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by DAVID LAVIS

INTRODUCTION

There exists a class $\{\mathscr{S}\}$ of systems, any member $\mathscr{S}$ of which can be regarded on the one hand as a *mechanical system* $\mathscr{S}^{(M)}$ and on the other as a *thermodynamic system* $\mathscr{S}^{(T)}$. The mechanical system $\mathscr{S}^{(M)}$ is characterised by its classical or quantum mechanical state which evolves with time according to the appropriate differential equation (Hamilton's equation or Schrödinger's equation respectively). The thermodynamic system $\mathscr{S}^{(T)}$ is characterised by the assumption that, if undisturbed for a sufficiently long period of time, it will attain a state called its *equilibrium state*. Such an equilibrium state is specified by a small set of parameters, these being interrelated by the laws of thermodynamics. The primary rôle of statistical mechanics is to interpret the parameters of $\mathscr{S}^{(T)}$ and to derive the relationships between them in terms of the properties of $\mathscr{S}^{(M)}$.

We may enquire whether this task could be performed only by a theory with a probabalistic component. One apparently obvious affirmative answer to this question would be of the following kind: 'Some probabalistic component is necessary because of the quantum nature of matter. Probability theory is involved because of its essential rôle in quantum theory'. Such an answer is inadequate on two counts. First because of the existence and relative success of classical statistical mechanics and secondly because of the dual rôle of probability theory in quantum statistics. From the point of view of this discussion quantum considerations are irrelevant and we shall henceforth suppose $\mathscr{S}^{(M)}$ to be a classical mechanical model. The question of the necessity or otherwise of *statistical* mechanics remains open and will arise in the course of the discussion.

It must be emphasised at the outset that the aim of this paper is to give a possible *rational reconstruction* of the current programmes of statistical

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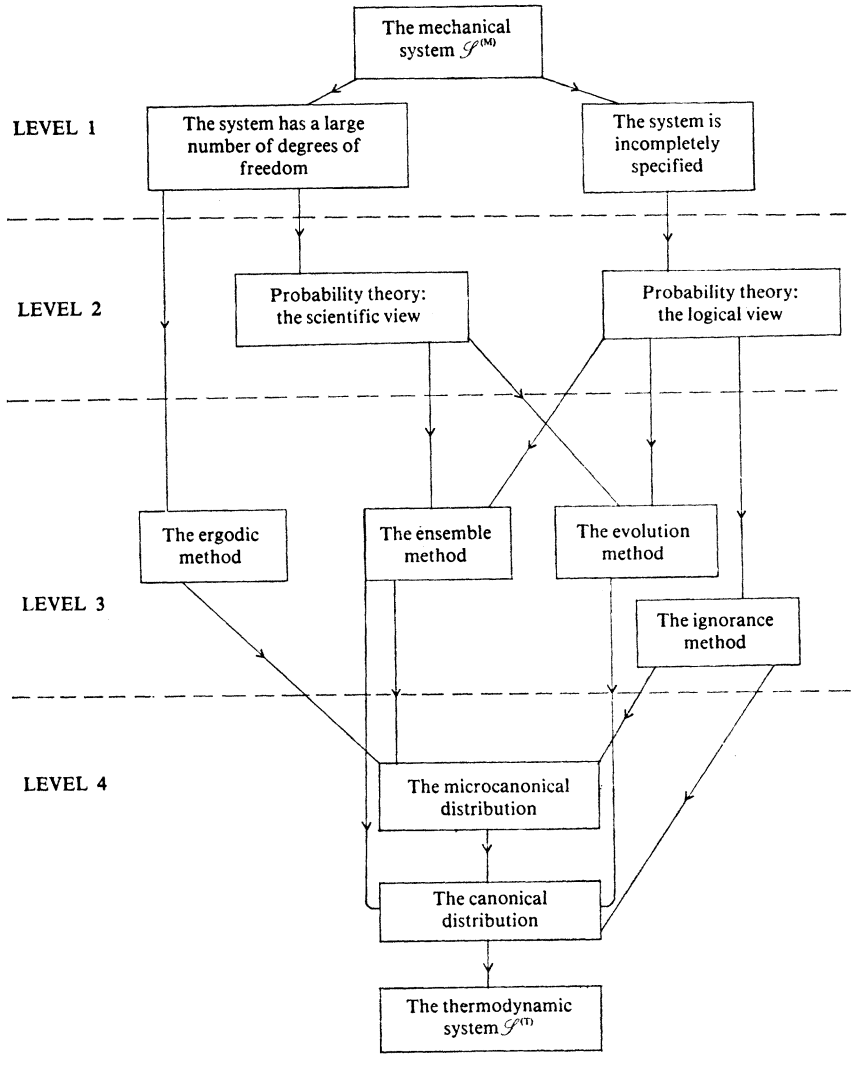
mechanics. It is necessary to stress the motive of rational reconstruction because the development of statistical mechanics has been such that a survey entirely in terms of the declared views of writers in the field would on the one hand be confusing and on the other leave many gaps. Certain



terms (*e.g.* 'ensemble') are used, as we shall see, in different senses by different writers. It is also the case that many of those most concerned with the development of statistical mechanics have left certain key aspects of their programmes implicit or ambiguous. This is particularly so with respect to their views on probability theory. The attempt has been made

therefore to construct the possible routes from mechanics to thermodynamics in terms of concepts rather than personalities. To aid this task the material of the discussion has been divided into four levels as shown in the diagram. Level 1 contains classical mechanics together with the two properties which would seem, separately or together, to characterise those mechanical systems which give rise to thermodynamic behaviour. Level 2 contains the philosophical positions with respect to probability theory which would seem to provide sufficient support for the construction of statistical mechanics.[1] Level 3 contains most of the disputed aspects of the derivation of statistical mechanics. It is in itself a mainly mathematical level but the choices between different approaches within it are to some extent determined by the philosophical considerations arising from level 2.[2] Level 4 is common ground for all workers in statistical mechanics. There are differences in the degree of mathematical sophistication with which the material is manipulated, but there is little doubt that the microcanonical and canonical distributions are a necessary part of equilibrium statistical mechanics.[3] The arrows in the diagram represent my personal opinion as to the possible rational routes from level 1 to level 4. Part of the purpose of this paper is to attempt to expose the weaknesses of these various routes. Since levels 1 and 4 present the least problems and since they represent the beginning and end points of all the programmes under discussion we shall consider them first, after which we shall deal with the problematic areas represented in levels 2 and 3.

LEVEL 1

Let $\mathscr{S}^{(M)}$ be a stationary Hamiltonian system of N identical microsystems (gas molecules, dipoles *etc.*) each with η degrees of freedom (translational, rotational *etc.*). The macroscopic dimension of the system is given by one extensive parameter $A^{(M)}$.[4] The system has the following properties:

(*i*) The state of the system at time t is given by the phase vector $(\mathbf{p}(t), \mathbf{q}(t)) = (\mathbf{p}_1(t), \mathbf{p}_2(t), \ldots, \mathbf{p}_N(t), \mathbf{q}_1(t), \mathbf{q}_2(t), \ldots, \mathbf{q}_N(t))$ which specifies a point in the $2\eta N$-dimensional phase space Γ, $\mathbf{p}_i(t)$ and $\mathbf{q}_i(t)$ being

[1] I agree with the view of Hobson ([1971], p. 33) that the subjective theory of Ramsey and de Finetti has no relevance to the physical sciences. The grouping of other points of view into two traditions, labelled 'logical' and 'scientific' follows the classification of Gillies [1973] except that he includes the subjective position within the logical tradition.

[2] Or, in the case of the ergodic method, by the attempt to by-pass level 2.

[3] This remark should not be taken to imply that no alternative link between mechanics and thermodynamics, avoiding statistical mechanics altogether, is possible (see p. 259, n. 2).

[4] For the sake of simplicity we consider only identical microsystems and only one extensive parameter. In general there may be more than one type of microsystem and more than one extensive parameter. Typical extensive parameters are the volume and the magnetic and electric moments of the system.

respectively the momentum and configuration vectors of the ith micro-system.

(*ii*) There exists a continuous differentiable Hamiltonian function H on Γ[1] and the evolution of the phase point in Γ satisfies *Hamilton's equation*

$$\frac{d}{dt}\ (\mathbf{p}, \mathbf{q}) = (-\nabla_q, \nabla_p)H(\mathbf{p}, \mathbf{q}). \tag{1}$$

It is convenient, although not essential, to suppose that the value of the Hamiltonian is the total energy of the system.

It is a standard result of the theory of differential equations that, given a point $(\mathbf{p}_0, \mathbf{q}_0)$ in Γ, there exists a solution of Hamilton's equation which determines a unique *path* of the system through $(\mathbf{p}_0, \mathbf{q}_0)$. The phase point of the system moves along the path, passing through $(\mathbf{p}_0, \mathbf{q}_0)$ at time $t = 0$. We have therefore a set of continuous mappings of Γ into itself parametrised by t. This set is called a *Hamiltonian flow*. An *integral* g of the equation of motion is a function of $(\mathbf{p}, \mathbf{q})$ and t whose value remains unchanged along a path. The equation to be satisfied by g is

$$\frac{\partial g}{\partial t} - \nabla_q H \,.\, \nabla_p g + \nabla_p H \,.\, \nabla_q g = 0. \tag{2}$$

A time independent integral is called a *constant* of the motion. The equation of motion will have $(2\eta N - 1)$ local constants of motion (constants which remain unchanged in value at least for limited periods of time and for certain regions of Γ). Of these there will be some which are constant throughout phase space and for all time; these are called *global*. A global constant of motion is called *isolating* if it defines a hypersurface in phase space. For a fluid system, consisting of particles which undergo perfectly elastic collisions at the boundaries of the container, the components of the total linear momentum will be local, but not global, constants. The Hamiltonian will however represent an isolating constant. A path of the system with at least one point on a particular energy hypersurface $\Sigma_E = \{(\mathbf{p}, \mathbf{q}): H(\mathbf{p}, \mathbf{q}) = E\}$ will lie entirely in that hypersurface.

In defining the mechanical system $\mathscr{S}^{(M)}$ we have simply outlined the general characteristics of a stationary Hamiltonian system. It is usually argued, however, that there is some additional feature peculiar to those kinds of mechanical systems which can be linked to thermodynamic systems, even though there is no general agreement on the nature of this feature. According to Grad [1967]: 'The single feature which distinguishes

[1] To be accurate we have of course a set of Hamiltonians parametrised by N and $\Lambda^{(M)}$. On these we impose the condition that H/N is finite in the thermodynamic limit $N \to \infty$, $\Lambda^{(M)} \to \infty$, $N/\Lambda^{(M)}$ finite. A detailed analysis of the mathematics involved in taking the thermodynamic limit is given by Ruelle [1969].

statistical mechanics from ordinary mechanics is the large number of degrees of freedom'. On the other hand there are those (*e.g.* Jaynes [1957], Hobson [1971]) who would deny that statistical mechanics is exclusively concerned with large systems. For them it 'is the study of incompletely specified systems' (Hobson [1971], p. 2).

LEVEL 4

For the thermodynamic system $\mathscr{S}^{(T)}$ the variables can be divided into two sets. There are the independent variables which, in an experimental situation are directly controlled by the experimenter. The remaining dependent variables will, for fixed values of the independent variables, change their values until they reach an equilibrium state, after which they remain constant. The thermodynamic system $\mathscr{S}^{(T)}$, at equilibrium, has the following properties:

(*i*) If undisturbed all variables of the system maintain constant values.

(*ii*) The macroscopic dimension of the system is given by one extensive parameter $A^{(T)}$ and there exists a 'generalised force' $F^{(T)}$ such that an increment of work dW, performed on the system by its environment, as it moves through a succession of equilibrium states increasing $A^{(T)}$ by $dA^{(T)}$, is given by $dW = F^{(T)}dA^{(T)}$.[1]

(*iii*) The thermodynamic energy U, the entropy S and the absolute temperature T are defined. Any incremental change of state (dU, dS, $dA^{(T)}$) for which the system moves through a succession of equilibrium states must satisfy the *fundamental thermodynamic relationship*

$$dU = TdS + F^{(T)}dA^{(T)}. \tag{3}$$

By including a discussion of the microcanonical and canonical distributions in level 4 (see diagram) we introduce, at this level, the mathematics of what is usually referred to as 'equilibrium statistical mechanics'. I argue that this is legitimate for two reasons:

(1) Although this work can be, and is, formulated in a variety of different ways, it is common to all attempts to relate $\mathscr{S}^{(M)}$ and $\mathscr{S}^{(T)}$.[2]

(2) The statistical connotation imposed on the mathematical structure, in most texts and on some interpretations, is not integral to it.[3]

[1] If $A^{(T)}$ is the volume then $F^{(T)}$ is minus the pressure exerted by the environment; if $A^{(T)}$ is the magnetic or electric moment then $F^{(T)}$ is the corresponding field. Again we have restricted the discussion to systems with only one extensive parameter. We shall also refrain from discussing systems which exchange matter with their environment.

[2] To my knowledge, the only exception to this is the attempt to justify (some parts of) thermodynamics using the methods of molecular dynamics (see *e.g.* Alder and Wainwright [1959], [1960], [1962]).

[3] I shall argue that it is one of the aims of the ergodic method to eliminate statistical connotations.

In other words what I wish to do, at this level, is to delineate those parts of the mathematics which do not depend on philosophical presuppositions. The questions on which there is real disagreement are contained in level 3. We now list the problems which, in a formal sense, will be resolved at this level. We need

(P1) A definition of equilibrium in terms of the properties of $\mathscr{S}^{(M)}$.

(P2) A connecting link between the macroscopic properties of $\mathscr{S}^{(M)}$ and $\mathscr{S}^{(T)}$.

The method of solution of these problems is on the following lines. Let ρ be a function of $(\mathbf{p}, \mathbf{q})$ and t which defines a *measure* on Γ. The measure $M[\gamma_t]$ of the set γ_t in Γ at time t is given by

$$M[\gamma_t] = \int_{\gamma_t} \Gamma\rho(\mathbf{p}, \mathbf{q}, t). \tag{4}$$

We suppose that the measure is normalised (*i.e.* $M[\Gamma] = 1$) and that the measure of any set γ_t as it moves with the Hamiltonian flow is *preserved.* It is not difficult to show[1] that a necessary and sufficient condition for the measure density function to be that of a preserved measure is that it satisfies *Liouville's equation*

$$\frac{\partial \rho}{\partial t} - \nabla_q \cdot (\rho \nabla_p H) + \nabla_p \cdot (\rho \nabla_q H) = 0.^{2} \tag{5}$$

We now consider the extended dynamic system $\{\rho, \mathscr{S}^{(M)}\}$ consisting of $\mathscr{S}^{(M)}$ together with the normalised measure preserving density function ρ. It is in terms of this extended system that P1 and P2 are solved. The solutions are as follows:

(S1) The system is in equilibrium if the measure density function is not an explicit function of time.

(S2) Related to any property $X^{(T)}$ of the thermodynamic system $\mathscr{S}^{(T)}$, with the exception of the entropy S and the absolute temperature T, there is for $\{\rho, \mathscr{S}^{(M)}\}$ a phase function $X^{(M)}$. The variable $X^{(T)}$ is given by the mean value of $X^{(M)}$ with respect to ρ, *i.e.*

$$X^{(T)} = \int_{\Gamma} d\Gamma \rho(\mathbf{p}, \mathbf{q}) X^{(M)}(\mathbf{p}, \mathbf{q}). \tag{6}$$

At equilibrium the thermodynamic entropy is given by

$$S = -k \int_{\Gamma} d\Gamma \rho(\mathbf{p}, \mathbf{q}) \ln \{c(N)\rho(\mathbf{p}, \mathbf{q})\}, \tag{7}$$

[1] The mathematics is the same as that used to prove the hydrodynamic continuity equation.

[2] Since $(-\nabla_q H, \nabla_p H)$ is an irrotational vector field Liouville's equation is identical to its adjoint, which is equation (2), the equation satisfied by integrals of the equation of motion.

where k is Boltzmann's constant and $c(N)$ is the Boltzmann correcting factor.[1]

If, as we assume, the value of the Hamiltonian H is the total energy of the system, then the phase function corresponding to the thermodynamic energy U is the Hamiltonian. With respect to the pair of variables $F^{(T)}$ and $A^{(T)}$ two situations can arise:

(*a*) If the system is mechanically isolated then $A^{(T)}$ is an independent variable, the corresponding phase function $A^{(M)}$ is a constant and we have $A^{(T)} = A^{(M)}$. The phase function corresponding to $F^{(T)}$ is $\partial H/\partial A^{(M)}$. This phase function will vary as the phase point moves along its path in phase space. An illustration of this situation is that of a volume of fluid in a container with rigid walls. Here the volume is the same, interpreted as either a mechanical or thermodynamic quantity. We see however that the force on the walls of the container arises from a large number of discrete impulses caused by the impacts on it of the particles of the fluid. The phase function corresponding to the pressure of the gas is the force per unit area averaged over the surface of the container. This quantity, which could be called the 'microscopic pressure of the fluid' will fluctuate with time unlike the corresponding thermodynamic pressure.

(*b*) If the system is in mechanical equilibrium with its environment then the generalized force $F^{(T)}$ is determined by the environment and it is the mechanical extensive variable $A^{(M)}$ which will fluctuate. This, for a fluid system, would correspond to the case where one wall of the container is replaced by a piston. The pressure of the fluid is now a constant, given by the force per unit area exerted from outside on the piston. The 'microscopic volume' of the fluid will now fluctuate as the piston vibrates under the influence of particle impacts.

Since equilibrium fluctuations of dependent variables can, for physical systems, be experimentally detected (see *e.g.* MacDonald [1962]) the mechanical viewpoint here represents a positive advance over that of classical thermodynamics.

There remains the problem:

(P_3) We need to know the equilibrium forms of the measure density function corresponding to particular thermodynamic conditions.

There are for any particular system a variety of possible thermodynamic conditions. In this paper we shall consider only two for which problem P_3 is solved in the following way:

[1] The precise form of $c(N)$, which is designed to avoid the difficulties of Gibbs's paradox and to give identity, in the case of a perfect gas, with the corresponding formulae of quantum statistics, is determined by the physical system under investigation. We do not need an independent formula for the absolute temperature. Once the form for entropy is established the temperature arises from the thermodynamic procedures.

(S3) *For an isolated system* with energy E the phase point moves entirely on the energy surface Σ_E. The natural (uniform) measure on the energy shell $\{(\mathbf{p}, \mathbf{q}): E-\frac{1}{2}\Delta E < H(\mathbf{p}, \mathbf{q}) < E+\frac{1}{2}\Delta E\}$ is preserved by the Hamiltonian flow. In the limit $\Delta E \to 0$ a preserved measure, called the *microcanonical distribution*, is induced on Σ_E in terms of which

$$X^{(T)} = \frac{1}{\omega(E)} \int_{\Sigma_E} \frac{d\Sigma_E}{|\nabla H(\mathbf{p}, \mathbf{q})|} X^{(M)}(\mathbf{p}, \mathbf{q}) \tag{8}$$

where

$$\omega(E) = \begin{cases} \displaystyle\int_{\Sigma_E} \frac{d\Sigma_E}{|\nabla H(\mathbf{p}, \mathbf{q})|} & E > 0 \\ 0 & E \leqslant 0 \end{cases} \tag{9}$$

is the structure function of the system.

For a system in thermal contact with its environment at absolute temperature T the measure density function is that of the *canonical distribution* which is given by

$$\rho(\mathbf{p}, \mathbf{q}) = \frac{\exp(-H(\mathbf{p}, \mathbf{q})/kT)}{\displaystyle\int_\Gamma d\Gamma \exp(-H(\mathbf{p}, \mathbf{q})/kT)}. \tag{10}$$

Use of the canonical distribution and the formulae (6) and (7) of S2 leads very simply (see *e.g.* Hill [1956]) to the fundamental thermodynamic relationship given above. We are therefore left with two problems. We need to justify

(P4) The use of the measure density function to relate the variables of $\mathscr{S}^{(T)}$ and $\mathscr{S}^{(M)}$.

(P5) The equilibrium forms for the measure density function.

These are the problems which must be tackled at levels 2 and 3. We should however note before passing to these levels that it is not essential to give independent justifications of the microcanonical and canonical distributions. A system in thermal equilibrium with its environment can be taken to be part A of an isolated system of which the remainder, part B, is taken to be the environment of A. If A and B are assumed to be only weakly interacting[1] then the canonical distribution can be derived by taking the asymptotic limit as B becomes infinite.[2] The basic problem is therefore the justification of the microcanonical distribution.

[1] The Hamiltonian of the total system is the sum of the Hamiltonians of A and B.

[2] Using the central limit theorem (Khinchin [1949]) or the method of steepest descents (Kubo [1965]) this can be shown on the basis of certain reasonable mathematical assumptions.

LEVEL 2

At this level we discuss the ways in which probability theory is used as a means of justifying the use of a measure density function to relate the variables of $\mathscr{S}^{(M)}$ and $\mathscr{S}^{(T)}$. As can be seen from the diagram the ergodic method is alone in its attempt to relate equilibrium thermodynamics and the underlying mechanical structure without resort to this kind of justification. It will not therefore feature in our discussion until level three. The common feature of all the approaches described here is that, on some interpretation or another, the measure density function emerges as a probability density function.

One of the difficulties of discussing the use of probability concepts in statistical mechanics is that, in much of the literature on the subject, these concepts are introduced in a rather informal manner. This is a tradition in statistical mechanics which dates from the works of Boltzmann ([1896]) and Gibbs ([1902])[1] and which persists to some extent until the present day. Apart therefore from those occasions when we are considering a writer who makes specific efforts to state his views on probability theory[2] we shall need to be somewhat tentative in classifying authors into one camp or another.

The Logical View

This may be characterised by the claim that we can 'cognise correctly a logical connection between one set of propositions which we call our evidence and which we suppose ourselves to know, and another set which we call our conclusions, and to which we attach more or less weight according to the grounds supplied by the first. . . . It is not straining the use of words to speak of this as the relation of probability. . . . No proposition is in itself either probable or improbable, . . . and the probability of the same statement varies with the evidence presented . . .' (Keynes [1921], quoted by Gillies [1973], p. 8). In the context of statistical mechanics it is perhaps more appropriate to refer to data or information rather than to evidence. A complete set of data for the mechanical system $\mathscr{S}^{(M)}$ would allow us to solve the equations of motion. The rationale for the use of probability theory, in the logical tradition, is therefore the need to deal with a system for which he information is incomplete (see diagram).[3] On

[1] With respect to Boltzmann and Gibbs this is not surprising in view of the time at which they were writing.

[2] This is true of those authors like Jaynes and Hobson who use the information theory approach.

[3] The logical view is sometimes referred to as the 'ignorance view' although, as we shall see, the ignorance method at level 3 is only one of the possible methods which can adopt this view of probability.

the basis of a particular set of data we must derive in some way the 'best' probability density function for the system. This point of view features in the development of statistical mechanics in two ways. In the first of these it is closely linked to the justification of the microcanonical distribution. It will be recalled that the microcanonical distribution purports to be that which is appropriate to an isolated system. The information which we have about such a system consists of some value E for the total energy. The Keynesian *Principle of Indifference* leads to the use of a probability density function zero outside of, and uniform within, the energy shell $\{(\mathbf{p}, \mathbf{q}):E - \frac{1}{2}\Delta E < H(\mathbf{p}, \mathbf{q}) < E + \frac{1}{2}\Delta E\}$[1] and from this we derive the microcanonical distribution in the limit $\Delta E \to 0$. This would seem to be the approach of Tolman ([1938]), although we must be rather careful in analysing his writings because of his use of the idea of ensembles (see below). A more recent and developed approach within the logical tradition is the ignorance method of Jaynes ([1957], [1965], [1967]) and Hobson ([1971]). These writers adopt a specific principle by means of which, given a set of data, a unique (best) probability assignment can be derived. For Jaynes this is the *Principle of Maximum Entropy*. He identifies the concept of entropy as defined by Shannon in information theory (see Shannon and Weaver [1949]) with entropy in statistical mechanics; the appropriate probability distribution is the one which maximises this entropy relative to the given set of data and the thermodynamic entropy is equal to the maximum value of the statistical mechanical entropy. Hobson's formulation differs from this in detail but is ultimately equivalent. He derives an expression for the *uncertainty* in a probability distribution and adopts the principle (called by him *Jaynes' Principle*) that the appropriate probability distribution is that which maximises the uncertainty relative to the given data. It is only at a later stage that identification is made between entropy and uncertainty. The advantage of Hobson's formulation, at this point, as compared to that of Jaynes, is that it avoids the immediate (and tempting) conflation of the information theory and thermodynamic concepts of entropy. Apart from these slight differences it is clear that, for both Jaynes and Hobson, the appropriate density for a system for which the datum consists simply in the restriction of the phase point to an energy shell is that given by the Principle of Indifference. Hobson claims (probably correctly, although see the discussion below) that Tolman [1938] shares his view that statistical mechanics is the study of incompletely specified systems. He also argues that Gibbs rejected both the ergodic method and the viewpoint that statistical mechanics is

[1] The uniform distribution over the energy surface Σ_E is not preserved by the Hamiltonian flow.

the study of large systems and that he must therefore have been to some extent an early member of the same school.

The Scientific View

This view may be characterised by the fact that it considers 'the theory of probability as a science of the same order as geometry or theoretical mechanics' (von Mises [1957], p. vii). In this tradition the probabalistic properties of the system under investigation emerge if we consider the results of a large number of identical[1] operations on the system. For von Mises (see *e.g.* von Mises [1957], p. 29) this large number of operations or events is the *collective*; the probability of a particular outcome is then defined as the limit of the *relative frequency* of this outcome in the collective, as the size of the collective increases to infinity. For Popper on the other hand (see Popper [1959]) the collective, rather than providing a means of defining probability, serves to reveal the *latent propensity* of the system to behave in a certain way.[2] The idea of the collective features in statistical mechanics in two, more or less distinct, ways. In the first of these the behaviours of the individual microsystems, or particles, constitute the events and the collective is the mechanical system as a whole. This is the point of view of von Mises, when he asserts (von Mises [1957], p. 182) that 'A volume of gas containing a great number of molecules appears . . . as a system not different in principle from the automatic lottery machine. . . .'[3] In this context we are concerned about assigning a probability density function to a single particle and the crucial characteristic of the system is that it has a large number of particles (or degrees of freedom). The second way in which the idea of the collective features in statistical mechanics is in the situation in which we are concerned about the properties, not of an individual particle, but of the whole system. We may, for example, be concerned with the total energy of the system. For a system of particles whose interaction is given in terms of a pairwise potential function, the total energy of the system is not reducable to the sum of individual particle energies and the von Mises viewpoint is inapplicable. The method here is to take the various possible behaviours of the whole system as the events and to consider a collective of macroscopically identical systems. This collective is called an *ensemble*. The idea of an ensemble of systems was introduced by Gibbs. His idea was

[1] Identical in the 'macroscopic' sense that repeated throws of the same die are identical.

[2] There are of course, besides the relative frequency and propensity interpretations, other variants of the scientific view (see Gillies [1973]).

[3] The automatic lottery machine is designed to mix the lottery slips by shaking in such a way as to make 'it impossible to follow the fate of one of them. . . . (It is provided with) some mechanism which would eject a lot through a funnel after a sufficient period of shaking the container' (von Mises [1957], p. 177).

that we imagine the phase space Γ to be filled with phase points of 'a great number of independent systems, identical in nature, but differing in phase' (Gibbs [1902], p. 5). Dividing the density of phase points by the number of members of the ensemble and taking the limit, in which the number of members of the ensemble and the density of phase points become large, their quotient remaining finite, produces a normalised density on phase space which is taken to be a probability density function. Although this way of producing the probability density function has a strong flavour of the von Mises relative frequency interpretation it is not entirely clear, from Gibbs' discussion, that this was his intention. It is certainly true, as Hobson points out, that Gibbs believed that 'The laws of statistical mechanics apply to conservative systems of any number of degrees of freedom, . . .' (Gibbs [1902], p. viii). But we have seen that a scientific interpretation of probability, using an ensemble, is not restricted to systems with a large number of degrees of freedom. It is only the von Mises viewpoint, which takes the system itself as the collective, which is so restricted. In the case where the ensemble is the collective, it is the number of members of the ensemble which is large. It could however be argued (and this I think is the essence of Hobson's point) that if we are to introduce probability at all then it must be because exact mechanical calculations are not viable. Since it appears that this inviability arises, either because of the large number of degrees of freedom, or because the system is not completely specified, then Gibbs must have taken the latter view with the concomitant logical approach to probability. In this case the ensemble must be regarded as a heuristic aid to understanding.

Since the time of Gibbs it has needed a considerable act of will on the part of teachers and researchers in statistical mechanics to avoid all references to ensembles, so much have they become part of the language of the subject. It is fairly clear that, for at least some writers of textbooks (*e.g.* Hill [1956]), the ensemble is a means of defining probability after the manner of von Mises. But in most cases its role is rather more confusing. Particularly interesting in this respect is the work of Tolman ([1938]). He begins his analysis by using an ensemble of systems in conjunction with the Principle of Indifference. He assumes that 'the phase point for a given system (of the ensemble) is just as likely to be in one region of the phase space as in any other region of the same extent which corresponds equally well with what knowledge we do have as to the condition of the system' (Tolman [1938], p. 60). This remark seems to support Hobson's contention that his view of probability is the logical one. It must however be born in mind that an important aspect of the logical view is that probability is a relationship between a set of data and our knowledge of a single

system. The weighted average of a phase function taken with respect to the probability density function is the expectation value which reflects in some way our expectations about the system, based on our knowledge. For Tolman this average is the *ensemble average*. For him it provides results which 'are to be regarded as true on the average for the systems in an appropriately chosen ensemble rather than as necessarily true in any individual case' (Tolman [1938], p. 63). This remark has an 'objective' scientific ring which accords ill with Keynes' comments on probability quoted above.

LEVEL 3

The Ergodic Method

Let γ be a subset of the phase space Γ which is invariant with respect to the Hamiltonian flow and let ρ be a time-independent density function on γ which is preserved by the flow and for which γ has total measure unity. It is supposed that $X^{(M)}$ is a phase function integrable over γ. It is argued that a measurement of the thermodynamic quantity $X^{(T)}$ corresponds to the average $\bar{X}(\mathbf{p}_0, \mathbf{q}_0, \tau)$ of $X^{(M)}$ over a period of time τ, computed along a path of the system beginning from the point $(\mathbf{p}_0, \mathbf{q}_0)$ in γ. It is assumed that τ is long with respect to (*a*) the microscopic correlation time, (*b*) the relaxation time of macroscopic variables and (*c*) the time taken to destroy purely local constants of motion. On the basis of these assumptions it is further argued that the result of the measurement is effectively the infinite time average obtained by allowing τ to tend to infinity. For this view of measurement to be meaningful it is of course necessary to show, not only that this time limit exists, but also that it is independent of the point $(\mathbf{p}_0, \mathbf{q}_0)$. Let $\bar{X}$ be the average of $X^{(M)}$ over γ with respect to the measure density function ρ. In terms of this the following results were proved by Birkhoff ([1931]):[1]

(*i*) $\lim_{\tau \to \infty} \bar{X}(\mathbf{p}_0, \mathbf{q}_0, \tau) = \hat{X}(\mathbf{p}_0, \mathbf{q}_0)$ exists almost everywhere in γ (*i.e.* except possibly for a set of measure zero with respect to ρ).

(*ii*) $\hat{X}$ is a constant of motion almost everywhere in γ.

(*iii*) $\bar{X} = \hat{\bar{X}} = \bar{\hat{X}}$.

Let us put aside, for the moment, any doubts which arise from the existence of exceptional points and examine how these results affect the definition of measurement. It is clear that (*a*) if $\hat{X}$ is a constant almost everywhere in γ then $\bar{\hat{X}} = \hat{X}$ and hence from (*iii*) $\hat{X} = \bar{X}$ holds almost everywhere in γ, (*b*) if $\hat{X} = \bar{X}$ holds almost everywhere in γ then $\hat{X}$ is a constant almost everywhere in γ. If $\hat{X} = \bar{X}$ holds almost everywhere in γ, for all

[1] Birkhoff's paper contains an explicit proof only of (*i*). Results (*ii*) and (*iii*) are trivial consequences of the main result.

phase functions integrable over γ, then the system is said to be *ergodic*. We see therefore that, for ergodic systems, we may (almost) legitimately write

$$X^{(T)} \doteq \bar{X} \tag{11}$$

which is the relationship (6) between $X^{(T)}$ and $X^{(M)}$ proposed in S2 level 4, with ρ identically zero at all points in Γ not belonging to γ.

It would be tempting to suppose that ergodicity has removed the statistics from statistical mechanics by establishing the proposed relationship between $X^{(M)}$ and $X^{(T)}$, with ρ as an uninterpreted measure density function used simply as a tool to calculate time averages. The difficulty in accepting this point of view arises if we consider what we are doing by neglecting the set of exceptional points. We are supposing that a measurement is never (or hardly ever) made on a system which at the beginning of the measurement has phase point $(\mathbf{p}_0, \mathbf{q}_0)$ belonging to that set of points of γ for which the infinite time average does not exist. In supposing that such a situation never in practice occurs we have tacitly assumed some probabalistic interpretation for ρ in terms of which sets of zero measure with respect to ρ have zero probability. Nevertheless, and accepting this slight obeisance in the direction of an interpreted probability, it would still seem to be useful to prove the ergodicity of a system.

The original *ergodic hypothesis* (usually attributed to Boltzmann, but see Brush [1964]) assumed that the path of the system passed through every point of γ. Since $\hat{X}$ is a constant of motion it is clear that this hypothesis is sufficient to establish that $\hat{X}$ is a constant on γ. It is equally clear, on measure theoretic grounds,[1] that the ergodic hypothesis is false. An alternative *quasi-ergodic hypothesis*, to the effect that the path of the system passes arbitrarily close to every point of γ, has not proved sufficient to establish ergodicity, although it is certainly necessary. There is however a condition, both necessary and sufficient, which is intuitively somewhat similar to the quasi-ergodic hypothesis. To prove the necessity of the quasi-ergodic hypothesis we would assume that, given a particular path l of the system, there exists a point P of γ for which a neighbourhood $\epsilon(P)$ of P contains no points of l. This is clearly impossible for an ergodic system since we could arbitrarily change the value of the phase function on $\epsilon(P)$,

[1] The path of the system is of measure zero in γ. A straightforward proof that the ergodic hypothesis is false is as follows. Let P and P' be two points of γ. Since the path of the system has a unique tangent direction at every point there are at most two arcs of the path joining P to P'. Let σ be an arc joining P to P' which is neither of the arcs of the path of the system. Now the points at which the path of the system intersects σ (if it does so) can be ordered with respect to their values of t and are denumerable. But for the ergodic hypothesis to be true the path of the system would have to pass through all the non-denumerable set of points of σ. (This is a similar argument to one used by the Ehrenfests ([1912], English edition 1959, footnote 98) to explain the difference between the ergodic and quasi-ergodic hypotheses.)

thereby changing the phase average but not the time average. The even stronger assumption, that γ can be decomposed into two invariant subsets of non-zero measure with respect to ρ, is clearly inconsistent with ergodicity by a slight modification of the same argument. *Metric transitivity*, which is defined to be the negation of this assumption, is therefore a necessary condition for ergodicity. That it is also a sufficient condition can be seen quite simply by the following argument. Suppose that $\hat{X}$ were not constant almost everywhere on γ, then γ can be decomposed into two invariant subsets of non-zero measure with respect to ρ according to the values of $\hat{X}$ and therefore it cannot be metrically transitive.

For the stationary Hamiltonian system $\mathscr{S}^{(M)}$, the Hamiltonian is an isolating constant of motion and the energy surface Σ_E is an invariant subset of Γ. If Σ_E is metrically transitive then the system is ergodic on Σ_E and the microcanonical distribution, given in S3 level 4, is proved (with the reservations described above with respect to exceptional points) by the ergodic method. From this the canonical distribution can be derived and the links between $\mathscr{S}^{(M)}$ and $\mathscr{S}^{(T)}$ are established.

Suppose that, besides the Hamiltonian, there exist other independent isolating constants of motion. In this case it is clear[1] that Σ_E cannot be metrically transitive and the development of statistical mechanics outlined above is invalid. Only in the case of a system of more than two hard spheres, contained within a parallelepiped box with perfectly elastic walls, has this been proved rigorously not to be so (Sinai [1967]).[2] In general the problems of proving the non-existence of additional isolating constants of motion is very difficult. It would therefore seem reasonable to investigate the consequences of their existence. This has been done by Lewis [1960]. Beginning with the set of hypersurfaces, which represent almost everywhere all isolating constants of motion, he showed that the system is ergodic on the set obtained as the intersection of vanishingly small shells defined with respect to each hypersurface, the measure being the uniform measure in phase space. On the basis of this it is possible to obtain generalisations of the microcanonical and canonical distributions. Unfortunately the form of thermodynamics developed from these distributions differs significantly from the standard form (Grad [1952]). In particular we have, rather than one parameter representing temperature, a whole range of parameters, one for each of the isolating constants of motion.

To circumvent the difficulties associated with metric transitivity and the possible existence of additional isolating constants of motion, attempts have been made to weaken the requirements of ergodicity in such a way

[1] Any other isolating constant of motion will divide the energy surface into two invariant subsets each of non-zero measure.

[2] See also the discussion of Sinai's results at the end of Farquhar [1967].

as still to satisfy the needs of statistical mechanics. It is not difficult to show (see *e.g.* Farquhar [1964]) that, for the measure density function ρ and the invariant subset γ, and for any $\epsilon > 0$,

$$\text{Measure}\left[(\mathbf{p}, \mathbf{q}): \left|\frac{\hat{X}(\mathbf{p}, \mathbf{q})}{\bar{X}} - 1\right| \geqslant \epsilon\right] \leqslant 1/\epsilon^2 \,\text{Variance}\left[\frac{X^{(M)}}{\bar{X}}\right], \quad (12)$$

where the variance is calculated using the measure density function ρ. In particular this result applies to the microcanonical measure over the energy surface Σ_E. In order for this result to be of any use for our purpose it is necessary to show that the right-hand side of equation (12) is small. This is certainly not the case for arbitrary phase functions and systems with any number of degrees of freedom. As we have already argued, the reason for the introduction of methods, other than direct integration, for dealing with the system $\mathscr{S}^{(M)}$ is, either that the system has a large number of degrees of freedom, or that it is incompletely specified. Since the assumption of incomplete specification seems to lead inevitably to statistical methods, it seems reasonable to see the use of the ergodic method as a consequence of the system having a large number of degrees of freedom. Up to this point in our discussion of the ergodic method this feature has played no rôle. But even in the case of systems with a large number of degrees of freedom it is not necessarily the case that the variance of $X^{(M)}/\bar{X}$ is small for all $X^{(M)}$. Khinchin [1949] was however able to show that if the Hamiltonian H and the phase function $X^{(M)}$ are both sums of contributions from the individual microsystems (sum functions) then the variance of $X^{(M)}/\bar{X}$ is of the order of $1/N$. The unwanted restriction represented by the Hamiltonian having to be a sum function has since been removed by Mazur and van der Linden [1963], who considered the asymptotic limit for N of sum functions for systems of particles interacting through short-range hard-core interactions. Their argument requires an assumption that the zeros of a certain polynomial related to the configurational integral of the system are not dense in intervals of the real axis. The difficulty again encountered with this approach is that we have in some way to know that sets of small measure with respect to ρ have small probability of occurrence.

The Evolution Method

Once some probability interpretation has been given to the measure density function ρ, the measure $M[\gamma_t]$ of any subset γ_t of Γ, at time t, will be the probability of the phase point of the system being in γ_t at that time. It is then clear why measure must be preserved by the Hamiltonian flow since, if the set γ_t evolves into the set $\gamma_{t'}$ at time t', the phase point will be in $\gamma_{t'}$ at time t' if and only if it is in γ_t at time t. The probability density

function must therefore satisfy Liouville's equation. We have defined equilibrium for the thermodynamic system $\mathscr{S}^{(T)}$ as the state into which $\mathscr{S}^{(T)}$ evolves if left undisturbed for a sufficiently long period of time. The most natural method of obtaining the equilibrium distribution would therefore seem to be to investigate the solution of Liouville's equation in the limit as t tends to infinity. This is part of the programme of the Brussels School of statistical mechanics (see *e.g.* Prigogine [1970], Balescu [1971]). These researchers trace the evolution of the Fourier coefficients of the probability density function in terms of the destruction and creation of interparticle correlations. They have succeeded in showing (at least for a certain class of interparticle interactions) that, in the thermodynamic limit, the dependence of the probability density function on initial correlations decays in the infinite time limit. In this time limit the probability density evolves to the canonical form. They would also claim to have resolved the *recurrence paradox* of Zermelo ([1896]) and the *reversibility paradox* of Loschmidt ([1876], [1877]). These paradoxes arise by counterposing, on the one hand the evolution to equilibrium of a thermodynamic system, and on the other the quasi-periodic and time-symmetric behaviour of a finite mechanical system. The recurrence problem is resolved by taking the thermodynamic limit in which the recurrence time becomes infinite. The reversibility problem is resolved by observing that, although the initial correlations can be neglected at any stage in the evolution of the system in the positive time direction, such a process is inadmissible if time is reversed because in this direction the correlations remaining from the initial state play an increasingly important rôle in the process by which the system is returned to its initial state.

These brief comments are not intended to do full justice to this approach to the solution of the basic problems of statistical mechanics. Particularly so since the evolution method is essentially an approach to the whole problem of the relationship between equilibrium and non-equilibrium situations, this being an area still plagued by fundamental disagreements. One thing however should be emphasised. The evolution method is not tied to any particular philosophy of probability. It needs only some interpretation of ρ as a probability density function in order to give it validity.

The Ignorance Method

This method, based as it is on a logical view of probability, relies on a principle by means of which, given a set of data, the appropriate equilibrium probability density function can be derived. We shall adopt the formulation of Hobson [1971]. As we have already indicated at level 2, he derives an

expression for the uncertainty in a probability distribution and adopts the principle that the appropriate distribution is that which maximises the uncertainty relative to the given data. He shows that, if we make certain reasonable assumptions regarding the nature of information measurement, and if we suppose that the most accurate measurement on the system is capable of locating the phase point in a cell of measure $c(N)$ then there is a unique formula for uncertainty given by

$$S(\rho) = -k \int_{\Gamma} d\Gamma \rho(\mathbf{p}, \mathbf{q}) \ln \{c(N)\rho(\mathbf{p}, \mathbf{q})\}. \tag{13}$$

The uncertainty is equated with the entropy, given in S2 level 4 equation (7), when ρ has been adjusted to maximise $S(\rho)$ with respect to the restrictions imposed on it by the available data.

Within the context of this approach, the purpose of statistical mechanics is to predict values for the results of measurements. The thermodynamic variable $X^{(T)}$ is taken to be the best prediction of a result of a measurement of the corresponding phase function $X^{(M)}$. Since however, from Tchebyshev's inequality for any $\epsilon > 0$,

$$\text{Probability}\left[\left|\frac{X^{(M)}}{\langle X\rangle} - 1\right| \geqslant \epsilon\right] \leqslant 1/\epsilon^2 \,\text{Variance}\left[\frac{X^{(M)}}{\langle X\rangle}\right], \tag{14}$$

where $\langle X\rangle$ is the expectation value of $X^{(M)}$, it is argued that $\langle X\rangle$ is the best prediction for $X^{(M)}$. The right-hand side of the relationship (6) in S2 level 4 is now, with ρ interpreted as a probability density function, the expectation value of $X^{(M)}$ and this relationship is given a justification. It is further argued that the variance of $X^{(M)}/\langle X\rangle$ is of the order of $1/N$ and thus that the predictions made will increase in accuracy as N increases. Although this can be established on physical grounds for certain phase functions[1] a general statement of this kind would seem to rely on the kind of result established by Khinchin and quoted, with respect to our discussion of equation (12), at the end of the section devoted to the ergodic method.

The great advantage, from a teaching point of view, of this method is that we are able to establish the microcanonical and canonical distributions with the minimum of mathematical manipulation. All we need is some simple applications of the method of undetermined multipliers. Its weakness is that it makes no proper connection between the idea of *information* and our detailed *knowledge* of the physical circumstances of the system under investigation. This weakness is well illustrated by the remark of Hobson ([1971] p. 84) to the effect that 'the microcanonical

[1] In the case where the phase function is the Hamiltonian the variance of $H/\langle H\rangle$ is equal to $kC_\Lambda(T/U)^2$, where C_Λ is the heat capacity of the system at constant $A^{(M)}$, and both C_Λ and U are of the order of N.

distribution is *generally regarded*[1] as being applicable to closed systems (*i.e.* systems having time-independent Hamiltonians), while the canonical distribution is *regarded*[1] as being applicable to systems in weak interaction with a second system, where the interaction is time-dependent but random (*i.e.* not precisely known)'. The point is that physical considerations of the type referred to in this quotation, must be built into the information *before* the distributions are derived. If this is not done certain paradoxical situations can arise. One such is contained in the following example[2] where for the sake of simplicity we consider a system with discrete energy levels:

> Given a system with non-degenerate energy levels $E_1<E_2<\ldots$. Suppose that we are first given the datum D, that the energy lies in the closed interval $[E_1, E_n]$. Then from Jaynes' principle the appropriate distribution is the discrete form of the microcanonical distribution
>
> $$\text{Prob } [E_j|D]=\begin{cases} 1/n & 1\leqslant j\leqslant n \\ 0 & \text{otherwise} \end{cases} \tag{15}$$
>
> Suppose now, to quote Hobson ([1971], p. 107) 'the energy E be measured and let the datum be $\langle E\rangle=U$, where U is given'. Referring to this new piece of datum as D' and using Jaynes' principle we now have the discrete form of the canonical distribution
>
> $$\text{Prob } [E_j|D \text{ and } D']=\begin{cases} \exp(-E_j\beta)/Z(\beta) & 1\leqslant j\leqslant n \\ 0 & \text{otherwise} \end{cases} \tag{16}$$
>
> where
>
> $$Z(\beta)=\sum_{j=1}^{n}\exp(-E_j\beta) \tag{17}$$
>
> and
>
> $$-U=\frac{\partial \ln Z(\beta)}{\partial\beta} \tag{18}$$
>
> Now
>
> $$\text{Prob } [E_j|D]=\sum_{D'}\text{Prob } [E_j|D \text{ and } D']\ \text{Prob } [D'|D] \tag{19}$$
>
> and since D' varies over all values of β, which may be supposed to have a density function $p(\beta)$, we have
>
> $$\frac{1}{r}=\int d\beta\, p(\beta)\ \frac{\exp(-E_j\beta)}{Z(\beta)} \qquad 1\leqslant j\leqslant n \tag{20}$$
>
> But for $j=1$ and all $p(\beta)$ except $p(\beta)=\delta_D(\beta)$
>
> $$\int d\beta\, p(\beta)\ \frac{\exp(-E_1\beta)}{Z(\beta)}>\int d\beta\, p(\beta)\ \frac{\exp(-E_1\beta)}{r\exp(-E_1\beta)}=\frac{1}{r} \tag{21}$$

[1] My italics.

[2] A form of this example was proposed by A. Shimony during a seminar at Chelsea College.

As indicated above, a way to resolve this paradoxical situation would be to divide information into two types: (*a*) The results of measurements. We may, for example, know the energy of the system or the temperature of a heat-bath in which the system is immersed. These are the kinds of data with respect to which uncertainty has been maximised. (*b*) General observations of a non-quantitative kind concerning the system. We may, for example, observe that the system is, as far as possible, thermally isolated, or we may observe that steps have been taken to ensure, as far as possible, that it is in thermal contact with its environment. In the above example D will properly consist, not simply of data concerning the range of permitted energy levels, but it will also tell us that an attempt has been made to isolate the system thermally, in which case $\Delta E = E_n - E_1$ should be small. Again D' will consist, not simply of the piece of datum $\langle E \rangle = U$, but will also include the information that the system is in thermal equilibrium with its environment. Thus the total information (D and D') will contain a contradiction and, if we wish to accept D' then D must be rejected as mistaken, invalidating the use of the conditional probability formula (19).

While this point may seem relatively trivial, and by no means to indicate a general failure of the method as a whole, it does need to be clarified in the writings of those who use the ignorance method as their approach to statistical mechanics.

The Ensemble Method

As we have already indicated in our discussion at level 2, the use (at least verbally) of ensembles in statistical mechanics is both nearly universal and shrouded with a certain amount of ambiguity. As a method of obtaining the microcanonical and canonical distributions it does however have the virtue of great simplicity particularly in the case of systems with discrete energy levels (see *e.g.* Rushbrooke [1949]). In fact the mathematical procedure is almost identical to that used in the ignorance method. The difference between these two methods arises when we come to interpret what in the ignorance method is the expectation value, featuring as the best prediction about a single system, and what in the ensemble method is the ensemble average representing a property, not of a single system, but of the ensemble as a whole. One apparent advantage enjoyed by the ensemble method in this connection (over both the ignorance and ergodic methods) is in its treatment of the problem of the possible existence of isolating constants of motion in addition to the Hamiltonian.

We have seen at level 4 that once a uniform distribution over an energy shell has been assumed the microcanonical and canonical distributions

can be rigorously derived. For a system for which only the energy is known the Principle of Indifference provides the required distribution. The impasse of the possible existence of additional isolating constants of motion, which brings the ergodic method to a halt, is here resolved in a very simple way. If we do not know the values of these constants (whether we suspect their existence or not) we ignore them because we no longer expect one single system to be precisely modelled by the ensemble behaviour.

The difficulty with this argument is that the only way to test predictions arising from statistical mechanics is to make measurements on an actual system. Now suppose that the phase function $X^{(M)}$ is an isolating constant of motion independent of the Hamiltonian. The ensemble average will predict the value for $X^{(T)}$, the thermodynamic quantity corresponding to $X^{(M)}$, by taking an average over all the possible values for $X^{(M)}$, whereas for any one system the value of $X^{(M)}$ will be a constant which may differ in any possible way from the ensemble average. To correctly model the behaviour of the system in question we should choose a subensemble with both H and $X^{(M)}$ fixed which brings us back to the problem of determining additional constants of motion. If this is not done it is difficult to see how ensemble averages can be related to experimental measurements. The problem becomes even worse in the case of entropy which is directly related to the properties of the whole ensemble through our choice of a distribution for phase points of the ensemble.[1] To refer to the equations resulting from statistical mechanics as 'analogues' of the corresponding thermodynamic equations (as do both Gibbs, ([1902], chapter 14) and Tolman ([1938], chapter 13)) serves simply to confuse the issues.

FINAL DISCUSSION

I have in this paper tried to distinguish the possible strategies in terms of which attempts have been made to base equilibrium thermodynamics on the structure of the underlying mechanical system. The four headings at level 3 (see diagram) do, as far as I can see, represent the four existing methods. At the present stage of statistical mechanics it would seem to be impossible to make a definitive choice between these methods except on philosophical grounds. (Personal adherence to one or other view of probability theory would lead to outright rejection of one or other of the methods.) Within its own terms of reference each of these methods has its strengths and weaknesses and it is the aim of this discussion to

[1] For a system with discrete energy levels the entropy is equal to $\lim_{n\to\infty} (k \ln \Omega)/n$, where n is the number of members of the ensemble and Ω is the number of ways of distributing these members over the energy levels.

summarise these, giving, where possible, some indications of how the weaknesses could be overcome.

The main strength of the *ensemble method* lies in its mathematical simplicity. It also gives at least the appearance of conceptual simplicity, especially if based on a scientific view of probability with the ensemble interpreted as a collective in the sense of von Mises. In this way the fact that the probability density function and the ensemble averages are properties of the ensemble is not essentially different from the view of von Mises ([1957], p. 12) that probability means 'the probability of encountering a certain attribute in a given collective'. The situation seems more difficult when we consider the entropy. This quantity is a property of the ensemble related to no phase function at the mechanical level of a particular system (compare equations (6) and (7)). It therefore cannot, even in principle, be envisaged as the result of a sequence of repeated measurements. It may be possible to overcome this difficulty by some change of philosophical position on probability (using for example Popper's idea of propensity in which probability is more closely related to an individual system) but I know of no discussion of this point.

For the *ignorance method* the probability density function is calculated by maximising the uncertainty relative to a particular set of given data. On the level of formal calculation this again gives a very simple method of obtaining the probability density function appropriate to the information that we have about the system. As we have seen there is a difficulty, well illustrated by Shimony's problem, if information is too narrowly interpreted. It does however seem possible to overcome this if we are prepared to include more general non-quantitative observations as part of the known data. A more important objection to this formulation relates to the dependence of the probability density function on the state of knowledge of the observer. This in turn means that the entropy of the system is dependent on this state of knowledge. This seems to imply an anthropomorphic view of entropy. Jaynes ([1965]) is fully prepared to accept this 'not only in the well-known statistical sense that it measures the extent of human ignorance as to the microstate. Even at the purely phenomenological level, entropy is an anthropomorphic concept. For it is a property, not of the physical system, but of the particular experiments you or I choose to perform on it'. The argument given by Jaynes for coming to this conclusion seem to rely on the observation that, whenever a measurement is made of the entropy of a system, only a subset of the possible variables of the system is taken into account. There will always be other thermodynamic variables which are implicitly assumed to remain constant. If we make an attempt to list all the variables of the system and to obtain a general formula for

the dependence of the entropy on the complete set then the task is, practically speaking, impossible. The entropy of the system will therefore be dependent on just those variables whose existence we choose to acknowledge and will thus be a function of the experiments we decide to perform. This argument seems to mix together two quite different problems: (*a*) the calculation of the entropy of a theoretical model, and (*b*) the correspondence between the entropy of a theoretical model and the measured entropy of a real system. We surely wish, for example, to say that the Sackur–Tetrode equation is an 'objective' formula for the entropy of a perfect gas in isothermal contact with its environment. The fact that no real system is a perfect gas is a distinct issue. In spite of these comments it must be admitted that the ignorance method seems, at least potentially, to be a consistent solution to the basic problem of relating mechanics and thermodynamics (not only at equilibrium but also in non-equilibrium situations (see Hobson [1971])). If we are inclined to reject it, it will ultimately be because we are not prepared to subscribe to this 'subjective'[1] view of classical physics.

The important common factor shared by the *ergodic and evolution methods* is their attempt to take seriously the dynamic character of the underlying mechanical model. Some difficulties of the ergodic method have been described. Briefly these are the problem of actually proving that a system is ergodic on the energy hypersurface (ergodicity on an invariant subset arising from the presence of other isolating constants of motion is not satisfactory for statistical mechanics) and the need to attach 'almost everywhere' conditions to the theorems which have been proved. With respect to the latter difficulty we find ourselves in the trap of having to assign zero probability to sets of measure zero in order to explain the prevalence of thermodynamic behaviour in real systems. This problem arises again in the context of equilibrium fluctuations. It is certainly possible, once a measure on phase space has been derived, to calculate the variance of phase functions. We need however to know that this variance gives us some information about the spread of experimental measurements about their mean. For this to be the case it is necessary that, in some sense, the measure function should be construed as representing the probability of the results of measurements. Otherwise the credit accorded to statistical mechanics for its prediction of experimentally detectable equilibrium

[1] 'Subjective' is the term used by Jaynes to describe his philosophical position on probability. Any false impression which may be gained from this terminology is corrected by Hobson who draws a clear distinction between the subjective (degrees of belief) interpretation of Ramsey and de Finetti and his own position (and that of Jaynes) which can be characterised by the quotation from Keynes given above (see also p. 257, n. 1).

fluctuations will be lost. The strength of the evolution method is that it makes a direct attack on the problem of the approach to equilibrium, deriving the equilibrium distribution as the long time limit of the solution of Liouville's equation. Its weaknesses are largely mathematical. By using, as it does, various types of perturbation expansion it becomes involved with uncontrolled approximations. It is difficult to obtain a clear insight into the significance of neglecting higher order terms in these expansions and it is virtually impossible to know whether their contributions to the evolution of the system are significant.

In conclusion it is worth emphasising that the purpose of this paper has been to attempt a rational reconstruction of *current* programmes for the foundations of statistical mechanics. It may be that some entirely novel approach, not envisaged here, will be developed in the future. In view of the successes of statistical mechanics at a practical level, it is difficult to believe that there will not come a time when the difficulties discussed here will be resolved. My own belief, for what it is worth, is that this resolution will come about from an approach which studies in detail the dynamic properties of the system. By this I do not of course mean that we should revert to attempts to solve the equations of motion. Apart from the practical impossibility of doing this, such a programme would contribute little to our understanding of the criteria for the class of mechanical systems giving rise to thermodynamic behaviour. It does however seem possible that a study of the qualitative properties of systems (see *e.g.* Abraham [1967], Arnold and Avez [1968]) will be able to give insights in terms of which the foundations of statistical mechanics can be better understood.

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