POINCARÉ RECURRENCE TIMES AND STATISTICAL MECHANICS

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ABSTRACT

The theory of almost-periodic functions is applied to the problem of the relation, conjectured by the Ehrenfests, between Poincaré recurrence times and the time over which averages of phase functions must be taken in order to approximate their limiting values for infinite time. It is concluded that the necessary averaging times might be very much longer than the Poincaré periods. Equality of ensemble averages and time averages would than carry no implications about equality of ensemble averages and experimental values. Two possible ways of understanding the success of statistical mechanics without recourse to ergodicity are then discussed. One of these interpretations has implications for the theory of irreversible processes and the problem of condensation, which are capable of being tested independently.

1. INTRODUCTION

One of the most serious objections[1-3] to the ergodic approach in statistical mechanics is the fact that, even if the equality of time averages and ensemble averages were demonstrated rigorously and universally, this result would be established only for averages over the times which would be required for the phase point to "explore" all the accessible regions of phase space. This time is presumably related to the Poincaré recurrence times,[4,5] which are enormous compared to the age of the universe for macroscopic systems. Recently, the suggestion has been made[6,7] that this objection may be answered by considering permutations of identical particles. The Poincaré periods should then be divided by N! in order to obtain recurrence times for observable quantities. This raises the question whether these "generic recurrence times" are sufficiently short to be comparable with the times involved in experiments, and whether averages over these times will approximate their limiting values for infinite time.

These questions are difficult to discuss in terms of classical theory, since phase space is not a metric space and there seems to be no canonically invariant way of defining "closeness of approach." Boltzmann's estimate of these times[5] ($>10^{10^{19}}$ years) was made by considering distances in coordinate space and momentum space separately. Poincaré's theorem,[4] on the other hand, involves only the invariant element of phase volume. Since the factor N! is in a sense a quantum effect, it appears more satisfactory to discuss these problems in terms of quantum theory. Here the norm $|\psi_i - \psi_j|$ provides an invariant meaning to the "degree of closeness" of two states.

The classical problem concerned a completely isolated system, restricted to a finite volume and a finite energy, therefore a finite phase volume.

The phase point of such a system must ultimately return to a neighborhood, of arbitrarily small phase volume $\delta\Omega$, of the initial point. We take as the corresponding quantum theory model an isolated system of finite size, for which all elements of the density matrix referring to energies greater than E_{max} are zero. The analog of recurrence in phase space will be taken as a recurrence of the expectation values of all observables. The problem then reduces to a transcription of known results in the theory of almost-periodic functions.[8]

2. ALMOST-PERIODIC FUNCTIONS

A set of real numbers $\{\tau_i\}$ is called relatively dense if there exists a number T such that every interval $t < \tau < t + T$ of length T contains at least one number of the set. A continuous function $f(t)$ is called almost periodic if for any $\varepsilon > 0$ there exists a relatively dense set of numbers $\{\tau_i\}$ such that $|f(t + \tau_i) - f(t)| \leq \varepsilon$ for $-\infty < t < \infty$. The τ_i are called translation numbers of $f(t)$ corresponding to ε. We denote by $T_0(\varepsilon)$ an interval such that every interval of length $T_0(\varepsilon)$ contains at least one translation number corresponding to ε.

It may be shown[8] that the class of almost-periodic functions is identical with the class of functions consisting of all finite sums

$$f_N(t) = \sum_{n=1}^{N} a_n e^{i\omega_n t} \tag{2-1}$$

when "closed" by the addition of all functions $f(t)$ which can be uniformly approximated by the f_N: $|f(t) - f_N(t)| \leq \varepsilon$ for all t. In (2-1) the a_n are arbitrary complex numbers and the ω_n are arbitrary real numbers.

In our physical problem, the density matrix at time t is given by

$$\rho_{nm}(t) = \rho_{nm}(0)\, e^{i\omega_{mn} t} \tag{2-2}$$

where the stationary states are defined by $H\psi_n = E_n \psi_n$, and $\hbar\omega_{mn} = E_m - E_n$. Only a finite number of the ρ_{nm} are different from zero, and therefore any expectation value

$$f(t) = \langle F \rangle = \mathrm{Tr}(\rho F) = \sum_{m,n} F_{mn}\, \rho_{nm}(0)\, e^{i\omega_{mn} t} \qquad (2\text{-}3)$$

is an almost-periodic function of t. Recurrence times then correspond to the simultaneous translation numbers of all functions of the form (2-3).

3. TIME AVERAGES

In classical theory, the statement that recurrence times are related to the period over which time averages must be taken in order to approximate their limiting values (henceforth called the averaging times), seems to be only a reasonable conjecture. In quantum theory, however, this becomes a theorem with surprising content. For every almost-periodic function, not only does there exist a mean value

$$Mf(t) = \lim_{T\to\infty} \frac{1}{T} \int_{\alpha}^{\alpha+T} f(t)\, dt \qquad (3\text{-}1)$$

independent of α, but it is also true[8] that for any $\varepsilon > 0$ we have

$$\left| Mf(t) - \frac{1}{T} \int_{0}^{T} f(t)\, dt \right| \leq \varepsilon \qquad (3\text{-}2)$$

whenever

$$T \geq \frac{4}{\varepsilon}\, T_0(\varepsilon/2)\, f_{max} ,$$

where f_{max} is an upper bound of $|f(t)|$ in $-\infty < t < \infty$. This result is surprisingly weak, since one might expect intuitively a much stronger statement, that the average over a translation number corresponding to ε would already approximate $Mf(t)$ to the order ε. Note, however, that $T_0(\varepsilon)$ might be very much greater than the first[9] translation number $\tau_1(\varepsilon)$ corresponding to ε, so that the behavior of $f(t)$ in $0 \leq t \leq \tau_1$ would not provide a "representative sample" of its behavior in all regions.[10]

This result applies also to the classical case, if we interpret the Poincaré recurrence theorem as implying that every phase function $F(p_i, q_i)$ is, by virtue of the equations of motion, an almost-periodic function of time.

One then sees that the averaging time for F might in fact be very much longer than the Poincaré periods. There is no guarantee that behavior during one recurrence time with given closeness of return provides a representative sample of behavior for all time. We conclude that no simple relation exists between averaging times and generic recurrence times, and consequently the averaging times should be studied on their own merits, without reference to Poincaré periods.

For any macroscopic system the averaging time for the quantities (2-3) will still be large. To take the simplest possible example, consider a "system" consisting of a single hydrogen atom moving in a cubic box of side 1 cm, and known to be in one of the two lowest energy states. The averaging time for this case, of the order of $h/(E_2 - E_1)$, turns out to be about 15 minutes. Every new particle added to the system, and every new energy level taken into account, will increase this by a large factor. When we have reached any realistic model, the averaging time will again be enormous compared to the age of the universe. It seems hardly worthwhile to work out a typical numerical value.

4. PHYSICAL INTERPRETATION

The times involved in experiments are shorter, by perhaps 10^{10} orders of magnitude, than the times required for a full exploration of the accessible classical phase space or quantum function space. Thus there can be no possibility of explaining the laws of thermodynamics on the grounds that every possible microscopic condition is approximated in succession during the time of observation. In spite of this, the experimental fact which has to be explained is not that the average behavior over an ensemble of similar systems follows the laws of thermodynamics, but rather that each individual system obeys these laws. We conclude that any explanation of the fact that ensemble averages correspond to experimental values, must be based on other properties than ergodicity.

It should be noted that justification of the methods of statistical mechanics, and explanation of their success, are entirely different problems. The former is very easy if we regard statistical mechanics as a form of statistical inference, and show[11] that its methods make full use of all

the available information. Whether the theory is successful or not, one cannot do better than this. However, until we have also explained the reasons for its success, we cannot claim to have any real understanding of statistical mechanics.

Any attempt to do this without making use of ergodicity leads one immediately into the deepest questions of interpretation. There are two directions in which one can proceed, depending on whether we accept the following assumption of realism: Every system is, at every time, in a single, definite microscopic state. In classical theory one would never question this, but in quantum theory the Einstein-Podolsky-Rosen paradox[12,13] shows that it is not to be dismissed as obvious. If we deny this assumption, we imply the possibility that an individual system may be, in some sense which is different from that of the principle of superposition,[14] simultaneously in many different microscopic states. The statement that a system has a given temperature because it is "in a Boltzmann distribution" might then have a definite operational meaning for a single system at a single time. If we admit this possibility, the problem is solved in a very simple way; we assume that interaction with a heat-bath eventually produces this condition. There are good reasons[15,16] for believing this can be justified quite generally. If all states of the system are in some sense present simultaneously with Boltzmann weighting factors, the identification of ensemble averages with experimental values is immediate, independently of ergodicity or, in fact, of any property relating to evolution in time.

It is to be emphasized that this interpretation, bizarre as it may seem, probably cannot be refuted by logic. Furthermore, a study of the Einstein-Podolsky-Rosen paradox will lead one to conclude that it is quite consistent with, if not indeed required by, the present interpretation of quantum theory. For example, the present theory allows the possibility that the system of interest σ_1 and a heat-bath σ_2 which have been in interaction in the past, but are now completely isolated from each other and from the rest of the universe, may be jointly in a pure state

$$\psi(1,2) = \sum_{n,m}{}' a_{nm}\, u_n(1)\, v_m(2) \qquad (4\text{-}1)$$

where $u_n(1)$ and $v_m(2)$ are possible state vectors of systems σ_1 and σ_2 respectively. This implies that system 1 is in some sense in each of the states $u_n(1)$, with a density matrix

$$\rho_{nk}(1) = \sum_m a_{nm} a^*_{km} . \qquad (4\text{-}2)$$

There is clearly no possibility of interpreting this density matrix as giving the relative frequencies with which system σ_1 occupies the various states successively; because of coherence properties implied by (4-1) which are in principle observable (by measurement of some joint property of the two systems), we must conclude that there is some objective sense in which system σ_1 is in all these states simultaneously. Thus the statement that an individual system is "in a Boltzmann distribution" at a given time does not contradict the mode of description provided by quantum theory.

In spite of this, and a certain attractiveness because of the simple way in which this disposes of difficult problems, we prefer to retain the assumption of realism, and to try to understand statistical mechanics on that basis. The remainder of this paper is based on the assumption of realism and represents what appears to the writer as the only possible way of understanding the success of statistical mechanics which is compatible with that assumption, and which does not make use of ergodicity. We do not, however, attempt to answer the question whether "microscopic state" is to be interpreted as a pure state of quantum theory.

5. MACROSCOPIC UNIFORMITY

Consider any experiment performed on a macroscopic system. It might be anything from a nuclear induction measurement to throwing a baseball. The initial conditions of the experiment never restrict the system to a particular microscopic state; it could be in any one of billions of possible states. Clearly, when we repeat the experiment we do not repeat the initial microscopic state. If, in spite of this, the result is reproducible, we must conclude that the same result would have been obtained for each of the great majority of the possible initial states. This is the principle of macroscopic uniformity. The properties for which it holds true are precisely those for which reproducible macroscopic experiments

are possible.

Given the principle of macroscopic uniformity, it follows that, whether a process in reversible or irreversible, in order to calculate any reproducible feature of it we could choose at random any one of the possible initial states and solve the equations of motion (for example, the time-dependent Schrödinger equation) for it. We would get the same results for any such state, unless we were unfortunate enough to choose, out of all the billions of possibilities, one particular state of the small minority for which the answer is different. The only thing which the use of a probability distribution over initial states accomplishes for us is that it protects us from that danger; in calculating the average over many possible states, we suppress this small minority. "Almost any" probability assignment for initial states, which gives the correct average values for the controlled or observed parameters, would lead to the same macroscopic predictions. The Boltzmann distribution, besides being mathematically convenient, is the broadest one (i.e., it has maximum entropy) for a given value of $\langle E \rangle$; therefore it is the one which affords maximum protection against minority states.

Because of the principle of macroscopic uniformity, the validity of statistical mechanics as a method for predicting experimental results in no way depends on the "correctness" of the Boltzmann distribution. It is rather the other way around; the Boltzmann distribution or a generalization thereof derives its validity as a tool for prediction from the fact that it is consistent with the measured values of temperature and other parameters, and it assumes nothing beyond that.[11] This remark carries many implications. In particular, if we adopt the view just expressed, it becomes necessary to discuss anew the meaning of experimentally measured temperature and entropy.

6. EXPERIMENTAL TEMPERATURE AND ENTROPY

In a thermodynamic experiment, a few degrees of freedom of a system are fixed by the experimental conditions, and a few others are observed, while the vast majority are neither controlled nor observed. Energy exchanged via controlled degrees of freedom is called work; energy exchanged via uncontrolled ones is called heat. Two systems are said to be at the same temperature if, when placed in weak interaction with each other, the net amount of energy which they exchange over long periods of time is small, of the order of the interaction energy. Numerical values of temperature are defined by the relative

amounts of energy which two heat baths interchange with a third system operating in a Carnot cycle between them. Since these are the only criteria used in experiments to measure temperature and heat, they must, according to the operational view of physics, be the only ones involved in the corresponding concepts.

We may say that the temperature of a system is known if we can predict correctly which one of a set of thermometers, showing different readings, will not exchange appreciable energy with it if brought into weak interaction. If the system is in a known microscopic state, we must surely be in the best possible position to make this prediction. Thus, an operationally defined temperature has a definite meaning even, or rather especially, in the case of a system in a known microscopic state. This is in sharp constrast to the often expressed view that the concept of temperature requires some degree of ignorance or "randomness." To say that a system has a given temperature because it is "in a Boltzmann distribution," or to say, "the system has random phases," is devoid of any meaning if we adopt the assumption of realism.

Conventional modes of expression often suggest that experimentally measured entropy represents the logarithm of the volume of phase space "occupied" by a system, or its degree of "disorder." From the present point of view, such statements also become meaningless. The experimental entropy is constructed from observed quantities, and would be exactly the same for any microscopic conditions which would lead to the observed values. Thus it is not required that the system actually "avail itself" of this full volume of phase space; very severe constraints on the possible states could exist without in any way affecting macroscopic observations. Suppose we have found the experimental entropy $S(\alpha_1 , \alpha_2 , \ldots)$ as a function of certain measured parameters α_i. This entropy measures the volume of phase space which is compatible with the α_i, and thus it measures our degree of ignorance as to the true state in the case where α_i provide the only available information about that state.

There is in principle no reason why we could not obtain additional information, on a microscopic level. Such additional information would, of course, not alter the experimental entropy if we continue to define it as $(S_{exp})_1 = \int dQ/T$. It would, however, enable us to define a new experimental entropy $(S_{exp})_2$, which embodies this information. A method of doing this is described in reference 11. In principle, the additional information would

always make possible more reliable predictions of the behavior of the system than are obtainable from the equations of thermodynamics. In practice, however, it would be found to be of very little value unless we wished to predict microscopic details of that behavior, or unless it showed us that the system was in a "minority state." The reason for this is to be found, again, in the principle of macroscopic uniformity, which shows that the additional information is usually irrelevant for macroscopic predictions. If this were not the case, macroscopic information would not suffice for predicting macroscopic behavior, and there could be no science of thermodynamics.

7. CONCLUSION

Although the assumption of realism implies that the principle of macroscopic uniformity must be true, the converse does not hold. Indeed, the principle of macroscopic uniformity, in a somewhat weaker form, has long been recognized. If we accept it, we can relax considerably the requirements for the possible interpretation discussed in Sec. 4. There is no longer any need for the system to be exactly "in a Boltzmann distribution." Any reasonable approximation to it will still lead to the same macroscopic predictions.

The interpretation of statistical mechanics based on the assumption of realism carries many implications for current unsolved problems in statistical mechanics.[17] In the following we point out two examples of the manner in which these problems change if we now interpret "microscopic state" as meaning a pure state of quantum theory.

A. Irreversible Processes. One of the fundamental problems of the theory of irreversible processes is how to find the ensemble which correctly represents a system in a nonequilibrium state. With our interpretation, however, there is no such thing as a "correct" ensemble; the notion is quite meaningless. Nevertheless, because of the principle of macroscopic uniformity, we conclude that the methods of maximum-entropy inference,[11] when generalized to the density matrix formalism, must provide a correct prediction of every feature of irreversible processes which is experimentally reproducible. The reason for this is that every property which is characteristic of the great majority of the possible states will emerge from this treatment with a sharp probability distribution. Thus the prescription for a general theory of irreversible processes becomes: For the initial time $t = 0$, find the density matrix which maximizes the entropy $S = -\mathrm{Tr}(\rho \log \rho)$ subject to all the constraints represented by the available information. The solution of $i\hbar\dot{\rho} = [H,\rho]$ with

this initial condition must contain the description of the irreversible process. In finding this solution, any approximation which does not alter the expectation values $\langle F \rangle = \mathrm{Tr}(\rho F)$ of the quantities which we wish to predict, are permissible regardless of what they do to $\mathrm{Tr}(\rho \log \rho)$. Thus, the adoption of a "coarse-grained density" is not something required by philosophical principles[7] concerning the accuracy of measurements; it represents simply the process of discarding, voluntarily, irrelevant information.

B. Condensation. In attempts to understand condensation since the time of van der Waals, the underlying idea has been that the phenomenon is basically a statistical one, which would be understood if only one could do a rigorous job of evaluating partition functions and passing to the limit $N \to \infty$. However, since condensation is an experimentally reproducible property, we are forced to conclude that it must be found, not only in some ensemble average, but it must be characteristic of each of the great majority of the pure states compatible with the conditions of the experiment. But if this is so, then condensation must be predictable already from a study of the properties of typical pure states, independently of any statistical consideration. As we lower the energy of a gas, we must reach a point where practically all of the possible stationary states correspond to a greater density of matter along the bottom portion of the container. Thus the problem of condensation becomes primarily one of physics rather than statistics.

We see that if we abandon the attempt to utilize ergodicity, and at the same time retain the assumption of realism, the fact that statistical mechanics is successful carries far-reaching implications which are capable of being tested independently. Conversely, if it can be shown that any of these implications, such as (A) or (B) above, is false, then it would appear that we must either abandon the association "microscopic state = pure state," or else return to the interpretation of Sec. 4.

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9. By this is meant the first nontrivial translation number, i.e., we do not count the translation numbers which occupy a neighborhood of zero. That the latter are formally translation numbers depends only on the continuity, not the almost-periodicity, of $f(t)$.

10. As a simple example showing why the stronger statement could not be true in general, consider the function $f(t) = e^{i\omega_1 t} + e^{i\omega_2 t} + e^{i\omega_3 t}$, where the frequencies are all incommensurable and $\omega_1 \ll \omega_2$, $\omega_1 \ll \omega_3$. Then if m, n are the smallest integers for which $|m(\omega_2/\omega_3) - n| \leq \varepsilon/4\pi$ and ω_1 is sufficiently small so that $n(\omega_1/\omega_3) \leq \varepsilon/4\pi$, the interval $\tau_1 = (2\pi n/\omega_3)$ is a translation number corresponding to ε. Clearly, however, in order to obtain a representative sample of $f(t)$, one must observe it for at least a time interval T so long that all three terms have completed nearly an integral number of cycles. This time is of the order of $T \approx (2\pi/\omega_1) \geq 4\pi\tau_1/\varepsilon$. As a second example, consider the case where ω_1 is very close to ω_2.

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