearly, the whole system of [Hamiltonian] equations splits into component systems each of which describes the motion of some separate particle and is not connect in any way with other particles[27]

In order to avoid this difficulty we must admit that the components are not totally separate but interact, exchanging energy in very small quantity with respect to the total energy of the system. Such components are called 'weakly coupled.' If the components are weakly coupled, the dynamic correlations that arise from their interaction are rapidly lost and their behavior is comparable to that of random variables. Then, the great number of degrees of freedom leads to the behavior described by the central limit theorem (Khinchin 1949, p. 159):

> With an ever increasing number of molecules, the correlation between the dynamical coordinates of any two of them becomes very weak; we have seen, in fact, that the correlation coefficient of two molecules tends to zero when n _ ∞ . Hence using a well known theorem of the theory of probability one can expect that the distribution of the sum functions for a large number of molecules will be, as a rule, similar to the Gaussian distribution

Thus, both the dynamic correlations between subsequent states of the same component and those between distinct components are progressively destroyed by the hypothesis of weak coupling of the components and the assumption of a large number of degrees of freedom. Khinchin's theorem is therefore asymptotic in two senses: first, it requires that the number of degrees of freedom tends to infinity, second, it requires that the time be sufficiently great to allow for destruction of the dynamic correlations between weakly coupled systems. Accordingly, by putting together the two conditions we can say that Khinchin's theorem is based on the *hypothesis of progressive*

[26] Khinchin (1949, pp. 67–68).
[27] See also Jancel (1963, p. 322).

annihilation of dynamic correlations. The statistical and asymptotic meaning of the theorem lies in this hypothesis.

4. Ergodic theory vs. Khinchin's approach: a comparison

Ergodic theory attempts to resolve the ergodic problem by using structural characteristics of the phase space of Hamiltonian systems and the hypothesis of the MT. From this point of view, the probabilistic aspect of the problem is clearly subordinate to questions of general dynamics. In contrast, Khinchin's approach is based on specific characteristics of systems of statistical mechanics with the aim of showing that these lead to a statistical behavior. In a certain sense, he reduces the dynamic questions to probabilistic questions. This relationship between ergodic theory and Khinchin's approach is illustrated well by the following consideration (Jancel 1963, pp. 26–27):

> It must be emphasized also that even though in the […] proof [of the Khinchin's theorem] a predominant role is played by statistical considerations based on the limit process $n \to \infty$, it does not impose any structure which is peculiar to the Hamiltonian of the system, apart from the canonical nature of the time–evolution; this point of view is contrary to that of Birkhoff theorem, where the statistical element is reduced to eliminating a set of zero measure, but where the conditions imposed on the structure of the system play an essential role

As we have seen, criticism of the ergodic theory revolve around the fact that this is principally a theory of the state of equilibrium. On the contrary, using concepts like annihilation of dynamical correlations, Khinchin's approach develops a point of view on the ergodic problem that is clearly shifted toward the non-equilibrium statistical mechanics. The hypothesis of annihilation of dynamic correlations, the large number of degrees of freedom and the derivation of approximate formulas for the calculation of phase averages are all typical instruments of non-equilibrium theories. Obviously, I'm not maintaining that Khinchin's is a theory of the state of non-equilibrium *strictu sensu*. His point of view, and herein lies the principal difference with ergodic theory, limits itself to a consideration of the state of equilibrium as *one of the states* that possesses certain characteristics, in which the system may find itself and not the *only one* worthy of attention. In the final analysis, in fact, Khinchin's approach consists of substituting the hypothesis of the MT – that regards geometry of phase spaces of a system in equilibrium – with the hypothesis of annihilation of dynamic correlations – that regards the physical evolution of a system in an arbitrary state. To better understand the meaning of this passage, it is helpful to introduce the distinction between 'diffusion hypothesis' and 'randomization hypothesis'.[28]

A diffusion hypothesis is a statement that expresses the following idea:

DH. *Sooner or later a system will pass through all the states of the system phase space*.

In the history of statistical mechanics, there are many examples of DH: the ergodic hypothesis or Gibbs' and Tolman's postulate of equi-probability *a priori* are perhaps the best-known cases. A randomization hypothesis, on the other hand, is a statement like the following:

[28] This distinction was introduced and explored in Badino (2005).

RH. *The evolution of the system from time t_0 to time $t_0 + dt$ is regulated by a stochastic process S.*

An example of RH is given by Boltzmann's calculation of the number of collisions. He assumes that the number of collisions that happen in an interval of time *dt* among molecules with a velocity v_1 and molecules with a velocity v_2 depends solely on the product of the respective total numbers of molecules.[29] It is evident that this assumption totally overlooks eventual dynamic correlations among the molecules. What relationship exists between DH and RH?

In the first place, it is clear that the DH is an extremely general statement, while the RH is very specific because it is valid for an initial instant t_0 and for a particular stochastic process *S*. Still, a DH is equivalent to stating that *the evolution of the system is regulated by some stochastic process that lasts over time*. In fact, DH maintains that the evolution of the system depends *only* on the probability of the states that this can assume, therefore it is the result of a stochastic process. This, however, does not tell us what this process is, but only that it is valid over time, or rather, that its conditions of validity are maintained indefinitely along the phase trajectory.

An RH, on the other hand, maintains that a particular stochastic process regulates an infinitesimal portion of evolution of the system. This specifies the nature of the process, but it is not at all implicit in this that the stochastic process will continue to be valid beyond that infinitesimal interval starting with the initial time t_0. Boltzmann was perfectly aware of this, in fact, he introduced the hypothesis of molecular chaos to allow that the assumption of the number of collisions was valid for the entire evolution of the system. A simpler example is the following. If I throw the dice once, I may think that its evolution is linked to the distribution of probability among the sides. But if I throw it a second time, it is not obvious that this assumption will continue to be valid. I could suppose that the result of the second toss depends on the way in which the first toss was done. If I admit that even the second toss depends only on the distribution of probability *a priori*, I am advancing an assumption that is completely different, that according to which the stochastic process is valid over time.

From this standpoint the relationship between DH and RH is clear. DH affirms that a certain stochastic process is valid over time, but it does not specify the nature of such a process. The RH, to the contrary, determines the specific characteristics of the process but is not valid indefinitely over time. Thus the DH requires an RH to be more specific, while the RH requires a DH to be valid over time.

On one hand, the MT is clearly a DH. As we have seen, this affirms that no integral of motion has been overlooked. Now, the phase trajectory must pass through all the states admitted by these integrals of motion, because if it passed through only a subset of them, we could define such a subset through a new integral of motion against the MT. On the other hand, the hypothesis of annihilation of the dynamic correlations that Khinchin proposes as an alternative to MT affirms the validity over time of a stochastic process. Even if Khinchin fails to distinguish clearly between DH and RH, he is well aware of the fact that his hypothesis of annihilation «represents the basic idea of» Boltzmann's molecular chaos.[30] Thus, his hypothesis has a meaning that is exactly analogous to the MT, as emerges also from the following consideration.

The property of sum-functions of having small dispersion remains valid even if a new integral of motion appears in the system. Still, in this case, the phase trajectory will be limited to a subset of the phase space and this subset will therefore have zero

[29] This is the so-called *Stosszhalansatz*, the assumption of the number of collisions.
[30] Khinchin (1949, p. 67).

measure with respect to phase space itself.[31] To avoid this problem, it is necessary that the conditions that allow for the success of Khinchin's stochastic process maintain themselves indefinitely, or rather, that the integrals of motion considered be all and only those that regulate the evolution of the system. This last assumption is precisely the MT.

What follows from this is that Khinchin's approach substitutes the MT with a hypothesis that has an analogous meaning. Inasmuch as this move leads to a scarce gain from the logical point of view, it is however very important for the interpretation of the ergodic problem. In fact, while the ergodic theory considered ergodicity as an additional hypothesis to the dynamic characteristics of the system and substantially disjointed from them, Khinchin shows the link existing between ergodicity and stochastic characteristics of evolution of a system in an arbitrary state. His point of view shifted toward non-equilibrium underscores the foundational role of ergodicity and in a wider sense of ergodic theory: furnishing a general condition of validity of the stochastic processes that regulate the processes in states of non-equilibrium.

5. CONCLUSIONS.

One of the most interesting foundational problems of statistical mechanics regards the embedding of equilibrium in the non-equilibrium theory. As we have seen, the analysis of the state of equilibrium often moves from suppositions that are difficult to reconcile with those at the base of non-equilibrium statistical mechanics. To try to recompose this fracture by bringing back a unity to statistical mechanics is a goal that is no less important than explaining the predictive success of phase averages. The distinction between DH and RH and the analysis of their relationships should be a step in this direction. Khinchin's point of view, it seems to me, asserts itself in this context. His approach tends to resolve the ergodic problem using suppositions and typical instruments of non-equilibrium statistical mechanics and the result is a weaker, but more interesting version of the ergodic theorem. Above all, it must be said that Khinchin has the merit of having developed the statistical meaning of ergodicity and the relationships that exist between this and the laws of evolution of systems more than with the geometric structure of phase space.

[31] Cf. Jancel (1963, pp. 36–37).

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