

Comments*

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My comments on Earman's paper will be very brief and those on Malament's somewhat more extended.

1. Comments on Earman's "Combining Statistical-Thermodynamics and Relativity Theory: Methodological and Foundations Problems"

The difficulties pointed out by Earman which one encounters in attempting to reconcile statistical mechanics with the special theory of relativity emphasize, once again, the very peculiar status of thermodynamics within the usual, hierarchically organized, structure of physical theories.

While thermodynamics is usually presumed to have a universality surpassing, perhaps, that of any other but the most fundamental of our physical theories - being applicable to the behavior of macroscopic materials, to electromagnetic radiation, and to phenomena on the range of the most submicroscopic (the use of phase-space in predicting cross-sections for scattering, for example) - it attains this universality not by being located at some fundamental or "deep" level in the hierarchy of theories related to one another by the usual process of reduction but, rather, by standing off on its own and cutting across the usual "vertical" organization of theories.

While some of the principles of thermodynamics, in particular the first law's statement of the conservation of energy, form an integrated part of the remaining body of physical theory (although as Earman has shown, even the division of energy into work and heat is not obvious in all cases), the most peculiarly thermodynamic concepts - equilibrium, irreversibility and entropy - do not fit in easily, either in their thermodynamic guise or explicated statistically, with the overwhelmingly larger part of physics.

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It is no great surprise that the naive attempts to find the right Lorentz transformations for the thermodynamic quantities resulted in radically opposed views each unsupported by any legitimate argument. Even in their most naive forms, as Earman points out, resort to the statistical interpretation of entropy and the underlying mechanical theory was necessary.

Our ultimate understanding of the source and nature of those aspects of the world described by thermodynamics or by the statistical theory to which it reduces still has a long way to go. It will have to account for the apparently mysterious fact that a theory, many of whose concepts are not intrinsically on a par with the other basic concepts of physical theory (requiring as they do a relativisation to modes of description, limitations on knowledge, etc.), and a theory whose explanatory basis seems to find the source of its own lawlikeness in features of the world denied just that lawlikeness by the underlying theory of the interaction of micro-constituents, turns out to be a theory whose range of applicability cuts across the usual subject matter demarcations which divide physical theory into neat compartments, and a theory whose universal applicability seems, at times, almost independent of the detailed nature of the underlying laws of interaction.

2. Comments on Malament's "Why Gibbs Phase Averages Work - The Role of Ergodic Theory"

From modern works on statistical mechanics, one might think the whole subject consisted in evaluations of canonical quadratures. Nowadays the ergodic problem is often forgotten and canonical averages are accepted because "they work." Such an approach, ready to assume any result for which some difficulty of proof turns up, breaks physics into disconnected fragmentary rules of thumb, forgetting that in physics it is no less important to understand than it is to calculate useful numbers. The only justification for using canonical averages lies in their ultimate bearing upon time averages. ([1], p. 29).

We are familiar with examples designed to show us that that which is sufficient for prediction may not be sufficient for explanation. From the barometric reading we can predict the storm and from the period of the pendulum infer its length, but the predictive basis hardly explains that which is predicted. From the thermal conductivity of a metal (in a reasonable range of values) we can, using the notorious Wiedeman-Franz law, predict its electrical conductivity, but this provides no explanation of the value of the latter conductivity at all. In general, non-causal connection, "wrong way" causal connection and phenomenological laws provide general classes of cases where prediction may be available without providing explanation.

In statistical mechanics (SM) there is much that we can predict: equilibrium interrelationships of thermodynamic parameters; small motion about equilibrium; general features of the approach to equilibrium when the non-equilibrium states are at least locally in equilibrium; some

qualitative features of phase-change, etc. But throughout the history of the theory again and again it has been felt that a perfectly adequate predictive device stands in need of backing up before it can be claimed to be part of a genuinely explanatory scheme.

The most general source of this felt disassociation between prediction and explanation in SM is probably this: Even the results of equilibrium theory must, in the final account, be explained in terms of the general non-equilibrium theory, with equilibrium taken as an explained ultimate state of evolution of a system. But the dynamic evolution of a system is governed not only by the laws of interaction of its micro-constituents, but by the initial conditions describing the initial state of the system as well. Now we cannot even descriptively and statistically characterize these initial states in general, having some access to this description only in such special cases as near equilibrium or locally equilibrium systems. But even if we could describe the initial microstate (by giving the class of such states some kind of statistical ensemble characterization), could we then *explain* it? It is almost as if our theory is in a classical schizophrenic double-bind, telling us to explain the progression toward equilibrium and the quality of this ultimate state, yet invoking initial conditions - exactly the sort of thing taken as a "given" and not explained in terms of the underlying micro-theory - as being essential for the quasi-lawlike explanations of SM itself.

Of course the way things are actually done is in a manner which attempts to evade to some degree this fundamental problem. Both for purposes of prediction and explanation we use what we know about how systems do behave to get some grip on the appropriate kinds of micro-behavior to look for. Thus, instead of deriving equilibrium from the theory in a fundamental way, we may presuppose that equilibrium does exist and then ask what the only appropriate statistical-mechanical description of such an invariant non-evolving state could possibly be. Again, in the non-equilibrium theory, instead of trying to solve, say, the Boltzmann equation in general we may assume, in the manner of Hilbert, Chapman and Enskog, that the evolution of the system can be described in terms of a small number of transport coefficients and then relate these to the statistical description of the underlying micro-structure.

Once we make such a move, however, we must then always be on the alert to ask ourselves, when the question is one of explanation, just what we have presupposed. While equilibrium theory may very well explain as well as predict some features of the equilibrium state, it does nothing to explain to us why equilibrium exists. Similarly, if we build the existence of transport coefficients into our non-equilibrium theory, their values and interrelations may very well be predicted and explained by our theory, but that there are transport coefficients at all will not be.

Over and above the fundamental problem in understanding explanation in SM there are other problems which are generated by the particular

structural features built into the theory as it has evolved. One of these we might call the problem of the "wrong statistical function". We are out to predict and possibly explain some thermodynamic feature of a system. To do this in SM we must associate (by identification or otherwise) the thermodynamic quantity with some quantity calculable from the micro-structure of the system and from some statistical distribution function plugged into the theory as an additional element; say, in the case of equilibrium, the micro-canonical distribution function. We find, however, that the quantity computed just doesn't seem, on reflection, to be the appropriate one to identify with the thermodynamic quantity, even given the most generous assumptions about the applicability of statistical methods in the first place.

As is well known Maxwell's original justification for the equilibrium momentum distribution was implausible. Boltzmann's primary position, never abandoned by him, was that the equilibrium distribution was to be derived as a consequence of the general dynamical theory. Under the influence of the early criticisms of the H-theorem he began the move from the earlier kinetic theory to a genuinely statistical SM. In this program the familiar derivation of the equilibrium distribution, as the one obtained by the overwhelmingly maximum number of permutations of the molecules in a cellularly partitioned molecular phase-space, was obtained. But that argument, aside from being inapplicable in the case of molecules with interaction potentials, itself presupposed the familiar "uniform" probability distribution among the total phases of the gas. Maxwell and Boltzmann both began the general program, later extended by Gibbs, of then identifying the thermodynamic parameters with phase-averages of micro-functions, using the "uniform" distribution in the system phase-space. Both Maxwell and Boltzmann realized, from the very beginning of this version of the statistical mechanical program, that some rationale was needed to justify this identification of measured thermodynamic quantities with mean values over an ensemble and both provided hints at such a rationale in the form of the ergodic hypothesis in the old sense of that term.

A thorough discussion of these issues was provided by the Ehrenfests in their famous review article. Basically the line taken there was that it was most probable values (over an infinite time) which could plausibly be identified with equilibrium values. The problem then becomes to rationalize the choice of distribution function in phase-space and the identification of mean values calculated by means of that distribution function with temporally most probable values. Even if one is satisfied with the identification of equilibrium values with the most probable values relative to some distribution, a distribution somehow or another rationalized, and doesn't insist on the move to most probable values in the sense of values held for the overwhelmingly greatest fraction of time, one still has the problem of showing that one's distribution function, the micro-canonical in the case of an isolated system, is nicely peaked about the mean and overwhelmingly so in the thermodynamic limit of a system whose degrees of freedom go to infinity in the familiar way.

Work on this latter problem, at least for the simplest case of the

ideal gas, was carried out by Khinchine in his attempt to make an "end run" around the ergodic problem. He hoped, by restricting attention to only certain functions of phase, but a class broad enough to include all those whose phase-averages were standardly identified with thermodynamic parameters, and by restricting attention to systems of vast numbers of degrees of freedom, to rationalize the usual statistical mechanical procedures without the then seemingly impossible task of showing a realistic model actually ergodic. He showed that for the standard micro-canonical distribution, in the thermodynamic limit, and for the case of the ideal gas, mean values were identical with most probable values. Lanford and others have now generalized these results to the case of gases whose potential energy is suitably symmetric and otherwise well-behaved.

Malament is now plausibly suggesting that we make use of these results not, as Khinchine hoped, to avoid the ergodic problem entirely, but to combine them with the recent successful attempt to show at least some models of gases ergodic to provide, finally, a rationale for the use of the micro-canonical phase-average in the equilibrium case.

In passing it is interesting to note how this suggested rationale for the standard equilibrium theory uses two results in a manner quite different from the intention of those who originally derived the results. While the proof of ergodicity was originally intended to rationalize the standard theory by showing that micro-canonical mean values were equal to infinite time averages, it is, instead a corollary of the main result which is used - the proof that in an ergodic system the micro-canonical ensemble is the only ensemble which is stationary and absolutely continuous with respect to Lebesgue measure. Infinite time averages are ignored altogether. While it was Khinchine's intention to circumvent the proof of ergodicity, it is now proposed to use his results on the structure of the standard distribution function in conjunction with ergodic results to rationalize the two-fold procedure of (1) adopting the standard ensemble distribution function and (2) then computing mean values with respect to it which are to be identified with thermodynamic parameters.

Malament, like many others, finds the old attempt to justify the standard methods by showing phase-averages equal to infinite time averages unsatisfactory as a rationale of the standard procedures. His doubts are fundamentally the view that it isn't plausible to take an infinite time average as the appropriate function of the micro-states to correlate with measured equilibrium values. But to what extent does this new rationale succeed in converting the usual procedures from a mere calculational device to a genuine explanatory scheme? I will only make a few tentative observations about this here.

(1) First of all there is the notorious problem of sets of Lebesgue measure zero. This approach first rationalizes the invocation of the standard ensemble by showing it to be uniquely stationary. If the system is ergodic the micro-canonical distribution function is the only stationary distribution function which assigns zero probability to a

system being in a set of measure zero. But why should we assume that sets of measure zero have zero probability? Without this assumption being made the number of alternative stationary distributions is obviously infinite. But this problem of ignoring sets of Lebesgue measure zero infects, of course, every ergodic approach, the traditional as well as this one.

(2) The kind of explanation being offered here is one of a conditional sort: given that equilibrium exists, what must it be like? Now equilibrium is a state which remains unchanged through time. Therefore our statistical analogues for the thermodynamic quantities must be temporally unchanging. But that by itself doesn't rationalize the choice of an ensemble invariant in time (and, hence, given the result of ergodicity for the system and the neglect of ensembles not absolutely continuous in Lebesgue measure, the usual distribution function). It only rationalizes the choice of an ensemble whose nature is such that mean values of the micro-functions associated with thermodynamic quantities are invariant in time. And we have little reason to believe that the usual distribution function will be the unique one with that feature.

But, of course, knowing the statistical nature of real equilibrium, complete with fluctuations, etc., we may instead take as our very notion of equilibrium the idea of a state, statistically characterized, whose means and all of whose moments are constant in time, giving us a temporally invariant characterization of fluctuation probabilities as well as of mean values. Then the ergodic rationale will (along with neglect of sets of measure zero) give us the usual distribution as the appropriate one to characterize equilibrium.

(3) The old ergodic theory had the virtue that in its terms the statistical assumptions were altogether eliminated except as an instrumentalistic device. Once mean values are identified with averages over infinite time spans and the latter taken to be appropriately identified with the thermodynamic quantities, no further questions about the role of the statistical assumptions remains.

In the new approach, however, the statistical assumption never really goes away. To be sure we are offered a rationale for choosing the distribution function we do. And we are given reason to associate the quantity we calculate (the mean value) with something at least a little more plausibly associated with the measured thermodynamic quantity than the mean value itself. The question "Why is Jones 5'9" tall?" does seem better answered by "Almost everyone is", than by "That's the average height in the population." After all, the latter could be true with everyone under 3' tall or over 7' tall! But there may still be questions to be discussed about the connection between such ensembles' most probable values and the values of parameters of individual systems which we actually measure. For example, in thinking that we have an explanation for the values this particular system possesses by noting that it is the "overwhelmingly most probable" value for the parameter, is it possible that we are once more using "most probable" in the sense of a

time ensemble and, by equivocation, identifying *that* with the, admittedly rationalized by temporal invariance, most probable value in the usual phase ensemble?

(4) This whole approach rests on the assumption that equilibrium exists and that what we want to do is assume its existence and then explain why it is like it is. But what we really want to know is *why* equilibrium exists. The present account, like all equilibrium statistical mechanics, goes as far as it can to disassociate equilibrium theory from the general dynamical problem of evolution. For predictive purposes this is unexceptionable. And, as far as it goes, there can be no complaint about a methodology which says: "Grant me that equilibrium exists and I will account for the specific nature of it."

But ultimately we will want an explanation of why systems evolve to equilibrium states and stay there, or, rather, of whatever special role equilibrium takes which replaces that rather naive notion of it. Such an explanation would require the invocation of the full dynamical picture of evolution. It would seem to require something more as well (solving the mystery of appropriate initial conditions). Where that would come from I have no idea.

(5) It ought to be kept in mind that the rationale Malament offers presupposes a proof that one's gas model is ergodic. In the case of realistic gas models we have no such proofs of ergodicity. It is a long way indeed from hard spheres in a box, for which Sinai has proven ergodicity, to the model of a gas whose molecules interact by means of some realistic potential.

The present approach does seem to have one additional virtue when compared to the older use of ergodic theory. The earlier rationalization of the methods of equilibrium SM makes no use whatever of (1) the large numbers of degrees of freedom of real systems or (2) the special nature of the phase functions we are interested in (their symmetry, for example). Sometimes it is claimed that the earlier rationalization can't be correct because it assumed too little! (On reflection this is a very curious objection and one worth some further thought.) The present approach does require us, as did Khinchine's, to invoke these two essential features and on that grounds alone will have more appeal to some than the earlier use of ergodic theory.

Editor's Note

*Malament's paper, given at the PSA Meeting and discussed in these comments, was not submitted for publication. Professor Sklar's comments are reasonably self-contained and were thought to be worth publishing even without one of the papers on which the comments are being made.

References

- [1] Truesdell, C. "Ergodic Theory in Classical Statistical Mechanics." In *Ergodic Theories*. (*Proceedings of the International School of Physics "Enrico Fermi"*, Course XIV.) Edited by P. Caldirola. New York and London: Academic Press, 1961. Pages 21-56.