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SCIENCE AND MATHEMATICS

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1. The Basis

An abyss opened up before my eyes when a famous mathematician told me once in a discussion of fundamental concepts of thermodynamics: "why do you search for definitions? You should just use the concepts and establish their meaning by usage." When I had recovered from the shock of this blasphemous attack at holy thermodynamics, I realized that this attitude was quite natural for a mathematician in our time. Since Gödel has blasted the idea of a consistent and complete set of axioms there has not been any hope for a closed, self-reenforcing structure in mathematics. Why should we search for such a structure in science if it cannot be realized even in mathematics?

Actually the problem of the foundation of science is quite different. Mathematics is a free creation of the mind, unencumbered by earthly ties of any kind. Science, however, has a fixed goal, the description of nature. Has such a very general, and therefore somewhat pale, idea enough life in it to produce a base sufficiently strong to carry the whole of science?

The problem goes back at least to Descartes. Hume as well as Berkeley proposed solutions that were both clear and internally consistent although they were entirely different from each other; they satisfied nobody. Hundreds of pages in Kant's "Critique of Pure Reason" demonstrate his gigantic struggle with the problem, which he called the existence of synthetic _a priori_ statements. But Kant's discussion, lengthy and cumbersome, contains the nucleus of a solution, which at once elucidates the difference of the foundation problem in science and in mathematics.

The solution[1] derives precisely from the fact that science is not autonomous (in the sense mathematics is) but has a predestined goal. It follows without question that a concept is part of the basis of science if I can show that it is inevitably required in the description of nature. The evidence that a concept is an indispensable tool is necessary and sufficient in selecting the basic concepts and building the foundation of science.

But can this evidence ever be established free of any doubt? Are we not plunging into the morass of scholastic philosophy? After all, this aberration was elaborate and logically consistent, and its concepts had only the one small defect of not corresponding with anything in the world of reality. The way to answer these doubts is the direct demonstration of those concepts that are indispensable tools indeed. Before we show these concepts, however, a few comments will be useful on how to find them.

2. The Method

In order to find the basic concepts of science we proceed by the rules of scientific research itself. That means in this case that we have to observe ourselves describing nature, to find the general features of any and all research, and to express the results in idealized terms.

All our concepts are idealized, not only those expressly labeled as such, as for instance the ideal gas or the ideal solution. The idealization of molecules as hard spheres is obvious, but a calorimeter is just as well an idealized thing and every experimenter tries hard to correct his immediate observations so that they are as close as possible to results that would be obtained by a perfect instrument (whose heat conductance would be infinite inside, zero outside). We cannot expect that the basic concepts are different and shall be satisfied with concepts that are idealized in the same sense as a calorimeter is an idealized concept.

It would be a mistake to make the validity of an idealization dependent on a pseudo-pragmatic definition such as: "An ideal calorimeter is the limit to which a set of improving constructions tend." An actual set of constructions may very well produce worse and worse instruments and lead to a wrong limit. If we press the condition "improving," the statement is empty, because it explains one unknown term by another. It would also be wrong to justify an idealization by the claim that the effects of small deviations from the ideal state always cause proportionate effects. The explosive power of a cargo of ammonium nitrate, set off catalytically by some impurity such as nitrite, is not proportional to the amount of the impurity present.

There is only one justification of idealization and numerous other steps in research: success in describing nature.

3. The Basic Concepts

For a moment let us forget all we know. Then let us open our eyes and start describing what we see. Immediately we realize that we must divide what we see in parts which we then can describe one by one. More than that. Our first description would be without any value if the described object were changing. For a valid initial description we have to keep an object in such a manner that it does not change. How to do this is a matter of experience. To find the properties of hot coffee we have to keep it in a thermos bottle. To maintain a document we put it into a strongbox. In order to preserve the battery of our car we prevent conducting connections of the positive pole with the car body.

Thus we need two concepts, which are coupled, object and isolation. If a part of the world can be isolated we call it an object. Isolating an object means to keep it under such conditions that it does not change whatever may happen in the rest of the world, i.e., in its environment. The conditions of isolation are established in every single case by experience.

In this first step we used precisely the method outlined before: we observed our actual procedure, extracted the most general features from it, and expressed them in clearly explained concepts. They are of course idealized. At the same time, there cannot be any doubt in the inevitable need of these concepts for the description of nature. Thus we have complied with the requirements that have been derived from Kant's work.

An exhaustive examination of all isolated objects is still far from a complete description of nature. We have to find the general features of interaction between objects and the general concepts required for describing interaction.

A simple gadget to establish interaction between two objects is a balance. A weight can be lifted or dropped according to our pleasure, i.e., the height of the weight above the table is a property of the weight. But when I put two weights on a balance their heights are not independent any more. Whatever the weights are, due to the design of the balance the sum of their heights above the table is constant. Similarly, we can put on an arbitrary electric charge on a storage cell or on a capacitor. The charge is therefore an independent property of one as well as the other. But as soon as we connect the two objects by wires, the sum of the two charges is fixed. As another example we take two cups, one containing a potassium chloride solution, the other a magnesium sulfate solution. We can change the concentration of either solution by adding or evaporating water. The water contents are properties of both solutions. But if we keep both cups in the same closed box the sum of the water contents is constant, though water may distil from one cup to the other.

The general characterization of interaction now is easy: An interaction means the imposition of a condition

$$F(x',x'') = 0 \tag{1}$$

on the properties x' and x'' of two objects. We can always transform the interaction variables in such a manner that on interaction their sum is constant

$$dx' + dx'' = 0 \quad . \tag{2}$$

The nature of the interaction condition (1) or (2) depends on the gadget which is used in establishing interaction. By experience we find different modes of interaction, mechanical, electrical, chemical, and so on. As soon as we consider several modes of interaction, the choice of the corresponding variables x_1, x_2, x_3 ... of an object must be restricted. An orderly description of different interaction processes requires that each must be examined by itself. If we investigate a capacitor with movable plates, we must be able to change it electrically with fixed plates; conversely we must be able to insulate it electrically while we change the distance of the plates. The electrical quantity which can be used is the charge; it remains constant during electrical insulation and can be changed by electrical interaction with fixed plates. The voltage would not be suitable since it changes in either mode of interaction.

We introduce therefore the concept of generalized coordinates as a set of orthogonal variables characterizing an object. "Orthogonal" means here that any coordinate can be changed in a corresponding mode of interaction while all other coordinates are fixed.

There is one mode of interaction without a corresponding coordinate, the interaction by contact or thermal interaction. We can prevent thermal interaction by enclosing the object in a vacuum jacket, crudely represented by a thermos bottle. A process in which thermal interaction is excluded, is called adiabatic. But there is no property which is always unchanged in any adiabatic process, and therefore there exists no generalized coordinate for thermal interaction. This is a specifically thermodynamic problem, which requires the two laws for a discussion.

If we have established interaction between two objects, there are three kinds of interactions that in view of the condition (2) may happen. They are

$$\text{(a)} \quad dx' > 0 \;; \qquad dx'' < 0 \tag{3}$$

$$\text{(b)} \quad dx' < 0 \;; \qquad dx'' > 0 \tag{4}$$

$$\text{(c)} \quad dx' = 0 \;; \qquad dx'' = 0 \;. \tag{5}$$

In the examples the balance beam may tilt to the left or right or stay in the middle position. An electric charge may flow from the storage cell to the capacitor or reverse, or no charge is transferred on establishing the connection. Water may distil over from the potassium chloride solution to the magnesium sulfate solution or reverse, or no water is transferred.

The third case (c) is called equilibrium. In the other two cases we say either that the generalized force f' of the first object is greater than the generalized force f'' of the second object, or reverse. The experimental decision whether case (a) or (b) or (c) is realized suffices to define the concept of the generalized force f conjugate with the coordinate x. All details concerning standards and calibration are arbitrary and present no essential difficulty. We compare any generalized force with a standard force, its subdivisions and multiples in the same manner we compare the length of an object with a standard meter or the hue of a dye with a standard color set.

There is one profound difference. Every measurement, i.e., comparison of forces is based on Eq. (5). The measurement therefore requires establishment of equilibrium. No other quantity in science, except temperature, is tied to this requirement.

In this whole discussion specific examples have been used only for illustration, never to carry the argument. The discussion therefore has been entirely general and the concepts introduced here are indispensable tools in the sense of Kant.

4. Thermodynamics and Other Sciences

Interaction by direct contact or thermal interaction can be prevented by enclosing an object in an adiabatic wall, which is a vacuum jacket or an idealized thermosbottle.

Work is now defined as the integral of a generalized force with respect to the conjugate generalized coordinate. The energy change E_F-E_I of an object going from an initial state I to a final state F is defined as the work done adiabatically upon the object by its environment. According to Carathéodory[2] the first law is expressed by the statement that the energy is a property of the object, i.e., the adiabatic work done upon it in the change I → F is always the same for a given initial and a given final state though it can be done upon the object in a variety of ways.

The entropy change of an object is then defined with the aid of the observation of the adiabatic change from A to B. If this change is spontaneous in the direction A → B, the entropy difference S_B-S_A is positive, and conversely. If the adiabatic change is reversible, we set S_B=S_A.

In order to define an entropy change quantitatively, we take into account that we have only a single independent variable of state left if we keep all coordinates fixed since in this case only thermal interaction is admitted. We choose the energy as the variable and represent the entropy change by means of a new function T as

$$dS = dE/T \tag{6}$$

where the small change indicated by d is performed at constant coordinates. The quantity T has the characteristics of temperature. This is shown by considering the transfer of heat (energy transfer without work) from one object (A) to another (B). This transfer proceeds spontaneously

$$dS = dE_A/T_A + dE_B/T_B = dE_A/T_A - dE_A/T_B > 0 \tag{7}$$

if T_A for the energy receiving object A ($dE_A > 0$) is smaller than T_B for the energy losing object B.

The entropy of any other state is measured by combination of such a purely thermal change with an adiabatic-reversible change for which the entropy remains constant.

It is a matter of taste whether or not these fundamental thermodynamic concepts should be included with the basic concepts of science. In any case, thermodynamics comprises our knowledge of equilibrium and of changes proceeding near equilibrium and thus may be considered to be the root of all physical sciences. From this common root sprout all branch sciences by extending their scope to non-equilibrium phenomena, kinetics and dynamics in mechanics and chemistry, molecular theory, and so on.

In an epistemological discussion, technology is included in science for a peculiar reason. In all natural sciences reproducibility of every observation is required. Therefore we must be able to change the state of any object to any state that is desired as an initial state for the repetition of an observation. But this is precisely the general problem of technology.

5. The Significance of the Basic Concepts

In view of this discussion it will be clear that the instruction given us by Kant leads indeed to the foundation of physical science. Numerous indications in the literature demonstrate the need for a straight and clear presentation of these foundations.

The most illustrious expression of this need has been given by Ehrenfest,[3] one of the most profound thinkers in the field of thermodynamics, in a discussion of the principle of Le Chatelier and Braun. He found that in this principle one needs a clear distinction between what today we call generalized coordinates and forces. But he did not find a fully satisfactory solution and frankly said so. Much later Planck[4] took up the question. Neither his paper nor the ensuing discussion[5] clarified the issue although it was felt that a much more important problem than the principle of Le Chatelier and Braun was involved.

It is strange to see that these difficult discussions would have been resolved in a few minutes had the eminent participants been aware of the need of equilibrium in the measurement of all forces. It appears that there has not been any possibility of recognizing this plain fact before it was epistemologically deduced.[1]

Due to a historical accident, generalized coordinates and forces have frequently been confused with extensive and intensive properties.[6] Most often, however, a clarification of these terms has not even been attempted.

The meaning of the term "work" has been repeatedly discussed in the literature. Gibbs apparently has never really tried to explain the meaning of work. A casual remark in a footnote[7] to a discussion of free energy says: "....the question is virtually, how great a weight does the state of the given body enable us to raise a given distance, no other permanent change being produced in external bodies?" This statement illustrates very well the change of free energy but it cannot be used for a general explanation of the term "work" because it sets up an open-ended research problem in every case. But attempts in the same direction have been made.[8] Even if they were successful, they would not solve the whole problem since we must introduce two of the concepts coordinate, force, and work. The third, of course, follows from the others.

6. The Application of Mathematics in Science

The basic concepts of science have been developed as the tools inevitably necessary for the goal of science, the description of nature. Mathematics has no such externally prescribed goal; its style of life is therefore different. In science, the foundation is clear and not subject to any possible doubt; but each single statement of substance is eternally open to re-examination and possible discard.[9] In mathematics any correctly derived single statement is removed from possible doubt, but the foundation is still under discussion.

In view of this essential difference mathematics cannot help science in fundamental questions. Mathematization of science, in particular of thermodynamics, is an illusion, notwithstanding its initiation by a great master.

There is a well known principal difficulty in applying mathematics to science. All our observations are affected by a finite error; the results are therefore expressed by rational numbers and they constitute a denumerable set. A digital computer with a sufficiently large memory can store the sum total of quantitative science. The utilization of the whole content of the memory without loss of information is a solved problem; there exist programs for computations with integers of any desired number of digits.[10] Thus we can, in principle, draw all possible conclusions without leaving the realm of rational numbers.

But almost all models we use in representing observations are constructed in a continuum. In other words, when we represent two observations in a diagram by drawing a straight line through them we add to the experimental information a number of points that exceeds by far the number of all rational numbers.

One may draw various conclusions from these facts. Nobody of course will wish to give up the wonderful shorthand of mathematics and in particular the operations requiring continuity. But we must realize that these operations in science require arbitrary assumptions which necessarily transcend any possible experience. In this situation it may be a good policy for scientists not to worry about the mathematical problems of the continuum.

Summary

The foundation of science, and of thermodynamics in particular, can be developed cogently and without arbitrariness by a procedure derived from Kant's epistemological discussions. The goal of science, description of nature, is externally given; it requires a set of basic concepts as indispensable tools. Mathematics has no similar externally given goal.

The consistent development of the foundation of science leads to the detection of gaps in thermodynamics and to the elimination of widespread errors.

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