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A Solution of the Restricted Ergodic Problem in Statistical Mechanics. (**)

Introduction.

As it is known [1], the aim of the ergodic theory in statistical mechanics is the investigation of the connection between phase-averages and time-averages of phase functions which represent physical (microscopic) quantities for a given mechanical system.

The phase-averages are taken as theoretical representations of physical (macroscopic) quantities; the time-averages as theoretical representations of experimental data (see [1] page 44).

In what follows we shall always assume the Hamiltonian function of the given mechanical system not to depend on time t explicitly.

Let V be any invariant part of the whole phase space Ω; then a group of transformations T_t (2) on V is defined by the solutions of the equations of motion (3). The time-average of a phase function $f(\omega)$ is then the limit:

$$\lim_{T\to+\infty} \frac{1}{T}\int_0^T f(T_t\,\omega)\,\mathrm{d}t\,,$$

we shall denote, as usual, this limit by $\hat{f}(\omega)$.

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Section (1) is by BRUNO FORTE, section (3) is by FRANCO STROCCHI, the remaining sections have been developed in collaboration.

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(2) If ω represents the initial state of the mechanical system, $T_t\,\omega$ represents the corresponding state at time t.

(3) Hence all these motions of the mechanical system may be represented theoretically by a stationary process (see [3]).

Now it is not self-evident that a macroscopic quantity must be related to the time-average of a phase function f, even if $\hat{f}$ is constant in Ω. The time-average, as defined above, might not be the right representation of a macroscopic quantity as resulting by measurements.

Nevertheless it is reasonable to suppose that any macroscopic physical quantity should be represented by a functional $F(f)$ of a phase (microscopic) function. The question is what properties should be postulated for this functional; the following ones seem to be natural:

a) For every phase function $f(\omega)$ in a given linear space E of phase functions defined on V, $F(f)$ is a real number.

b) The functional $F(f)$ should be linear.

c) If $f(\omega) = 1$ everywhere in the given invariant part V of the phase space Ω, it should follow that $F(f) = 1$.

d) Let U_t be the transformation of $f(\omega)$ defined by $U_t f = f o T_t$, then $F(f)$ should be invariant with respect to U_t, that is $F(U_t f) = F(f)$.

e) If everywhere in V $f(\omega) \geqslant 0$, then also $F(f) \geqslant 0$.

Following these ideas we shall state in the next section a theorem whose importance in any ergodic theory is apparent.

1. - A basic property of the time-averages.

Let us agree to denote with $m(A)$ a finite invariant measure of any set A in a given σ-field of subsets of the invariant part V of Ω.

Let this field include V.

Consider the linear space $\mathcal{E}_V$ of the integrable functions $f(\omega)$ for which the time-average $\hat{f}(\omega)$ (exists and) is constant on V. The time-average $\hat{f}(\omega)$ $\left[\text{equal to the phase-average: } \overline{f}(V) = \frac{1}{M(V)} \int_V f(\omega)\, \mathrm{d}m\right]$ of any function $f(\omega)$ in $\mathcal{E}_V$ is just a functional $\Phi(f)$ on $\mathcal{E}_V$ which fulfils all the above stated requirements.

We shall show that the time-average is the unique functional on $\mathcal{E}_V$ which fulfils the requirements a), b), c), d), e).

As is known, if τ is any time interval and $T_\tau = T$ the corresponding transformation, the group property of the T_t' s implies $T_{i\tau} = T^i$ for every integer i. Then for every function $f(\omega)$ in $\mathcal{E}_V$:

$$\hat{f}(\omega) = \lim_{n \to +\infty} \frac{1}{n} \sum_0^{n-1}{}_i\, f(T^i \omega). \tag{1.1}$$

Hence fixing our attention on a point ω in V, given $\varepsilon > 0$ there is an integer $\bar{n}$ such that:

$$\left| \frac{1}{\bar{n}} \sum_{0}^{\bar{n}-1} {}_i f(T^i\omega) - \Phi(f) \right| < \varepsilon . \tag{1.2}$$

Suppose now that there is a fuctional $\Psi(f)$ different from $\Phi(f)$ fulfilling the same requirements.

From b) and e) we have:

$$\left| \Psi \left\{ \frac{1}{\bar{n}} \sum_{0}^{\bar{n}-1} {}_i f(T^i\omega) - \Phi(f) \right\} \right| \leqslant \Psi \left\{ \left| \frac{1}{\bar{n}} \sum_{0}^{\bar{n}-1} {}_i f(T^i\omega) - \Phi(f) \right| \right\} . \tag{1.3}$$

Hence:

$$\left| \Psi \left\{ \frac{1}{\bar{n}} \sum_{0}^{\bar{n}-1} {}_i f(T^i\omega) - \Phi(f) \right\} \right| < \varepsilon , \tag{1.4}$$

and taking into account b), c), d)

$$| \Psi(f) - \Phi(f) | < \varepsilon . \tag{1.5}$$

From the arbitrariness of ε, the relation (1.5) proves our statement (4).

Out of any ergodic theory we may remark that this theorem asserts in particular: the unique way to obtain an invariant with the specified requirements from a phase function $f(\omega)$ is by taking the time-average:

$$\hat{f}(\omega) = \lim_{n \to +\infty} \frac{1}{n} \sum_{0}^{n-1} {}_i f(T^i \omega) .$$

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(4) See the similar problem in the theory of invariant integration on a topological group [4].

2. - The « restricted » ergodic problem.

As it is known the solution of the ergodic problem, given by BIRKHOFF, VON NEUMANN and HOPF is not satisfactory from a physical point of view. In fact the BIRKHOFF condition cannot be checked system by system, as this would require the knowledge of the solutions of HAMILTON's equations. On the other hand, metrical transitivity is not a common property for physical systems and it should be postulated just as was the ergodic hypothesis.

Now the metrical non-transitivity of physical systems does not exclude the existence of phase functions the time-averages of which are independent of the trajectories in phase space, and therefore equal the phase-averages. Only this assertion can be made: if a system is not metrically transitive *not all* the integrable functions are such that

$$\hat{f} = \bar{f}. \tag{2.1}$$

From this it follows that metrical transitivity has not a deep physical meaning. Therefore one can look for a weaker condition implying that eq. (2.1) is satisfied only by functions representing physical quantities. This is indeed the only requirement to be made in order to set up the foundations of statistical mechanics. In fact the experimental data prove the evolution of the system towards equilibrium states, only in the sense that *certain* physical quantities, after long time, assume constant values which are practically independent of the initial conditions.

Thus the aim to be pursued is to prove the « ergodicity » of the system with respect to some particular phase functions. That is, we have to find a condition on a single phase function in order that we have $\hat{f} = \bar{f}$.

The requirements we make about this condition of ergodicity are the following:

1) The particular structure of the given function must be taken into account.

2) The aforesaid condition must be strictly related to the physical properties of the system for which eq. (2.1) has to be proved.

3) An essential rôle must be played by the Hamiltonian of the system. In fact we can treat an assembly of particles as a statistical system only if an interaction between them, although weak, is present.

4) It must be possible to check the fulfillment of the above condition without necessarily solving the equations of motion as it was the case of BIRKHOFF condition.

5) It must be taken into account the possibility of confining eq. (2.1) to some particular subregions V of phase space. In fact the time-average $\hat{f}$ may be independent of the initial state only under suitable restrictions, i.e. only if one is dealing with states characterized by some qualitative physical properties.

For the sake of brevity we shall call this approach to ergodic theory *the « restricted » ergodic problem*. Before showing a possible solution of this problem, we shall prove some mathematical assertions dealing with abstract measure theory.

3. - A theorem of decomposition of integrals.

Let Ω be the $2n$ dimensional phase space of the system. It is known that the transformation T induced by HAMILTON's equations is measure preserving (LIOUVILLE's theorem).

Now let Σ be a $(2n-1)$-dimensional surface invariant under T. Clearly the transformation T does not preserve the ordinary LEBESGUE measure on Σ.

However we can use a measure (5) on Σ which is preserved under T. This measure is so defined: if $K(q/p) = \text{const.}$ is the equation defining Σ and $K(q/p)$ is a time-independent integral of motion, the measure of the set $\Sigma' \subset \Sigma$ is:

$$m(\Sigma') = \int_{\Sigma'} \frac{\mathrm{d}\Sigma}{|\operatorname{grad} K|} . \tag{3.1}$$

All this has suggested the following theorem.

Let $(\Omega, \mathfrak{F}, m)$ be a mensural space and $\mathfrak{L}$ a set of functions integrable in $(\Omega, \mathfrak{F}, m)$. Every element $f \in \mathfrak{L}$ may be written as a function of $\varphi_1, \ldots, \varphi_h$, with $\varphi_i \in \mathfrak{L}$, $(i = 1, 2, \ldots, h)$, i.e.

$$f = \psi(\varphi_1, \ldots, \varphi_h) .$$

One has

$$\int_{\varphi^{-1}(B)} f \, \mathrm{d}m = \int_B \psi(\varphi_1, \ldots, \varphi_h) \, \mathrm{d}M , \tag{3.2}$$

(5) See KHINCHIN ([1], page 34).

where B is a BOREL set of R^h, $\varphi^{-1}(B)$ is the set of points

$$\left\{ \omega \in \Omega : P \equiv (\varphi_1(\omega), \ldots, \varphi_h(\omega)) \in B \right\},$$

M is the measure induced on the BOREL sets of R^h by the relation

$$M(B) = m(\varphi^{-1}(B)) .$$

Now, as it is known from measure theory, if $\psi(\varphi_1, \ldots, \varphi_h)$ is an integrable function in $(R^h, \mathfrak{B}, M)$, one has

$$\psi(y_1, \ldots, y_h) = \lim_{\delta \to 0} \frac{1}{m(\varphi^{-1}(I_\delta))} \int\limits_{\varphi^{-1}(I_\delta)} f \, \mathrm{d}m , \tag{3.3}$$

almost everywhere. Here I_δ is a neighbourhood of $P = (y_1 = \varphi_1, \ldots, y_h = \varphi_h)$. On the other hand if M is an absolutely continuous measure, it may be represented by a density function $F(y)$, i.e.

$$M(B) = \int\limits_B F(y) \, \mathrm{d}y . \tag{3.4}$$

Here $\int \mathrm{d}y$ denotes the ordinary LEBESGUE integral in R^h, and

$$F(y) = \lim_{\delta \to 0} \frac{M(I_\delta)}{M'(I_\delta)} , \tag{3.5}$$

with M' being the usual LEBESGUE measure in R^h.

Therefore we have

$$\int\limits_{\varphi^{-1}(B)} f \, \mathrm{d}m = \int\limits_B \psi(y_1, \ldots, y_h) \, F(y) \, \mathrm{d}y ,$$

where $\psi(y)$ and $F(y)$ are defined by eqs. (3.3), (3.5).

The above result may be easily extended to the case in which M is not an absolutely continuous measure. We may write

$$\int\limits_{\varphi^{-1}(B)} f \, \mathrm{d}m = \int\limits_B \psi(y) F(y) \, \mathrm{d}y ,$$

where $F(y)$ is now the distribution corresponding to the measure M.

We now specialize the previous results to the phase space. Let $f(x_1, \ldots, x_n)$ and $y_i(x_1, \ldots, x_n)$ $(i = 1, \ldots, n)$, be arbitrary functions defined in $\Omega \subset R^n$. We assume that

$$f = \psi(y_1, \ldots, y_n) .$$

Then

$$\int_\Omega f(x)\,\mathrm{d}x = \int_{y^{-1}(B)} f(x)\,\mathrm{d}x = \int_B \psi(y)\,\mathrm{d}M ,$$

where B is the set of points $\{P \equiv (y_1(x) \ldots y_n(x)) \in B;\ x \in \Omega\}$, i.e. $y^{-1}(B) = \Omega$. M is the measure induced on R^n by the usual LEBESGUE measure m in Ω:

$$M(A) = m(y^{-1}(A)) ,$$

with $A \subset B$ and $y^{-1}(A) = \{x \in \Omega,\ P \equiv (y(x)) \in A\}$.

Now let I_δ be a neighbourhood of $P = (y_1 = c_1 \ldots y_n = c_n) \in R^n$.

Then

$$m(y^{-1}(I_\delta)) = \mathrm{d}V = \frac{\mathrm{d}c_1}{|\operatorname{grad} y_1|} \cdots \frac{\mathrm{d}c_n}{|\operatorname{grad} y_n|} .$$

Therefore the density function $F(y)$ is given by

$$F(y) = \left[\prod_1^n {}_i\, |\operatorname{grad} y_i|\right]^{-1} .$$

Concluding we obtain

$$\int_\Omega f(x)\,\mathrm{d}x = \int_B \psi(y) \prod_1^n {}_i \frac{\mathrm{d}y_i}{|\operatorname{grad} y_i|} . \tag{3.6}$$

This equation is particularly interesting when only $j < n$ of the new variables y_i are considered. Then one has

$$\int_\Omega f(x)\,\mathrm{d}x = \int_B \psi(y) \frac{\mathrm{d}y_1 \ldots \mathrm{d}y_j}{|\operatorname{grad} y_1| \ldots |\operatorname{grad} y_j|} \cdot \frac{\mathrm{d}y_{j+1} \ldots \mathrm{d}y_n}{|\operatorname{grad} y_{j+1}| \ldots |\operatorname{grad} y_n|} ,$$

and using eq. (3.6),

$$\int_{\Omega} f(x)\,\mathrm{d}x = \int_{R'}\int_{S} \frac{f(x)}{\prod_1^j{}_i\,|\operatorname{grad} y_i|}\,\mathrm{d}S\cdot\mathrm{d}y_1 \ldots \mathrm{d}y_j\,.$$

Here $\mathrm{d}S$ is an element of the surface S with equations

$$y_i = c_i \qquad (i = 1 \ldots j)\,.$$

4. - The ergodic problem and the constants of motion.

The previous result suggests a useful decomposition of the integral defining the phase-average $\bar{f}$ of a functions f. In fact one has

$$\int_{\Omega} f(x)\,\mathrm{d}x = \int_{R'}\int_{S} \frac{f(x)}{\prod_1^j{}_i\,|\operatorname{grad} H_i|}\,\mathrm{d}S\cdot\mathrm{d}H_1 \ldots \mathrm{d}H_j\,, \tag{4.1}$$

where $H_i =$ const. are j time-independent integrals of HAMILTON's equations.

Clearly

$$\bar{f}_{H_i=c_i} = \int_{S} \frac{f(x)}{\prod_1^j{}_i\,|\operatorname{grad} H_i|}\,\mathrm{d}S \Bigg/ \int_{S} \frac{1}{\prod_1^j{}_i\,|\operatorname{grad} H_i|}\,\mathrm{d}S$$

is the phase-average of f on the surface $H_i = c_i$, as defined by KHINCHIN. Therefore eq. (4.1) states that $\bar{f}$ is the mean value of the phase-averages $\bar{f}_{H_i=c_i}$ evaluated on the integral surfaces, according to KHINCHIN and LEWIS (see [2]).

All this suggests a way of further restricting the ergodic problem.

The mechanical structure of the system, its Hamiltonian or its equations of motion may supply some global information about the solutions (without knowing them directly). For example some constants of motion may be known

$$H_i(q,\ p) = c_i \qquad\qquad (i = 1,\ 2,\ \ldots,\ j)\,.$$

Then we may further restrict the ergodic problem by requiring that $\hat{f}$ is independent of the initial state only when dealing with points on an integral surface. Thus a phase function, not ergodic on all phase space, may become so on each integral surface $H_i(q/p) = c_i$ $(i = 1, 2, ..., j)$, i.e. it may be

$$\hat{f} = \bar{f}_{H_i = c_i} = \int_S \frac{f(x)}{\prod_1^j{}_i |\operatorname{grad} H_i|} \mathrm{d}S \Big/ \int_S \frac{1}{\prod_1^j{}_i |\operatorname{grad} H_i|} \mathrm{d}S .$$

Clearly it follows from the previous theorem that if f is ergodic on Ω, it is so on each integral surface too. Therefore the above restriction does not alter the meaning of the ergodic theorem and in some special cases it may be a closer adherence to the physical problem.

In fact it might be impossible to prove the ergodicity in Ω, as this would imply the same behaviour for systems starting from far different initial conditions. This would clearly go beyond what is required by experimental facts; the evolution towards equilibrium is indeed the same for most of the physical systems, only under certain restrictions on the initial conditions.

On the other hand a limitation of the region V, on which the ergodicity of f is required, must be expressed by a condition covariant under canonical transformations. This is necessary in order that a physical interpretation of the theory is possible. In particular the above condition must be covariant under the canonical transformation induced by HAMILTON's equations. This implies that V is defined by surfaces invariant under HAMILTON's transformations, i.e. by constants of motion. Thus the way suggested by the mathematical theorem of sect. 2, is also justified on physical grounds.

5. - A sufficient condition for ergodicity.

We look for a condition which assures the ergodicity of f on the integral surface $V(H)$, $(H_i = c_i,\ i = 1 \ldots j)$. Clearly the phase-average on $V(H)$ is a function of $H_1 \ldots H_j$ alone. Thus a necessary and sufficient condition of ergodicity is that

$$\hat{f} = \varphi(H_1 \ldots H_j) . \tag{5.1}$$

On the other hand the time-average $\hat{f}$ with respect to a certain path may be represented in the following way. We consider the image of f on R^1 and divide R^1 into small intervals all of length δ. With varying time and with respect to a given solution $q = q(t)$, $p = p(t)$, the phase function $f(p, q)$ may be represented by a running point P_f on R^1, moving with velocity $\mathrm{d}f/\mathrm{d}t$. Then $\hat{f}$ may be written in the form

$$\hat{f} = \lim_{\delta\to 0}\lim_{n\to+\infty} \frac{1}{\sum_0^n{}_i \tau_i} \sum_0^n{}_i \left(f_i + \frac{\delta}{2}\right)\tau_i ,$$

where f_i is the left extreme of the interval containing P_f at the time $t = \sum_0^i{}_j\tau_j$ and τ_j is the time spent by P_f in the interval (f_j, f_{j+1}),

$$\tau_j = \left[\left(\frac{\mathrm{d}f}{\mathrm{d}t}\right)_j\right]^{-1}\delta .$$

Here $(\mathrm{d}f/\mathrm{d}t)_j$ denotes the time derivative of f, with respect to the given solution $q = q(t)$, $p = p(t)$, evaluated at a proper point in the interval (f_j, f_{j+1}).

Then if $\left(\frac{\mathrm{d}f}{\mathrm{d}t}\right)^{-1}$ does not depend on the particular path $q = q(t)$, $p = p(t)$, the same is true for τ_i, so $\hat{f}$ is independent of the solutions and eq. (5.1) is satisfied. The physical meaning of this condition is that any surface $f = \text{const}$ is crossed by the trajectories always in the « same way », independently from the crossed point on it. Hence $\mathrm{d}f/\mathrm{d}t$ is constant when $f, H_1 \dots H_j$ are so. This requires that the $2n$-dimensional gradient of $f, H_1 \dots H_j$ is parallel to the gradient of $\mathrm{d}f/\mathrm{d}t$, i.e. from the equations

$$(4.2) \qquad \sum_0^n{}_h \lambda_h \frac{\partial f}{\partial x_h} = 0, \qquad \sum_1^n{}_h \lambda_h \frac{\partial H_i}{\partial x_h} = 0 \qquad (i = 1, \dots, j),$$

it must follow

$$(4.3) \qquad \sum_1^n{}_h \lambda_h \frac{\partial}{\partial x_h}\left(\frac{\mathrm{d}f}{\mathrm{d}t}\right) = 0 .$$

This implies the vanishing of the determinant

$$(4.4) \qquad D_1^2 = \left| \frac{\partial(f, [H, f], H_1, \dots, H_j)}{\partial(x_1, \dots, x_n)} \right|^2 .$$

When the additional condition

$$(4.5) \qquad D_2^2 = \left| \frac{\partial(f, H_1, H_2, H_3, \dots, H_j)}{\partial(x_1, \dots, x_n)} \right| \neq 0$$

is satisfied, eq. (4.4) is perfectly equivalent to eqs. (4.2), (4.3). On the other hand if $D_2^2 = 0$ and $H_1 \dots H_j$ are all independent, then f is a constant of motion dependent on $H_1 \dots H_j$ and clearly $\hat{f} = f_{H_i = c_i}$.

6. - Conclusions.

With our sufficient condition for the ergodicity of a microscopic function we have partially solved the restricted ergodic problem in the statistical mechanics of energy preserving systems; on the other hand we have characterized a linear space of functions for which $\hat{f} = \text{const.}$ on well defined and physically significant subsets of the phase space Ω. We are sure now, on the basis of what is expounded in section (1), that the statistical assertions on the macroscopic quantities represented by the phase averages of these particular microscopic quantities $f(\omega)$ may be experimentally verified.

We hope moreover that the linear spaces of functions which satisfy our condition are sufficiently wide to include all the microscopic quantities of physical interest.

What one may say about the restricted ergodic problem for dissipating systems is still an unsolved problem.

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Sommario.

Sulla base di una formulazione più generale del problema ergodico di Birkhoff gli Autori assegnano nuovi fondamenti al problema ergodico ristretto. Dopo alcune considerazioni sulle proprietà principali delle medie temporali e delle medie in fase, gli Autori presentano una soluzione fisicamente significativa di tale problema.

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