

# THE CONCEPTUAL STRUCTURE OF PHYSICS

LASZLO TISZA

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LASZLO TISZA

*Department of Physics and Research Laboratory of Electronics, Massachusetts Institute of Technology,  
Cambridge, Massachusetts*

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## INTRODUCTION

THE systematization of the theories of physics can be attempted along two different lines. A classification is either based on the logical conceptual structure, or else follows the pattern of classification of the objects that are of principal interest in the theory.

The most important example of the first procedure is provided by late 19th century physics which is divided into mechanics, electrodynamics, and thermodynamics. This logical structure, and particularly the program of ultimate unification by reduction to classical mechanics, was shattered by the crisis that marked the transition from classical to modern physics. At any rate, the practical needs of contemporary research shifted the emphasis to the second of the abovementioned methods of systematization, within which one speaks of the physics of elementary particles, nuclei, molecules, fluids, solids, plasma, and stars (to mention only some of the most important divisions). Further subdivisions have been considered which depend on the expanding range of knowledge. Thus, one has not only the physics of semiconductors and masers, but also the physics of elementary particles in various ranges of energy.

Both methods of organization satisfy specific and important needs. On the one hand, the classification by objects of interest is indispensable for making specialized knowledge possible. However, the totality of physics presented in this fashion has an encyclo-

pedic character and is far beyond the grasp of an individual. On the other hand, the classical method of organization according to logical structure exhibits the simplifying and unifying power of high-level abstractions. This feature presumably accounts for the appeal of classical physics, which endures even in the face of breakdowns and limitations.

Of course, the unifying power of the classical logical structure is severely limited. The difficulties stem primarily from the fact that this structure centers around Newtonian mechanics as the basic discipline. The situation was characterized by Einstein<sup>1</sup> as follows:

"In spite of the fact that, today, we know positively that classical mechanics fails as a foundation dominating all physics, it still occupies the center of all of our thinking in physics. The reason for this lies in the fact that, regardless of important progress reached since the time of Newton, we have not yet arrived at a new foundation of physics concerning which we may be certain that the manifold of all investigated phenomena, and of successful partial theoretical systems, could be deduced logically from it."

During the quarter of a century that elapsed since Einstein wrote these lines, the discrepancy between the classical mechanical thinking and the formal development of physics has further increased. At the same time there is no decisive advance in the emergence of a new comprehensive foundation that can be accepted with assurance.

The purpose of this paper is to describe a new technique of logical analysis that is to bring about a more harmonious relation between conceptual thinking and formal developments. However, this is to be achieved within a program the scope of which is much more modest and manageable than the one hinted at by Einstein.

We propose to sort out and improve the logical structure of the existing, empirically verified theories. The establishment of a new foundation is the expected outcome rather than the prerequisite of this procedure.

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<sup>1</sup> A. Einstein, *J. Franklin Inst.* **221**, 349 (1936). Reprinted in A. Einstein, *Ideas and Opinions* (Crown Publishers, Inc., New York, 1954), p. 300.

The problem is to take advantage of the use of high-level abstractions while minimizing the risks inherent in their use. Successful abstractions have a predictive value of unexpected scope that greatly exceeds the range of their original empirical foundation. This situation often produces an unjustified confidence in the absolute validity of the theory. Yet not even the most perfect agreement between theory and experiment, extending over a wide range, provides a guarantee against the appearance of an essential disagreement as the range of experience is extended even further. The resolution of such disagreements may require the reconceptualization even of those theories that have been confirmed by experiment.

As a protection against the ossification of successful theories, we propose to make the connection between basic assumptions and experimental predictions sufficiently manifest, in order to facilitate a continued readjustment of the basic assumptions to the expanding range of experience. The use of deductive systems is an important device for achieving this goal.

The basic disciplines of classical physics are indeed organized as deductive systems. However, during the 19th century when the three major classical disciplines assumed their definitive form, the nature of deductive systems was still very incompletely understood.

The modern conception of deductive systems to be used in this paper is in some of its main aspects diametrically opposed to the classical one. Traditionally, deductive systems are used to organize knowledge that is already well substantiated. It is deemed essential to start from a basis that is safe from any emergency that might call for its revision. Of course, the origin of this reliable basis was an ever unsolved mystery. For existing systems that have been accepted as entirely dependable, the problem seems to be merely a recondite philosophical quest for the justification of something about which there is no real doubt anyway. However, in the present state of physics the problem of foundations manifests itself in the painful absence of a dependable starting point for developing important theories of practical interest.

Accordingly, the present effort is directed mainly toward the clarification of the problem of foundation. We shall attempt neither to justify the traditional foundations, nor to advance any new foundations on the basis of *a priori* plausibility. The method to be used is the *explicit* recognition and the systematic improvement of the logical structure that is *implicit*

in the existing experimentally supported theories.

We abandon the traditionally static, not to say dogmatic, relation between postulational basis and system. In the present approach the basis is tentative and subject to change if this leads to an improvement of the system in accounting for experimental facts. This feedback from system to basis leads to the dynamic, evolutionary adjustment of the system to a widening range of experience. Instead of assuming that deductive systems have to be perfect in order not to collapse, the present method of analysis deals with imperfect systems. In fact, one of the tasks of the method is to locate and eliminate imperfections. In view of this situation, we shall refer to this method as *dynamic logical analysis*, or the *dynamics of deductive systems*.

Section I of this paper contains a survey of the dynamic principles for the construction of deductive systems. These principles are not new, they have been developed in great detail in mathematical logic, and the empirical aspects of deductive systems have been investigated within logical positivism. The novelty of our presentation is therefore only a matter of selection and emphasis, and, last but not least, the contention, and, we hope, the demonstration that these principles are of practical use.

The actual construction of physically relevant deductive systems along these lines is, of course, a rather tedious enterprise. However, two instances have been actually produced thus far. First, the macroscopic thermodynamics of equilibrium,<sup>2</sup> briefly MTE, and the statistical thermodynamics of equilibrium,<sup>3</sup> briefly STE.

The axiomatizations of these well-known theories demonstrates the fact that the application of modern logical principles leads to a considerable restructuring—even of classical disciplines that seemed to have assumed a fairly rigid pattern.

It is an important insight of mathematical logic that each deductive system contains primitive concepts that cannot be defined by conventional means, but are implicitly defined by the deductive system as a whole. This "definition by postulation" of primitives, so important in modern mathematics, will be shown to be valuable also in physics. While recognizing the basic identity of the method in both disciplines, one should also take note of a difference stemming from the fact that the deductive systems of physics are always supplemented by rules of correspondence which establish a link with experience. Mainly as a consequence of this connection, most

<sup>2</sup> L. Tisza, Ann. Phys. (N. Y.) **13**, 1 (1961).

<sup>3</sup> L. Tisza and P. M. Quay (to be published).

concepts of physics evoke in the mind images or models, for which the postulates are presumably true statements. Although this intuitive aspect of the abstract concepts of physics is important for many reasons, the relations between experiment, intuitive models, and deductive systems are intricate, not unique, and hard to state in precise terms. The method of definition by postulation is an effective tool for clarifying the semantic ambiguities that arise out of this situation.

The fact that primitive concepts assume a precise meaning only relative to the deductive system into which they are incorporated, can be aptly referred to as the *relativity of concepts*.

An apparent difficulty for the deductive method is that most of the basic disciplines, say classical mechanics, thermodynamics, quantum mechanics, are too ramified and diverse to be compressed within the confines of a rigorously built deductive system. We propose to overcome this difficulty by constructing a cluster of deductive systems, even for representing one basic discipline.

Since, as we have pointed out, each deductive system implicitly defines its own set of primitive concepts, the increase in the number of systems is tantamount to an increase in the number of fundamental concepts that are defined relative to a particular context specified in terms of a *deductive system*. For this reason, we designate the procedure leading to a collection of deductive systems as *logical differentiation*.

The conceptual wealth brought about by the method of logical differentiation provides us with all the freedom we may need to adjust our deductive systems to a variety of experimental situations.

However, if the analysis should stop at this point, one might feel that the freedom in the formation of deductive systems has been carried too far, since it seems to lead to a proliferation of basic concepts. Actually, however, this process is held in check by the second stage of our procedure, the *logical integration* of deductive systems. This is a procedure which, to our knowledge, is advanced here for the first time.

The problem of logical integration arises from the methodological postulate that the various deductive systems are to express various aspects of the same reality. The reference to "reality" is apt to provoke queries of a philosophical nature. However, for the purposes of this paper it is satisfactory to interpret the statement above simply as follows. The separation of phenomena into "mechanic," "electric," "thermodynamic," etc., each described in terms of several deductive systems, is an abstraction. Real

phenomena exhibit all of these aspects at once, and the various deductive systems should be applicable in conjunction with each other, and hence should be compatible.

The program of logical integration, pursued by ensuring compatibility or mutual consistency of deductive systems, is the central issue of this paper.

In Sec. II we examine the logical requirements under which two systems, strictly speaking inconsistent with each other, can nevertheless be made compatible for empirical purposes. In this procedure we assign a central role to a simple relation that is the prototype for such relations that exist, say, between relativistic mechanics (RM) and classical mechanics of particles (CMP), or quantum mechanics (QM) and CMP. Here and in what follows, the capitalized abbreviations refer to deductive systems, and are explained in the block diagram (Fig. 1). This diagram represents the integrated system of the major deductive systems of physics, obtained by the repeated application of our fundamental relation. We note that this relation is asymmetric: In an appropriate limiting case one of the systems, to be called *dominant* or *fundamental*, reduces to the *derivative system*. The trend towards the integration of the existing deductive systems can be conceived of as the driving force leading to such highly abstract and fundamental systems as RM and QM. In this integration process, the arbitrariness in the selection of single deductive systems is drastically reduced. It appears that taking cognizance of the *relative character of concepts* is the prerequisite for establishing increasingly *objective* and unique *integrated logical structures*.

We shall refer to the doctrine that calls for the establishment of such structures as are represented in Fig. 1 as *integrated* or *consistent pluralism*.

The problem of logical integration does not arise in mathematics. Even though some of the deductive systems are related to each other, in general, each deductive system of mathematics constitutes a universe of discourse of its own. Therefore, it is not surprising that the intersystem relation of Sec. II has not been discussed in mathematical logic.

We consider now the relation of our method of logical integration to that which is implicit in classical physics. The classical method of integration has a *monistic* character: The consistency of physics is achieved by singling out one of the existing deductive systems as "fundamental," while all other systems are considered "phenomenological," to be "justified" by reduction to the fundamental system. The concepts of the latter are the only ones directly related to "physical reality." Problems, which seem to play

a key role in the reduction of phenomenological systems to the fundamental one, are accorded the status of *fundamental problems*.

From the time of Newton until the end of the 19th century the fundamental deductive system was assumed to be classical mechanics. The ideal monistic organization of physics was mechanistic. As the shortcomings of classical mechanics became evident, unified field theory and quantum mechanics were supposed to play the same fundamental role.

Although the monistic philosophy stimulated many brilliant achievements and scored interesting partial successes, the idea was never more than a program, its ultimate feasibility a matter of metaphysical conviction.

The monistic mechanistic metaphysics was indeed criticized from the positivist empiricist point of view. It was pointed out in essence that: (a) There is no reason why an expanding range of experience should be reducible to a system distilled from past experience, and (b) the narrowness of the alleged fundamental system is in striking contrast with the conceptual wealth of the systems to be reduced.<sup>4</sup>

The suggested alternative is the *positivist*, or *operational method*, according to which, abstract concepts should be introduced only if directly anchored in experimental operations. This procedure, at least in its more extreme versions, would discourage the introduction of high-level abstractions for the consistent organization of a wide range of experience. The positivist approach played an important liberating role in stimulating the development of modern physics along lines which were inconsistent with the mechanistic logical structure.

Nevertheless, operationalism has its unsatisfactory aspects. It leads to a highly fragmented state of physics that could be aptly described as *eclectic*, *nonintegrated pluralism*. Moreover, a close adherence to the operational principle is no more feasible than a strict adherence to the mechanistic organization. Actually, the practice of physics, at present, is an uneasy compromise between monistic unity and the diversity of eclectic pluralism. The exact nature of this compromise eludes precise formulation.

Even a most cursory inspection reveals that our integrated pluralism differs in essential respects from all versions of nonintegrated pluralism, and also from the classical monistic structure, although the difference is more subtle. It is possible, and the author

finds it most likely, that the procedure of logical differentiation and integration will ultimately lead to a single system that dominates all other systems. Even if this conjecture should turn out to be correct, the present situation is very different from the one postulated in the monistic view according to which we are *already in possession of the most fundamental deductive system*. The present method has an open-ended character, greatly in contrast with the traditional idea of the deductive method, according to which everything is implicit in the already available basis. In a certain sense we are dealing with an *inverse deductive* method. Starting from the experimentally tested low-level abstractions, we search for the basis from which the former can be derived.

The first two sections of the paper are written in a manner which, we hope, is detailed enough to convey a reasonably definite idea of the logical equipment which we propose to use. The remainder of the paper is devoted to applications of this equipment. Since the potential scope of these applications seem to be quite extensive, our account of it is necessarily sketchy, it merely prepares the ground for further elaborations.

The applications can be, by and large, grouped into two categories; The first is only a better systematization of existing knowledge, whereas the second leads to genuinely new results. Although traditional logical analysis was brought to bear only on the first type of problem, in the present approach the two are closely related to each other.

As a first step we have a crude systematization of the major systems of physics represented in the block diagram of Fig. 1. The blocks symbolizing theories are connected by various symbols representing the logical relations defined in the first two sections. Strictly speaking, these symbols have a precise meaning only if the theories are represented in terms of reasonably rigorous deductive systems. Generally speaking, this condition is not satisfied, but some of the theories, say, those related to classical fields, are so well organized, that a more rigorous axiomatization is unlikely to affect the situation substantially. For cases of this sort, the block diagram can be considered as a table of contents for a novel type of encyclopedia of theoretical physics. Also, the first three sections should provide sufficient instructions for the specialist who might wish to axiomatize his own field of interest. The requirements of mutual consistency provides certain "boundary conditions" for this endeavor, but conversely he might generalize, widen, and certainly enrich the block diagram itself. Clearly, the latter does not constitute a rigid "grand

<sup>4</sup> The second argument is, at present, entirely obvious if the fundamental system is classical mechanics or unified field theory. The case of quantum mechanics is more subtle and we shall return to it in Sec. IV.

scheme" that one would have to accept in its totality at the outset.

A particularly interesting case falling into the second category is thermodynamics. Recently two axiomatizations of this discipline were developed, the first, MTE, leads to a restructuring of the macroscopic theory,<sup>2</sup> the second, STE, to an extension into the statistical domain.<sup>3</sup> It is our contention that implicit in these theories is a conception of the structure of matter that is in a way complementary to the mechanistic one implicit in CMP. At least potentially, this conception seems to be more microscopic than the mechanistic one and provides a more satisfactory transition to quantum mechanics than the historical path emphasizing the connection with CMP. The substantiation of these claims is, of course, a very extensive project the outline of which is contained in Sec. IV. The details are being developed in a series of papers, of which references 2 and 3 are the first two. At this point, we advance two remarks that might serve to explain our statement to some extent. CMP can be conceived as the conceptualization of astronomy, a macroscopic observational discipline, while thermodynamics is the conceptualization of chemistry, an experimental discipline dealing with structural transformations. The mathematical equipment of CMP is essentially the theory of differential equations, that of thermodynamics is mathematical statistics. To insert statistical elements into differential equations has a disruptive effect on the formalism. This seems to have been the reason for Einstein's objections to the statistical aspects of quantum mechanics. In contrast, differential equations may appear as limits of stochastic difference equations and can also be inserted in other ways into mathematical statistics. Hence this change in point of view opens up the possibility of a constructive solution of the famous Einstein-Bohr controversy.<sup>5</sup> In particular, we shall formulate a second principle of causality that is characteristic of the thermodynamic theories and that is in contrast to the traditional mechanistic principle.

The switch from differential equations to mathematical statistics profoundly affects the type of questions that have to be admitted as legitimate in physics. Whereas it is traditionally emphasized that quantum mechanics restricts the range of measurements that were thought to be possible within CMP, it has not been brought out that quantum mechanics renders many real measurements possible

that were not even conceivable within the classical theories. It is apparent from these remarks that the present point of view is not without its philosophical implications. A few of these we shall discuss in Sec. V.

### I. DYNAMICS OF A SINGLE DEDUCTIVE SYSTEM

Deductive systems play a central part in the forthcoming discussion and we shall first summarize their properties, to the extent that these are relevant for our purposes.

A deductive system is a structure of concepts and propositions ordered according to the following principles. Complex concepts are explained in terms of simpler ones and, in the last analysis, the whole conceptual structure is derived from a few *primitive concepts*, or briefly, *primitives*. Definitions of this sort will be denoted as *synthetic definitions*. Similarly, complex propositions or theorems are inferred from simpler ones and are finally anchored in *postulates*.

The primitive concepts and postulates of the system will be briefly referred to as its *basis* or *foundation*. The *basis* has to be supplemented by rules governing the derivation of theorems and the formulation of synthetic definitions. In some respects a deductive system can be considered as a language; the aforementioned rules constitute its grammar.

The experimental relevance of the deductive systems of physics is conveyed by *rules of correspondence or coordination* that establish a relation between the conceptual elements on the one hand, and the objects of our common experience on the other. In general, the rules of coordination relate substantial parts of several deductive systems to extensive classes of measurements. It is seldom, if ever, possible to provide a convincing and direct experimental proof of the postulational basis.

In principle, we have to specify also the disciplines preceding the one under consideration, which are to be used freely. For the systems of physics, parts of logic and mathematics are such prior disciplines. However, these need not be explicitly listed for the current discussion.

We shall call the sequence of steps connecting the basis with a theorem a logical chain, or briefly, a chain. Symbolically,

$$T[C;P;D]$$

denotes a theorem  $T$  derived from the postulates  $P$  and involving the primitive concepts  $C$ , through the intermediary of a specified sequence of steps constituting a derivation  $D$ .

The logical content of the formula  $T[C;P;D]$  can be expressed as follows: The theorem  $T$  is at least as

<sup>5</sup> *Albert Einstein: Philosopher-Scientist*, edited by P. A. Schilpp, (The Library of Living Philosophers, Evanston, Illinois, 1949).

true as the postulates entering its argument. In other words, the acceptance of  $P$  implies the acceptance of  $T$ , but the converse is not true. It is often possible to prove the same theorem within different systems.

In discussing systems as a whole we can take one of two possible attitudes symbolically represented in the following formulas:

$$S = S\{C;P\} , \quad (1.1)$$

and

$$S = S\{C;P;D\} , \quad (1.2)$$

respectively. We shall refer to (1.1) as the *logical composition* of the system. It contains the entire basis that generates the system, whereas in a chain we insert only those concepts and postulates that are necessary for the completion of the proof. In principle, the basis determines the complete logical potentialities of the system, and formula (1.1) expresses the important fact that the basis is, in a way, the nucleus that succinctly contains the entire system, which is often too extensive to be apprehended otherwise.

Evidently, deductive systems contribute most effectively to the economy of thought. Yet one should not lose sight of the fact that statements about the potentialities of a system have often a speculative character. It is not always obvious whether persistent difficulties of solving a problem are only of a technical-mathematical nature, or whether they stem from the inadequacy of the basis.

Therefore, in a more conservative vein, it is sometimes useful to refer to a system in terms of Eq. (1.2). In other words to consider the system as the collection of theorems that has actually been derived at a particular stage of the historical development.

The construction of a deductive system essentially consists of the selection of the basis and the derivation of chains leading from the basis to theorems which, in turn, are related to observations. Thus, three distinct fields are open for logical analysis. The first pertains to the origin of the chains and consists of the evaluation and justification of the basis; the second is concerned with the rules for the derivation of the chains from a given basis, while the third deals with the rules of coordination that relate the end points of the chains to experiments. Of the three possible lines of inquiry, we shall be concerned here with only the first.

The second line of study deals with the routine operations of deriving theorems from a fixed basis. This corresponds to the conventional idea of the "deductive method." We need not enter into the discussion of this aspect of the problem, partly because

it has been thoroughly investigated within traditional logic, and partly because the standards of formal rigor emerging from these discussions are actually too high for the purposes of physics. For these purposes, the use of a reasonably precise mathematical formalism seems amply sufficient.

Although the third type of study, pertaining to the rules of coordination, is of considerable interest, we shall not enter into its discussion now. The rules of coordination are of a subtle nature; they contain abstract concepts on the one hand, and terms describing apparatus and objects of our common experience on the other. The disentangling of these various ingredients involves difficult epistemological problems. The more one ponders about these matters, the more surprising it seems how well these problems are handled in actual practice. However interesting it might be to clarify the logical basis of this highly intuitive activity, it seems unlikely that such a logical analysis could be of any real help to the experimental physicist at the present time.

The case for logical analysis is much more favorable when we turn to the first of the above mentioned problems and inquire into the meaning of the bases of deductive systems and the justification of their selection in preference to other possibilities.

In the discussion of the basis, the first problem to be considered is the clarification of the meaning of primitive concepts. Forming the point of departure for the synthetic definition of complex concepts, barring circularities, primitives cannot be defined in terms of even simpler concepts. Thus arises the paradoxical situation that the most important concepts of physics, or of any other science for that matter, cannot be defined along traditional lines.

The current attitude with respect to the paradox of undefinable concepts varies widely. Perhaps, the most frequent procedure is to cover up the difficulties by pseudo-definitions that fail to convey any precise meaning. At the other extreme is acceptance of the difficulty as inherent in the situation.<sup>6</sup>

There have also been attempts to explain the meaning of primitives in terms of "operational definitions," or rules of coordination. This program was never actually carried out in detail. In the author's opinion, the difficulties encountered are of a fundamental nature. The primitives form the beginning of the chains, while the connection with experi-

<sup>6</sup> "My own pet notion is that in the world of human thought generally, and in physical science particularly, the most important and most fruitful concepts are those to which it is impossible to attach a well-defined meaning." H. A. Kramers, *Motto of Collected Scientific Papers* (North-Holland Publishing Company, Amsterdam, 1956).



ment occurs at the end points. We clearly have two problems: the meaning of the primitives, and the experimental verification of the theorems. The power of experiment in deciding among competing assumptions will be greatly increased if the meaning of these assumptions is clear.

We propose to solve the problem of primitives by using the method of "definition by postulation" that is widely practiced in mathematics. According to this procedure, primitive concepts remain undefined in the synthetic sense, but their use is specified in terms of the postulates of the deductive system of which they are the ingredients. In fact, these postulates provide the instructions for the use of the primitives in forming the chains, and hence the observable prediction of the system.

Thus the precise meaning of the "undefined" primitive concepts is contained implicitly in the entire deductive system symbolically represented by its "formula"  $S = S\{C;P\}$ . We shall refer to this formula as the *analytic definition* of the concepts  $C$ .

Of course, we cannot expect a system to define a satisfactory set of concepts unless the formalism of the system is consistent.

The method of analytical definition is undoubtedly very abstract and is usually supplemented by the introduction of ideal objects, or intuitive "models" used as the interpretations of the primitive concepts. In this interpretation the postulates have to be true statements. Such intuitive notions are very useful and are instrumental in suggesting the experimental methods for the verification of the theory. Nevertheless, this use of models has many pitfalls. Their meaning is often not as clear as one might wish, and models that are intuitively accepted, or at least favored, are often oversimplified as compared with the theory to be interpreted.

In the presence of such difficulties, falling back on the method of analytic definitions may be the only recourse. In this way, we can establish the precise meaning of such concepts as "space," "time," "particle," etc. The problem of defining these by conventional means is complicated by the fact that these terms are currently used in the context of different deductive systems, such as classical, relativistic, and quantum mechanics. The method of analytic definitions makes it evident that the meaning of words denoting primitive concepts undergoes substantial changes as the context changes from one deductive system to another, or even as a deductive system is modified under the impact of expanding experience. Analytic definitions are most appropriate for handling these semantic difficulties which are quite

baffling on the level of verbal arguments. It appears that primitive concepts have a definite meaning only *relative* to a particular *context* characterized with precision by a deductive system and its formula.

We now turn to the problem of the justification of the postulational basis. First of all, we recognize that the basis is hypothetical, selected on intuitive grounds without any claim of *a priori* justification. Being arbitrary, the basis is not unique and there are in general several competing possibilities to account for the same class of phenomena. The relative merits of the various bases are evaluated *a posteriori* on the strength of the system generated by them. While the theorems within a system are justified by reduction to the basis, this situation is now reversed and the basis is justified by the system as a whole. If need arises, the basis is improved by feedback coupling from the developed system. Thus the circularity of reasoning, carefully eliminated from the intrinsic structure of the system, reappears "in the large" in the dependence of the basis on the system as a whole. This circularity is not "vicious," and can be handled to great advantage for the improvement of the system.

*Concordance* with experiment is of overriding importance for the evaluation of deductive systems. We shall not even consider systems unless concordance with experiment is ensured for a significant range.<sup>7</sup> Nevertheless, this empirical requirement is not sufficient by itself. The main reason is that the same experimental facts can be conceptualized in radically different ways, and we need criteria for selecting among the various possibilities.<sup>8</sup> The problem is to identify those highly abstract concepts that are most effective in creating order within the chaos of raw experimental facts, described in terms of low-level abstractions. In order to facilitate such judgments, it is desirable to have criteria for deciding in an objective fashion whether, and to what an extent a theory is *fundamental*, *phenomenological*, *ad hoc*, or merely an instance of curve fitting. It is also desirable that these criteria be more specific than a requirement of "simplicity."

Although we cannot expect to establish hard and fast rules for deciding such questions, we shall arrive

<sup>7</sup> Concordance is not an absolute concept, but is *relative* to a certain range. A further discussion of this point is found in the next section.

<sup>8</sup> This can be made plausible in terms of the following simple example. A finite portion of a plane can, within finite accuracy, be approximated by an infinite variety of surfaces of small curvature. Hence, plane geometry can be replaced for empirical purposes by an infinity of Riemannian geometries. This argument is easily adjusted to other deductive systems such as classical mechanics.

at workable criteria from the examination of the logical structure of the theories. This structure is evaluated in terms of such basic properties as the *consistency*, *independence*, and *comprehensiveness* of the axioms. We note that in virtue of formula (1.1) we can make such statements equally well about the basis and about the system. Moreover, these properties arise both in intrasystem and intersystem relations. The latter are of particular importance for the purposes of this paper.

If two chains have been found within a deductive system, one of which is the assertion, the other the negation of the same theorem, we are faced with an *inconsistency*. A system is consistent if it contains no inconsistency. The negative character of this definition renders the branch of mathematical logic dealing with the scope and limitations of proofs of absolute consistency extremely difficult.

Therefore, we hasten to point out that we shall accept the consistency of dependable deductive systems without known inconsistencies on pragmatic grounds. Our concern will be a much more manageable problem, the *mutual consistency* of two systems to be considered in the next section.

We turn now to the discussion of the *independence* of the postulates.

Let us suppose that a logical chain is discovered connecting a statement  $P_0$ , formerly believed to be a postulate, with the rest of the postulates:  $P_0[C, P]$ . In such a case we say that  $P_0$  is dependent on the rest of the basis. If it is impossible to find such a chain,  $P_0$  is independent.

It is seen that dependence is as tangible a relation as inconsistency, whereas independence shares the elusiveness of consistency. Economy requires that various postulates of a deductive system be independent of each other. However, under static conditions the dependence of an axiom on the rest of the basis is an esthetic flaw rather than a serious defect.

The situation is different under dynamic conditions. In the case of imperfect systems it is important to know that certain postulates are independent of each other and can be independently rejected or retained as the system is revised.

The problem of independence is particularly interesting as an intersystem relation. The question to be decided is whether or not one deductive system is reducible to another.

Another important property of a postulational basis is its *comprehensiveness*. By this we mean the explicit formulation of all of the *essential* assumption actually involved in the development of the system.

The application of the criterion of comprehensive-

ness clearly involves an important element of judgment. Comprehensiveness can be overdone and the proliferation of trivial postulates could degenerate into hair splitting. A positive sign that the addition of a heretofore hidden assumption to the basis is worthwhile, is obtained if the denial or modification of the postulate in question generates a new and interesting system. Significant examples of this sort were demonstrated by Hilbert<sup>9</sup> who found that Euclid's axiomatization of geometry is not comprehensive. He proved the independence and significance of the additional axioms by developing consistent geometries in which these postulates are negated.<sup>10</sup>

We shall see in Sec. IV that the situation is somewhat similar in thermodynamics. The new development of the subject is brought about by modification of postulates that were not explicitly formulated in the classical theory.

## II. INTERSYSTEM DYNAMICS

The dynamic interaction between a deductive system and its foundation leads to occasional revision of the latter. Often the revised system is in every respect superior to the earlier one, and completely replaces it in the living structure of physics.

However, there arise situations in which the old system cannot be dismissed as a historic relic, but has to be used along with the improved system. The joint use of different deductive systems for describing different aspects of reality raises novel problems of logical integration.

In preparation for this discussion we consider in this section, two principles that ensure the compatibility of certain types of deductive systems. It is an interesting fact that the formal logical aspects of these compatibility conditions can be recognized within a model of transparent simplicity. The same formal conditions can be given different concrete interpretations and used to handle most intricate situations.

The model in question is the practical (physical) geometry of a spherical surface, in other words geodesy. The physicist-geometer can avail himself of two abstract geometrical systems, to wit spherical, and plane geometry. From the point of view of the abstract mathematician the two systems are different and a discourse has to be completed in one or the

<sup>9</sup> D. Hilbert, *Die Grundlagen der Geometrie* (B. G. Teubner, Leipzig, Germany, 1956), 8th revised edition. English translation of the first edition (The Open Court Publishing Company, LaSalle, Illinois, 1899, reprinted 1950).

<sup>10</sup> Consistency is used here in the relative sense. The new geometries can be mapped into Euclidian geometry. Any inconsistency in the former would imply an inconsistency in the latter.

other system. The consistent use of the two systems for the description of the real, physical sphere depends on a number of circumstances.

In the first place, we establish a hierarchy between the two systems: We stipulate that in case of conflict spherical geometry should have priority. We express this by saying that spherical geometry is the *dominant* system, and plane geometry is called either *derivative*, *subordinate*, or *degenerate*.

We shall refer to the relation of these systems as supplementary *relation*, or briefly, *supplementarity*.

The second point is a clarification of what constitutes a "conflict" between the systems. In the mathematical sense a conflict always exists; however, in physical geometry we dismiss it as empirically irrelevant if it falls below the finite accuracy of the measurements which the theory is supposed to describe. The accuracy of measurement cannot be improved over the diffuseness set by thermal noise.

Somewhat more generally, we proceed to formulate a principle to which the rules of coordination have to conform. Experiment provides us with the values of continuous variables within a certain accuracy. However, the analysis of mathematical physics would be extremely cumbersome and lose much of its precision if the finite width of continuous parameters corresponding to empirical quantities were to be observed at every step. In actual practice, the segments of finite widths are sharpened into definite points of the continuum for the purposes of the analysis. However, the results obtained have no physical meaning unless they are sufficiently insensitive to the actual unsharpness of the continuous parameters.<sup>11</sup>

Mathematical solutions satisfying this requirement will be called *regular*. Solutions that change their essential features when the fictitious sharpening is given up will be referred to as *singular*. They are devoid of physical meaning except as possible stepping stones to more realistic results. The requirement that mathematical solutions be regular in order to have a physical meaning will prove to be of great importance and deserves to be called a principle, the *principle of regularity*.

The second point concerns the question of *scale*. Spherical geometry is characterized by an absolute unit of length  $R$ , the radius of the sphere. If  $R \rightarrow \infty$ , the sphere degenerates into the plane, the dominant

into the supplementary system. Let the linear dimension of a geometrical figure be  $a$ , then the parameter  $a/R$  appropriately expresses the deviation of spherical from plane geometry. It becomes meaningful to say that for small values of the parameter ( $a/R \approx \epsilon \ll 1$ , where  $\epsilon$  is the unsharpness of the parameter because of the inaccuracy of the measurement or because of noise) the subordinate system is asymptotically valid. Otherwise we have to fall back on the dominant system.

It is interesting to note that within plane geometry there is no absolute unit and it is meaningless to speak about small or large figures. All theorems are invariant under a transformation consisting of a change of the unit of length. We say also that plane geometry is *scale invariant*, or, it contains the theorem of similarity.<sup>12</sup>

The transition from the subordinate to the dominant system marks the breakdown of scale invariance. At the same time, however, the dominant system is characterized by an invariance of a novel type. In spherical geometry we have invariance of curvature. The more subtle invariances of the dominant systems of physics will be considered in Secs. III and IV.

In the course of historical evolution the dominant system has to be established by generalizing the subordinate system that reached what we shall call a *marginal breakdown*. In general, this is a task of great difficulty. While the converse procedure of arriving through a limiting process from the dominant to the subordinate system is a great deal more straightforward, even this transition is not without pitfalls.

Just as the sphere does not contain the infinite plane, so spherical geometry does not contain plane geometry. While the limiting process  $R \rightarrow \infty$  transforms every theorem of spherical geometry into one of plane geometry, the converse is not true. Thus the important laws of similarity of triangles and other figures have no counterpart in spherical geometry. The possibility of deriving such theorems is a new discovery, possible only in plane geometry. We shall see that the situation is quite similar for other pairs of dominant-supplementary theories.

We shall say that the inconsistency between the subordinate and the dominant system is *under control*, or that the *inconsistency* is controlled, if the range of validity of the subordinate system is known, and within these limits the compatibility with the dominant system is ensured.

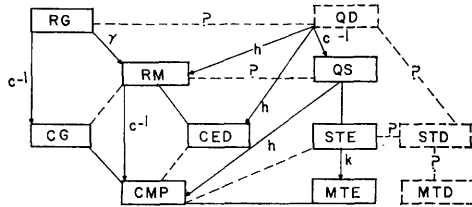
<sup>11</sup> See R. Courant and D. Hilbert, *Methoden der Mathematischen Physik II* (Verlag Julius Springer, Berlin, 1937), p. 176. Léon Brillouin, *Science and Information Theory* (Academic Press Inc., New York, 1962), 2nd ed. Chapter 21.

<sup>12</sup> E. P. Wigner, Proc. Am. Phil. Soc. 93, 521 (1949).

### III. LOGICAL INTEGRATION

Table I contains a simplified, symbolic representation of the integrated structure of systems that results from the application of the principles discussed in the last two sections. Although this structure, briefly, the *block diagram*, is still incomplete and tentative, it is adequate to provide the point of departure for our discussion. We have to remember that our method is set up to eliminate the shortcomings of the initially posited structure rather than to perpetuate them.

The block diagram can be discussed in different degrees of detail. On the most superficial level the theories associated with the various "blocks" are interpreted along traditional lines as suggested by their designation listed in Fig. 1. It will be recognized that the theories connected by arrows are indeed in a supplementary relation with each other, and the limiting processes leading to the derivative systems



—COMPATIBILITY - - - CONTROLLED INCONSISTENCY, —> SUPPLEMENTARY RELATION —?— INCOMPLETELY UNDERSTOOD RELATION

FIG. 1. Block diagram representing tentative structure of physics. Explanation of symbols designating deductive systems:

CMP	Classical mechanics of particles,
CMP ( $\mu$ )	Classical mechanics of particles (microscopic interpretation of particles),
PhCM	Phenomenological classical mechanics,
CG	Classical gravitational theory,
CED	Classical electrodynamics,
RM	Relativistic mechanics,
RG	Relativistic gravitational theory,
TD	Thermodynamics,
MTE	Macroscopic thermodynamics of equilibrium,
STE	Statistical thermodynamics of equilibrium,
MTD	Macroscopic thermodynamics,
STD	Statistical thermodynamics,
QM	Quantum mechanics,
QS	Quasistatic quantum mechanics,
QD	Quantum dynamics,

are formally associated with the vanishing of the absolute constants indicated in the diagram.

Maybe, the most significant aspect of the block diagram is that it exhibits CMP as derivative to several systems and dominant to none. This is in complete contrast with the logical structure hypothesized in classical physics in which CMP should have been dominant to all the other deductive systems of

physics. We shall use the discussion of the block diagram to sketch some of the refocusing that is made necessary by the changed role of mechanics.

In the current section we shall deal primarily with the relations involving CM, CED, and RM. These relations are fairly well understood and our brief discussion serves mainly to clarify our terminology in handling this situation; moreover it provides the prototype for the discussion of the more problematic relation among CMP, STE, and QM in Sec. IV.

If the discussion of the block diagram is to go beyond the broadly qualitative state, the theories have to be represented as deductive systems. This form of organization is not current in physics at the present time, and the traditional axiomatizations that are available, say for thermodynamics, do not satisfy the requirements of the present program.

Attempts to remedy this situation by up-to-date axiomatization bring to focus another complication. Most of the basic theories of Table I are too ramified and diverse to be compressed within the limitations of a rigorously built deductive system. However, these difficulties can be overcome by using a multiplicity of deductive systems, even within one basic theory. The establishment of this more intricate logical structure is in each case a major enterprise. In Sec. IV we summarize the specific problems that were encountered in MTE and STE.

In this section we first consider the case of CED, which is much simpler because the elaboration involves no departure from traditional lines of thought. A satisfactory axiomatization could be centered around Maxwell's equations, or an appropriate variational principle. The properties of material media are to be accounted for only phenomenologically; a microscopic description is outside the scope of CED.

If we let the light velocity  $c \rightarrow \infty$ , CED reduces to electrostatics (ES) which can be considered as a derivative system of the dominant CED. Even maintaining  $c$  finite, we obtain a series of theories classified in terms of  $\lambda/a$  and  $\omega$ , where  $\lambda$  and  $\omega$  are the wavelength and frequency of the electromagnetic disturbance, and  $a$  is a length specifying the size of the apparatus.

Additional possibilities arise if polarization and coherence properties are taken into account. However, we do not enter into these details at this point, and confine ourselves to the specification of a simple structure in Fig. 2.

It is apparent even without a detailed study that these theories are in supplementary relation to each other and CED is dominant to all. Thus the intrinsic logical structure of CED is somewhat of the type

represented in Fig. 1 for physics as a whole, with the exception that the latter is not (yet?) derived from a single dominant system.

The block diagram of Fig. 1 represents, in a way, a structure of low "logical resolution," which, if the

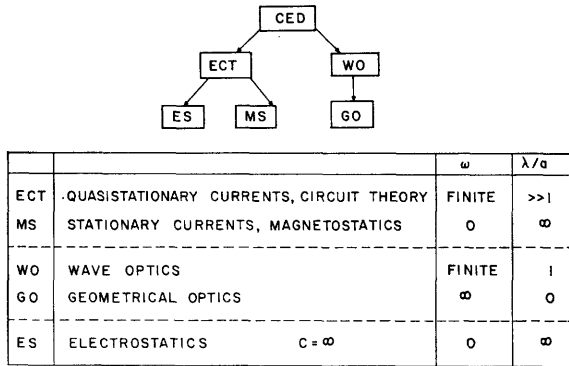
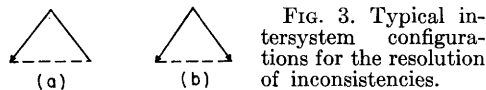


FIG. 2. Structure of classical electrodynamics.

need arises, may be supplemented by a "logical fine structure."

Although the intrinsic logical structure of CED would deserve a detailed study, this is not important for the purposes of the present paper.

A characteristic feature of the block diagram is the occurrence of a "triangle" formed by three deductive systems, the relations of which are represented in one of two alternative forms:



In either case, the base of the triangle is formed by two systems that are mutually inconsistent with each other. This incompatibility is resolved by a third system which is either dominant to both of the original systems, or dominant to one and consistent with the other.

It is interesting to look at this logical constellation from the point of view of historical evolution. It is a historical fact that the incompatible systems are the first ones to appear on the scene. Their incompatibility, represented in the diagram by a broken line, constitutes a "line of stress," which is resolved by the discovery of the dominant system. The inconsistency is thus brought under control in the sense explained at the end of Sec. II. For the sake of concreteness, we single out the systems CM, CED, and RM for a more detailed discussion. These systems are related to each other according to the pattern of Fig. 3(a).

The fact that RM and CM are in a dominant-supplementary relation to each other is obvious. There is, in fact, a close mathematical analogy between the relativistic and Newtonian kinematics on the one hand, and spherical and plane geometry (see Sec. II) on the other. The absolute constant is the velocity of light  $c$ , the dominant invariance principle is *relativistic invariance*. The scale invariance of the supplementary system CM manifests itself, e.g., in the linear law of the vector addition of velocities.

On the other hand, RM is consistent with CED rather than dominant to it, since the velocity of light  $c$  maintains its finite value. The limiting process  $c \rightarrow \infty$  leads to electrostatics, a highly degenerate part of CED.

The touchstone for the mutual consistency of CM and CED is the solution of two basic problems. The first is the fast motion of charged particles in the electromagnetic field. The second is the effect of the motion of the frame of reference of the observer on electromagnetic phenomena, including optics.

Historically, the study of both problems contributed essentially to the discovery of RM. In particular, Lorentz developed the theory of the electron in the electromagnetic field. However, this line of thought was complicated by uncertainties pertaining to the structure of the electron.

Einstein's great discovery was that the second of the aforementioned problems can be solved in phenomenological terms without involving assumptions concerning the structure of matter. The inconsistency of CM and CED was brought under control, in the sense explained in Sec. II, by giving up the space-time structure of CM in favor of that implicit in CED. Thus the intersystem relation between CM and CED was inverted and it was the latter that assumed the dominant role. More precisely, CED could be supplemented consistently by a mechanics (RM) that is dominant to CM. The expectation that all of physics, and in particular CED, is reducible to CM, was therewith disproved.

The establishment of RM led also to a consistent solution of Lorentz's problem of the motion of charged particles. However, it is not easy to delimit the phenomena in such a way as to stay clear of quantum effects and the subtler aspects of the consistency of the RM of the electron are still under discussion.<sup>13</sup>

The restructuring of physics connected with the recognition that the concepts of CMP do not have the expected fundamental character is a complex

<sup>13</sup> F. Rohrlich, Ann. Phys. (N. Y.) **13**, 93 (1961).

enterprise. For the purposes of discussion, it is convenient to divide the problem into three main divisions:

- (i) Kinematics, or space-time structure,
- (ii) Dynamics, the concept of force,
- (iii) The structural properties of matter.

The abovementioned analysis leading to RM corresponds to item (i) of this classification.<sup>14</sup>

The Newtonian concept of *force* as an universal idea suffered its first setback as the action at a distance of electrostatics and magnetostatics was replaced by the Faraday-Maxwell field. This process can be considered as the resolution of the inconsistency of the partial theories of electricity and magnetism by the dominant CED.

This process was continued as the Newtonian theory of gravitation CG was replaced by the relativistic theory. We note that this replacement was necessary, since the inconsistency of CG and RM had to be resolved by the dominant RG.

In contrast, the present analysis does not require the development of a unified field theory in which RG and CED are consolidated into a single system. In the first place, there is no manifest inconsistency to be resolved in this case. And second, a unified theory of interactions cannot fail to consider chemical effects, which in turn are intimately connected with the structural problems of matter.<sup>15</sup> The discussion of these is our next objective.

Up to this point our analysis is not in disagreement with commonly held view. We conclude this section with an item that may be considered controversial.

It was emphasized above that Einstein's analysis leading to RM is phenomenological. However, the analysis has one aspect, the well-known inference about the nonexistence of the ether, which transcends this limitation. While it is correct to say that there is no place for the ether in RM and CED, this concept has other implications which require further study from the point of view of our present knowledge.

The rejection of the ether concept is based on the fact that the assumption of a local flow velocity is inconsistent with RM, inasmuch as it would allow us

to assign velocities that moving bodies have with respect to an ether, stationary or otherwise. This, in turn, is contradicted by experiment.

It was pointed out by Dirac<sup>16</sup> that, though this inference seemed cogent in 1905, it is no longer convincing at present. The point is that within the classical theory a fluid is necessarily endowed with a local flow velocity, but this is not the case in QM. Thus an electron in an atomic *s* state does not possess a well-defined velocity.

It is instructive to discuss this matter in a more general context, since it lends itself to the illustration of our method of clarifying the meaning of primitive concepts. The problem of the "existence of the ether" is to be considered as a counterpart to the problem of the "existence of the atom." Texts of modern physics invariably argue that the answer to the first is in the negative, to the second, in the affirmative.

There is indeed convincing experimental evidence for the granular structure of matter. However, this is only a qualitative statement that is to be supplemented by the establishment of the laws governing the behavior of these "granules." Those denying the existence of atoms were right in the sense that the assumption of *c-atoms* obeying CMP are inconsistent with the facts of chemistry.<sup>17</sup> This statement is compatible with the existence of *q-atoms* obeying QM.<sup>18</sup>

The situation is similar with the ether. In an intuitive sense the ether was called upon to fill many roles. We may classify these along the threefold division invoked above in connection with the problems of mechanics:

(i) In kinematics the ether meant the existence of an absolute frame of reference. In view of RM the existence of such an ether is to be ruled out.

(ii) In dynamics, the most conspicuous role assigned to the ether was that of being the carrier of electromagnetic effects. Einstein pointed out that this notion is superfluous, although later, he came out in favor of the ether in connection with RG. We refer to the discussion of this point in a recent paper by Holton,<sup>19</sup> and in particular to the references given in his footnote 24.

(iii) The role of ether in the structural properties of matter is the most neglected aspect of this con-

<sup>14</sup> This statement is slightly oversimplified. The  $E = mc^2$  relation involves in a broad sense the concept of matter.

<sup>15</sup> Chemical interactions occur on the molecular, atomic, nuclear, and elementary particle levels. We claim that these varied effects have some common features to justify the use of a generic terminology. We shall attempt to support this point of view in the next section. This point of view is by no means generally accepted. Molecular chemical forces are usually considered as mere instances of electromagnetic interaction. The point that we emphasize, however, is that these interactions assume quite novel features if injected into the quantum-mechanical theory of the structure of matter.

<sup>16</sup> P. A. M. Dirac, *Nature* 168, 906 (1951).

<sup>17</sup> E. Mach, *Prinzipien der Wärmelehre* (Johann Ambrosius Barth, Leipzig, Germany, 1896), pp. 354-364.

<sup>18</sup> In the next section we shall subdivide QM into QS and QD, and accordingly we shall have to distinguish *qs* particles and *qd* particles.

<sup>19</sup> G. Holton, *Am. J. Phys.* 28, 627 (1960).

cept, and the one that is of the greatest interest in the present context.

The point to be realized is that the problem of structure has two aspects: (i) Starting from elementary particles we may build up complex structures and in particular the pseudo-continuum of macroscopic bodies. (ii) The elementary particles in their turn may be built up as the excitons of a hypothetical continuum, the ether.

The attempt of accounting for atoms as vortex rings is a theory of this sort. The failure of this theory is inconclusive, since it is based on the classical  $c$  ether. It is an open question whether an ether concept could be defined within QD to describe the creation and destruction of elementary particles. To dismiss the possibility of a  $qd$  ether because of the inadequacy of the  $c$  ether would be as unwarranted as to declare ultimate  $q$  particles nonexistent because of the nonexistence of ultimate  $c$  particles.

#### IV. MECHANICS, THERMODYNAMICS, AND QUANTUM MECHANICS

##### A. Introduction

We now turn to the central theme of our discussion and consider the problems related to structure. The empirical discipline dealing with the structural forms of matter and their transformations is chemistry.<sup>20</sup> Thermodynamics, in the broadest sense of the word, is a conceptualization of this discipline in much the same way as classical mechanics is the conceptualization of astronomy.

Of course, the space-time detail provided by the description of structure in classical thermodynamics is severely limited. We claim that there are two complementary methods for overcoming this limitation. The first is the traditional method of mechanical models, the second proceeds by the gradual deepening and extension of the thermodynamic conceptual framework.

Our main purpose is to sketch the second method (Secs. IV.C and IV.D), but for contrast it is important to sum up the essence of the first (Sec. IV.B).

We denote the microscopic interpretation of classical point mechanics by  $CMP(\mu)$ , a symbol explained more precisely in Sec. IV.B. In this theory, matter is assumed to consist of invariant point particles that trace precisely defined trajectories. Hence the space-time detail built into the theory is the highest conceivable. This amount of detail is not only unneces-

sary, but it leads to implications that are contrary to experiment.

The present conceptual discussions of quantum mechanics are still decisively influenced by the accidents of its origin. Since the space-time detail is overstated in  $CMP(\mu)$ , quantum mechanics appears as a theory that imposes limitations on the possibilities of measurement.

We claim that the alternative approach that arrives at quantum mechanics by an increase of the space-time detail of thermodynamics conveys a more germane conception of the meaning of quantum theory as an enrichment and sharpening of common experience.<sup>21</sup>

Of course, even in order to consider this alternative approach we have to revise some of the generally accepted ideas concerning the nature of thermodynamics. We start with the noncontroversial statement that thermodynamics is the theory that is always in close contact with measurement. During the last century atomic phenomena were beyond the reach of the available experimental techniques, and hence it was concluded that thermodynamics should not involve any reference to microscopic entities. This attitude was correct under the existing conditions; however, the notion that thermodynamics is inherently macroscopic is an unwarranted generalization.

If thermodynamics is indeed a theory of measurement, it has, at present, to be substantially generalized in order to match the advances of experimentation into the microscopic domain.

This means that we have to give up the idea that thermodynamics is merely the mechanics of systems of very many degrees of freedom, and we have to identify the more genuinely distinctive features of the two disciplines. This we can achieve by the technique of logical differentiation, as applied particularly to thermodynamics.

As a first step in this direction, we have to recognize that the classical theory of equilibrium is a blend of two essentially different logical structures: We shall distinguish the theory of Clausius and Kelvin, on the one hand, from that of Gibbs, on the other.

In the first of these theories the thermodynamic system is considered as a "black box" and all relevant information is derived from the amount of energy absorbed or provided by idealized auxiliary devices, such as heat and work reservoirs, coupled to the

<sup>20</sup> We shall make a few remarks about biological problems in Sec. IV.E.

<sup>21</sup> Whether or not this alternative approach would have been historically possible is irrelevant for the present discussion. We structure the transition from thermodynamics to quantum mechanics by exploiting all of the advantages of hindsight.



system. The main achievement of this theory is the establishment of the concepts of internal energy and entropy from observable mechanical quantities.

This is the situation that serves as the point of departure for the Gibbs theory. Attention is now turned toward the system; the concepts of internal energy and entropy are taken for granted and are used to provide a more detailed description of the system in equilibrium, which includes its chemical and phase structure.

The logical mathematical structure of the Clausius–Kelvin theory was clarified in the axiomatic investigation of Carathéodory.<sup>22</sup> We shall speak of the Clausius–Kelvin–Carathéodory theory, briefly CKC.

Elsewhere<sup>2</sup> we have developed the axiomatics of the macroscopic thermodynamics of equilibrium, briefly MTE, that bears a somewhat similar relation to the Gibbs theory.<sup>23</sup> In that paper, the main emphasis was on the theory of phase equilibrium in which MTE represented improvements over the classical theory. In the present context these improvements appear only as incidental benefits of the improved logical structure. The main point is that basically the same experimental material and very nearly the same formalism are accounted for in a different conceptual language that is in some respects richer than either CKC or  $\text{CMP}(\mu)$ . Whereas MTE cannot be reduced to  $\text{CMP}(\mu)$ , it is, logically speaking, an “open system” that readily admits a consistent deepening and expansion in the statistical and quantum-mechanical direction and leads to the dominant systems STE and QS.

In statistical mechanics it is often assumed that the main aspects of the program of reducing thermodynamics to mechanics are unchanged as classical mechanics is replaced by quantum mechanics. This is, of course, a possible way of structuring the situation. We shall attempt to show, however, that an alternative approach is more illuminating.

In the first place, the conceptual basis of  $\text{CMP}(\mu)$  is very simple, and the mechanistic reduction of MTE would require the elimination of much of its conceptual subtlety. In contrast, the transition from MTE to STE and QS involves an increase in conceptual wealth and sophistication.<sup>24</sup>

In Sec. IV.B we shall discuss the so-called fundamental problems of the mechanistic system. Our

main thesis is that, in general, these problems are fundamental only in the context of  $\text{CMP}(\mu)$ . Moreover, we warn against the all too common tendency of identifying the mechanistic scheme with that of common experience.

Sections IV.C and IV.D deal with the conceptual structure of thermodynamics and quantum mechanics. The two sections differ inasmuch as Sec. IV.C is devoted to quasi-static problems, whereas the role of time is more explicit in Sec. IV.D.<sup>25</sup> The time-dependent problems are still incompletely understood and will be discussed here only in a heuristic vein.

The forthcoming discussion is only a program in which innumerable details have to be filled in. The present paper is confined to such arguments that arise from the conceptual reinterpretations of the existing formalism. However, the increased intuitive insight gained in this process is suggestive of new developments within the formalism itself. The process of logical integration leading to QD is clearly unfinished.

## B. Classical Mechanics

According to arguments advanced in the general part of this paper, the term “mechanics” has a definite meaning only as the designation of a deductive system, or as a collection of deductive systems that arise as a result of logical differentiation.

The available axiomatizations of mechanics do not satisfy our requirements, since they have not been devised to differentiate between various disciplines that all go by the designation “mechanics,” even though not all of them are consistent with each other. The following sketchy discussion provides only the raw material for a future axiomatics, but its precision is sufficient for the present exploratory study.

The starting point of our discussion is the analytical dynamics of mass points in the Hamiltonian, or some equivalent form to which alone we accord the status of a fundamental deductive system included in the block diagram (Fig. 1). We shall refer to this part of mechanics as the classical mechanics of particles, briefly CMP. This theory deals with isolated systems of invariant structureless particles that cannot be created or annihilated. These particles differ from geometrical points only in that they have masses and act as force centers. The kinematics of the

<sup>22</sup> C. Carathéodory, *Math. Ann.* **67**, 355 (1909).

<sup>23</sup> J. W. Gibbs, *Collected Works* (Yale University Press, New Haven, Connecticut, 1948), Vol. I.

<sup>24</sup> This state of affairs would seem to violate the traditional requirements of conceptual *simplicity* and *economy*. However, these requirements can easily be carried *ad absurdum*, if taken in an absolute sense rather than judged relatively to achievement.

<sup>25</sup> We use the term “quasistatic” in the sense that we consider primarily states of equilibrium and transitions between them. This meaning is different from that of the “quasistatic path” of CKC. We shall refer to the quasistatic and dynamic theories as QS and QD, respectively. Also, we use QM in a generic sense for quantum mechanics.



system is based on Newtonian space-time structure and obeys Galilean relativity. An instantaneous state is described as a point in phase space; a mechanical process is a trajectory in this space. The dynamics is specified in terms of the Hamiltonian, a function of the instantaneous phase-space coordinates of the particles; the forces are conservative, of the "action at a distance" type.

The concept of mass points is an idealization, but there are two kinds of rules of correspondence for connecting the theory with observation.

In the *macroscopic interpretation* the mass points arise through concentrating the masses of *well-separated* objects in their center of mass. CMP provides, then, the translational motion, while the intrinsic properties of the objects are either considered irrelevant, or are referred to other theories, such as chemistry and generalized thermodynamics.

In an essentially different *microscopic interpretation*, the formalism of CMP is combined with a rudimentary atomic theory. Using the terminology of Sec. III, we assume that matter consists of  $c$  particles. We shall refer to the theory that has the formalism of CMP, but in which the point masses are interpreted in this microscopic fashion as  $\text{CMP}(\mu)$ , and the symbol CMP will be used to designate the macroscopic interpretation only.

The reason that CMP is accorded a fundamental status is due to the validity of a series of important general theorems.

Using a plausible terminology, we say that the conceptual input of the theory is a set of invariant mass points with their instantaneous state in  $\Gamma$  space, while the output consists of additional invariants, the integrals of motion, and the principle of mechanical determinism provided explicitly as the  $\Gamma$  trajectory.

Among these theorems, the principle of mechanical determinism deserves special attention because its basic feature has been applied far beyond the scope of classical mechanics. A formulation that gives justice to this wider range of application states in essence that causal chains are conditioned by the *exhaustive specification* of the initial states of the systems involved.<sup>26</sup> In the cases of CMP and  $\text{CMP}(\mu)$  the specification extends to the phase-space coordinates of all point masses of an entire isolated system. If, as usual, the system is coupled to its environment, then the initial state of the environment has to be

also completely specified; in practice this is an impossible task. Therefore, in the strict sense, mechanical determinism is empirically meaningful only for systems that are effectively decoupled from their environment. Evidently the case of planetary systems plays a uniquely favorable role in this respect.

The wealth of general theorems of CMP is in curious contrast with the scarcity of soluble special problems. In fact, the case of two mass points interacting with central forces is the only rigorously soluble problem in the theory.

It is of obvious interest to extend the range of CMP by making it more flexible in handling concrete problems. Apart from such important technical devices as perturbation theory, this extension can be achieved very effectively by joining to the basis of CMP additional assumptions that are of a more or less phenomenological nature. We shall refer collectively to a number of deductive systems that are obtained by joining one or more of the following assumptions to the basis of CMP as phenomenological classical mechanics (PhCM):

- (i) Potential energies specified phenomenologically rather than in terms of particle coordinates,
- (ii) Continuous distribution of matter resulting in the mechanics of rigid bodies, fluids, and elastic media,
- (iii) Dissipative forces,
- (iv) Statistical assumptions,
- (v) Assumptions of nonholonomic and rheonomic constraints.

While PhCM is of very great practical importance, this extension of the scope of the theory invalidates the general theorems of CMP. In fact, dissipative forces invalidate the constancy of the integrals of motion; and the manipulation of constraints substitutes one phase space for another, while a mechanical process is a trajectory in a fixed phase space.

The statistical assumptions that could conceivably be used in connection with CMP are of two sorts. First, one might consider an ensemble of identical systems with a probability distribution function of their representative points in  $\Gamma$  phase space at a given instant. The statistical assumptions of the second kind (stochastic assumptions) involve probabilities at a time  $t$  conditioned by the known states of the systems at an earlier time  $t_0$  (transition probabilities). Although CMP is entirely neutral with respect to the distribution of initial states and any assumption of this sort can be consistently joined to it, stochastic assumptions are inconsistent with mechanical determinism.

<sup>26</sup> We are using the terms "causality" and "determinism" as synonyms. Such usage is encouraged by the fact that CMP has only a single mechanism for the precise interpretation of both concepts. In reality, the terms in question suggest different meanings, and indeed we shall provide distinct interpretations for them in the thermodynamic theory.

The feasibility of the classical reduction program hinges on the solution of a number of problems that are considered to be fundamental relative to the mechanistic program. The most important of these are: (a) stability; (b) hydrodynamics, including dissipative and stochastic effects; and (c) manipulation of constraints. These are, of course, closely connected with the assumptions of PhCM listed above.

The problem of stability was a stumbling block for the theory. Postulating appropriate phenomenological forces did yield stability for a limited number of structures without ever explaining a fraction of the facts of chemistry. After the discovery of the role of Coulomb forces among particles, even this limited result was found to be precluded by Earnshaw's theorem.<sup>27</sup>

The most successful contributions to the reduction program fall into class (b). The rigorous approach to these problems is based on the qualitative observation that systems of many degrees of freedom starting from an arbitrary initial state and evolving in a deterministic fashion seem to exhibit a randomization, as far as a macroscopic observer can ascertain. This randomization is only an *appearance* and the latent memory of the initial state manifests itself in the Poincaré cycles.

Although it is plausible that conservative systems do often behave in such a fashion, it is very difficult to state these ideas in quantitative terms. Moreover, the methods necessarily ignore the principle of regularity, and therefore often have an unrealistic character. In view of these difficulties, it became customary to develop theories of dissipation by adding stochastic assumptions to the theory. This procedure can be pragmatically justified by reference to the fact that real systems are always subject to random perturbations. Instead of reducing randomness and dissipation to dynamics, one studies the interplay of randomness and dynamics. Many of the existing theories that make use of randomness assumptions can be integrated into STD, although they do not contribute to the classical reduction problem.

We turn finally to the problem of constraints. At first sight this problem does not seem to arise in CMP( $\mu$ ), since walls, other constraints, and the experimenter himself consists of atoms, and all could be included in the system and described in a super phase space. Hence the reducibility to mechanics can be upheld, but only at the price of giving up the separation of the object of experimentation from the experimenting subject.

At this point we are reminded of the fact that CMP is the conceptualization of astronomy, an *observational* science.

We shall avoid all these paradoxes in thermodynamics and quantum mechanics which can be considered as conceptualizations of chemistry, an *experimental* discipline.

### C. From Thermodynamics to Quantum Mechanics. Quasistatics

We shall develop the conceptual structure of a generalized thermodynamics that extends in successive approximations from a purely macroscopic theory (MTE) through statistics (STE) to quantum mechanics (QS). MTE and STE have been treated in more detail elsewhere.<sup>2,3</sup> At all three stages we confine ourselves to describing states of equilibrium, although we do allow for transitions among these states without describing them in detail. We shall refer to theories of this type as *quasi-statics*.

Equilibrium is a primitive concept analytically defined in terms of a deductive system, and thus will be redefined for each of the theories considered.

As we have mentioned in Sec. IV.A the conceptual structure of MTE is in practically every respect complementary to CMP( $\mu$ ).

Instead of building up systems out of mass points, in MTE one builds them out of "cells" that cover a certain region in space. We refer to the cells as *simple systems*, or *subsystems*, and to a collection of cells as a *composite system*.

The independent variables of the theory are additive conserved quantities, briefly, additive invariants  $X_1, X_2, \dots$ .<sup>28</sup> Composite systems are specified by sets of  $X_1^a$  ( $i = 1, 2, \dots, a = 1, 2, \dots$ ), where the subscript  $i$  designates the types of variables, and the superscript  $a$  refers to the subsystems of the composite system.

Explicitly, the  $X_i$  are the volume  $V$ , the internal energy  $U$ , and the mole numbers of the independent chemical components  $N_1, N_2, \dots$ . In spite of a superficial similarity, energy and mole numbers play a role in MTE that is very different from that in CMP( $\mu$ ). In mechanics energy is not additive, and it is only the nonadditive contribution, the interaction potential that leads to the coupling of different systems. We shall see that in MTE the most characteristic coupling comes about through the exchange

<sup>27</sup> W. T. Scott, Ann. J. Phys. 27, 418 (1959).

<sup>28</sup> The number of the invariants  $X_i$  is significant; it involves the concept of thermodynamic degrees of freedom and leads to the phase rules. <sup>2</sup> We ignore these matters here for the sake of brevity.

of energy and of other additive invariants.<sup>29</sup>

The mole numbers  $N_i$  have an essentially different meaning in MTE and in CMP( $\mu$ ). The most significant aspect of this difference is not in the shift from moles to molecules, since this is a simple scaling by Avogadro's number. In a context that does not involve numerical calculation, the same notation can be used interchangeably in both senses without risk of confusion. The important point is rather that the numbers of molecules of CMP( $\mu$ ) are absolute invariants, the molecules themselves cannot be created or annihilated. In contrast, MTE deals with molecules that are subject to chemical change. Hence, the numbers of the molecules of chemical species, or briefly *species*, are in general not invariants.

The situation is different with the numbers specifying the amounts of the independent chemical components, or briefly *components*. These are constructed to be the invariants of the relevant chemical reactions and thus they qualify as the additive invariants of MTE.

Needless to say, "molecule" stands here for any kind of discrete lump of matter that has a definite identity and is subject to transformation into other "molecules." In addition to conventional molecules we have atoms, ions, radicals, nuclei, and elementary particles.

An important implication of the foregoing discussion is that the numbers  $N_i$  are, in general, only relative invariants and the entire formalism of MTE is only relative to the set of chemical reactions that have been used to define the independent components. The formalism is to be adjusted to any change brought about in the set of reactions.<sup>30</sup>

We turn now to the discussion of processes. In CMP( $\mu$ ) all processes are alike, inasmuch as all of them are  $\Gamma$  trajectories. In MTE we have processes of different types and this variety is further increased in the deeper, dominant theories to be considered later.

An important type of process is the transfer of a

quantity  $X$  from the subsystem  $a$  to  $b$  during an arbitrary, fixed time interval.

The transfer quantity corresponding to the energy, with all of the other  $X$ 's fixed, is called *heat*.

*Walls* are the boundaries separating two systems which completely prevent the passage of one or more additive invariants, say  $X_\lambda$ , regardless of the nature of any system that may be adjacent, but permit free passage to all others, say  $X_k$ . The wall is *restrictive* of the  $X_\lambda$  and *nonrestrictive* of the  $X_k$ . Walls are said to exert *passive forces* on the distribution of the additive invariants. The restrictions on a system imposed by its walls are referred to as *constraints*.

It is most natural to think of a wall as a physical system with definite conductivity properties with respect to energy and matter (diffusion). Such systems are idealized as walls in MTE if their conductivities can be approximated as zero or infinite with respect to the time scale of the experiments considered. Alternatively, however, a wall may also be a mathematical surface. Thus a closed mathematical surface is restrictive of volume and allows us to define an open thermodynamic system that exchanges energy and mass with its surroundings. An important type of "wall" is provided by phase boundaries.<sup>2</sup>

Finally, the concept of thermodynamic process is easily extended to chemical reactions. In this case the molecular potential barriers stabilizing chemical species play the role of walls. As a last resort, all walls (except of course mathematical surfaces) depend on molecular potential barriers that may, or may not, be macroscopically organized.

We call *thermodynamic operations* any imposition or relaxation of a constraint through the uniting or subdividing of systems, or the altering of the type of any of its walls. In the presence of the existing constraints some of the variables  $X_\lambda^a$  are constant. We call these *fixed variables*. Those that are not entirely determined by the constraints are the *free variables*  $X_k^a$ . As a rule, we shall use Greek and Roman subscripts to denote fixed and free variables, respectively. The various admissible values of the free variables are called *virtual states*. The processes leading from one virtual state to another are *virtual processes*.

The distinction of thermodynamic operations and processes is a characteristic feature of the present approach. The admission of thermodynamic operations into the framework of the theory allows one to account for experimental procedures that have no place within CMP( $\mu$ ) because they correspond to transitions from one  $\Gamma$  space to another. Thus

<sup>29</sup> A second type of coupling is conveyed by surface forces such as elastic and Maxwell stresses. All apparent action-at-a-distance forces should be put in this form. Thus, surface forces described by scalar pressure integrate easily into the formalism, and the displacement of a boundary between two systems can be considered as an exchange of volume. For stress tensors shape effects involving distant parts of the composite system may come into play which complicates matters considerably. We exclude these situations in the present discussion in which we aim only at the clarification of the most characteristic features of MTE.

<sup>30</sup> While there is no way of selecting absolute invariant species or components in molecular and nuclear chemistry, such absolute invariants are likely to govern the transformation of elementary particles.

thermodynamics allows us to formally account for manipulation on thermodynamic systems. In particular, such manipulations may be performed on systems in the course of a measurement.

Yet the insistence on operations as contrasted with processes does not necessarily require the intervention of an experimentalist, and does not introduce more subjective elements into the theory than are warranted by the nature of the situation considered.

Thus in the case of chemical reactions and phase transitions, supplying catalysts or inhibitors that speed up or slow down the rates of reactions is the corresponding thermodynamic operation. In an automatic chemical plant, and even more in biochemical processes, the "operations" become effective without the interference of an experimentalist and it may be more adequate to speak of parametric processes which *control* or *govern* other processes. This is quite in line with the use of these terms in cybernetics.<sup>31</sup>

According to the present approach, the relevance of the cybernetic concepts mentioned is not confined to applications in engineering and in biology. These concepts play a fundamental role, even in the microscopic approach to the dynamics of structure. This conclusion is confirmed and extended in our interpretation of quantum mechanics.

Another implication of the foregoing remarks is that we can use both the mole numbers of species, or those of components in our formalism, provided that we remember that the former are free and the latter are fixed variables. Of course, the distinction between these two classes is not absolute, but is relative to the specific conditions that govern reaction rates.

Although thus far we have been describing the conceptual raw material of MTE, we note that our discussion is equally valid with respect to STE, the statistical thermodynamics of equilibrium. However, the two theories diverge in their formalization of equilibrium.

We arrive at the concept of equilibrium by noting that the foregoing considerations leave the values of free variables undetermined. However, in isolated composite systems there are, in addition to the "passive forces" exerted by constraints, also "active forces" originating in the intrinsic dynamics of the system which bring about a *quiescent equilibrium* in which the free variables take on asymptotically constant values.

Although the trend toward equilibrium is the basic experimental fact underlying thermodynamics, the

concept of equilibrium is nonetheless quite elusive, since there are no purely observational means for deciding whether an apparently quiescent system has actually reached equilibrium or is merely stranded in a nonequilibrium state while imperceptibly drifting toward equilibrium.

In the classical approach one meets this difficulty by advancing comparatively weak statements. Thus, in essence, the second law asserts the impossibility of processes in which systems drift away from equilibrium, but it does not claim that equilibrium is actually reached. The difficulty with this method is, however, that few if any significant results can be derived from these postulates without using a number of additional assumptions concerning the properties of material systems, such as the existence of homogeneous phases, validity of equations of state, and the like, which implicitly assume that equilibrium is reached. Since these assumptions are of limited validity, the rigor of the theory which the painstaking establishment of the universal principles was meant to ensure is considerably impaired.

In contrast to the classical procedure, we postulate in MTE that systems do reach their equilibrium and that the equilibrium values of the free variables are picked out from the set of virtual states by an extremum principle. The extremal function for this principle is the *entropy function*; the extremum is, by convention, a maximum.

For simple systems the entropy function is a first-order homogeneous function of the additive invariants

$$S = S(X_1, X_2, \dots) \quad (4.1)$$

and satisfies certain regularity conditions. It is convenient to number the variables so that  $X_1 = U$ .

The entropy function of a composite system is the sum of the entropies of its subsystems. The entropy maximum principle is written formally as

$$S(X_\lambda) = \max_k \{S(X_k|X_\lambda) = S(\bar{X}_k, X_\lambda), \quad (4.2)$$

where  $X_k$  and  $X_\lambda$  symbolize all of the free and fixed variables, respectively, and the  $\bar{X}_k$  represent the values of the  $X_k$  for which the maximum in (4.2) is attained and which appear experimentally as the equilibrium values of the free variables.

The entropy is a primitive concept of MTE and is defined implicitly in terms of the maximum principle (4.2). At the same time, the validity of this principle is associated in the observational domain with the establishment of equilibrium. The aforementioned difficulties inherent in the equilibrium concept are now solved as follows. The implications of the

<sup>31</sup> N. Wiener, *Cybernetics* (J. Wiley & Sons, Inc., New York, 1961), 2nd ed.

formalism of MTE are not to be taken as the prediction of the *actual* behavior of a given system, but rather as a statement of the *normal equilibrium* behavior. The comparison of the observed behavior of systems with the theoretical normal equilibrium yields a set of practical criteria for deciding whether or not equilibrium prevails.

To be sure, within MTE these criteria are, strictly speaking, only of a *necessary* character. In order to clinch the argument by establishing *sufficient* criteria, we have to use the methods of STE and QMS. We shall return to this question below.

Relation (4.1) is usually called the fundamental equation (f.e.). It has the remarkable property of containing all of the thermostatic information about the system. It can be visualized as a surface in the space of the variables  $S, X_1, X_2, \dots$  to which we shall refer as the Gibbs surface in *Gibbs space*.

It is convenient to assume, first, that the f.e. is given, and to return later to the combined experimental-theoretical task of establishing it for concrete systems.<sup>32</sup> With the f.e. known, in principle, it is possible to develop the implications of the maximum principle (4.2). Let the entropy of a composite system in equilibrium be  $S_i$ . Consider any kind of a thermodynamic operation in which some of the internal constraints of the system are relaxed, and thus the manifold of virtual states is increased. With the increase of the set of comparison states, the maximum (4.2) either increases or remains unchanged. Denoting the entropy in the relaxed equilibrium state  $S_f$ , we have

$$\begin{aligned} \text{(a)} \quad S_f &> S_i, \\ \text{(b)} \quad S_f &= S_i. \end{aligned} \tag{4.3}$$

or

In case (a) the relaxation of constraints triggers a process leading to a redistribution of the additive invariants, that is, to a new equilibrium. This process involves the increase in entropy:

$$DS = S_f - S_i. \tag{4.4}$$

The symbol  $D$  indicates an actual change in contrast to virtual changes denoted by  $\Delta$ .

In case (b) the relaxation of constraints leads to no process at all.

Simple as these statements are, they have broad implications that enable us to assess the relation of MTE with reality, that is, with experience understood in the broad sense of the word.

The fact that case (b) does indeed occur indicates that the value of the entropy and the entire for-

malism of MTE is insensitive to the distinction of whether or not a certain value of a variable is held constant by active or by passive forces. This feature of MTE is not rigorously concordant with experience, since the active forces that bring about the asymptotically constant values of the free variables also produce fluctuations, while the passive forces, or constraints, preclude fluctuations.

Remarkably enough, this limitation of validity hardly affects the usefulness of MTE. In the first place, fluctuations are often of negligible importance. Even more noteworthy is the fact that the marginal limitations of MTE are easily removed by refinement rather than disruption of its foundations.

Case (a) involving an increase of entropy leads to even more searching questions. How did the temporal concept "increase" suddenly emerge in the theory that does not even contain the concept of "time"?

Formally, the entropy maximum principle (4.2) is nothing but the well-known simple result of the calculus of variations according to which the maximum of a functional does not decrease as the set of trial functions is increased. The temporal aspect enters the picture through the interplay of operations and processes. If the relaxation of constraints leads to  $S_f > S_i$ , then this operation triggers a process in which the potentiality of a system for a new equilibrium is realized.<sup>33</sup>

The process itself has no counterpart in the formalism of MTE. The representation of this system reappears in this theory only after the new equilibrium is reached. This happens at a time that is *later* than the instant when the operation was performed. This is the point where the concept of temporal ordering enters the theory.

The description will continue to be valid until another operation triggers a new process. The representation of the system in disconnected time intervals is quite analogous to the spatial representation in terms of disjoint cells. All this may be summed up by saying that the system is described in a four-dimensional piecewise continuous space-time manifold. With each four-dimensional cell there is associated a point of Gibbs space, a set of numbers  $S, X_1, X_2, \dots$  specifying the equilibrium distribution of the relevant additive invariants.<sup>34</sup>

<sup>33</sup> At least this happens in what we call the normal equilibrium case. The alternative possibility is that the system remains stranded in the initial state that is now no longer an equilibrium, or in some intermediate frozen-in nonequilibrium state.

<sup>34</sup> This combination of the space-time manifold with Gibbs space constitutes the rudimentary elements of a nonlocal field theory.

<sup>32</sup> In order to avoid repetition, we shall consider the empirical foundation only in the context of STE.

The simple interplay between operation and process can be iterated to produce the description of complex situations that will be discussed somewhat further in Secs. IV.D and IV.E.

The above-mentioned classification of thermodynamic operations into classes (a) and (b) is important enough to be designated by special terms. We say that an *operation* is *irreversible* if it produces an entropy increase  $DS = S_f - S_i$ . This quantity is called the *measure of irreversibility*. An *operation* is *reversible* if it does not produce an entropy increase. Reversible operations occur in pairs; the relaxation and the reimposition of the same constraint that can be repeated indefinitely without producing any change in the system, except for the admission or suppression of fluctuations, a distinction not registered within MTE. We note that, in contrast to the usual procedure, we distinguish reversible and irreversible operations, rather than processes. The processes of the type considered thus far are all irreversible.

It is natural to ask two questions at this point. (i) How do we define irreversible thermodynamics, or, as we prefer to call it MTD, if irreversibility enters already so decisively in MTE? (ii) How do we arrive at the quasistatic processes of the CKC theory?

The answer to (i) is that the relaxation of an old to a new equilibrium is indeed considered both by MTE and by MTD, but the two theories differ in the detail of the description. In particular, MTD considers the relaxation time and to some extent the intermediate nonequilibrium states.<sup>35</sup>

The answer to (ii) is obtained by means of the following construction. A simple system can be coupled to a sequence of auxiliary systems, so that each operation triggers a process. A sequence of such operations and processes is called a *path* that is not uniquely specified by the initial and the final states. In particular, by increasing the number of well-chosen intermediate operations, the total measure of irreversibility can be decreased below an arbitrary threshold. In this limiting sense one can speak of reversible paths. These reversible paths, which are rather complex constructs in MTE, are the basic concepts in the CKC thermodynamics.

The entropy maximum principle states in essence that, given the nature of the systems involved in terms of their f.e., the fixed variables determine the equilibrium values of the free variables. Whether or

not these equilibrium values are unique and under what conditions is not a matter of postulation but can be deduced from the theory. The clarification of this issue is indeed its main achievement. It appears that the abovementioned equilibrium values are almost unique with some qualifications that will be stated below. This result we have called<sup>2</sup> the principle of thermostatic determinism.

The entropy maximum principle is used to define in a well-known fashion the concepts of stable and metastable equilibrium.<sup>36</sup> The formalism, as it has been sketched thus far, is too scanty to carry us much further. It can be made considerably more flexible by transforming the f.e. to other sets of independent variables. Each of these transformations has an intuitive interpretation and extends the scope of the formalism to another class of experimental situations.

The first step in this transformation theory is to solve the f.e.  $S = S(U, X_2, X_3, \dots)$  for the energy

$$U = U(S, X_2, X_3, \dots). \quad (4.5)$$

We shall refer to the formalism based on (4.1) and (4.5) as the *entropy* and *energy schemes*, respectively. Formally, the transition from (4.1) and (4.5) consists merely of the rotation of the Gibbs space, thereby resulting in the interchange of the roles of  $S$  and  $U$  as dependent and independent variables, and the two schemes are consistent with each other. In particular, they lead to equivalent stability criteria.

At the same time the transition to the energy scheme brings about a significant extension of the types of processes that are accounted for. The formalism is set up in terms of processes that conserve the independent variables summed over the composite system. Hence, in the entropy scheme we have energy conservation; the manipulation of the constraints do not involve any work and irreversible operations trigger irreversible processes. In the energy scheme, the total entropy is conserved, and hence operations<sup>37</sup> are reversible, but involve work performed on or by the environment.

We shall refer to the two kinds of processes as *entropic* and *energetic* processes, respectively.

An important extension of the formalism of MTE is the introduction of the intensities. These can be

<sup>35</sup> We note that MTD deals also with situations that do not connect an old with a new equilibrium, such as stationary currents and time-dependent environments.

<sup>36</sup> We note that the former is still not an *absolute* stability in the sense that every statement of MTE is relative to the choice of independent components, determined in turn by the set of relevant reactions. In principle, most if not all stable states can become metastable if the proper catalysts are added.

<sup>37</sup> In the energy scheme operations and processes are inseparably tied up. We may use the terms interchangeably.

defined in either scheme as the conjugate variables to the  $X_i$ :

$$P_1 = \frac{\partial U}{\partial X_1} = \frac{\partial U}{\partial S} = T, \quad P_i = \frac{\partial U}{\partial X_i}, \quad i \geq 2, \quad (4.6)$$

$$\pi_1 = \frac{\partial S}{\partial X_1} = \frac{\partial S}{\partial U} = \frac{1}{T}, \quad \pi_i = \frac{\partial S}{\partial X_i}, \quad i \geq 2. \quad (4.7)$$

Here,  $T$  is the thermodynamic temperature, the other  $P_i$  are negative pressure and the chemical potentials. Moreover,

$$\pi_i = -P_i/T, \quad i \geq 2. \quad (4.8)$$

In order to appreciate the significance of the intensive variables, it is convenient to single out one cell of a composite system for detailed consideration, and join all the others to provide the "environment" of this system. We require also that the over-all size of the environment be very large, in the limit infinite, compared with the system of interest. The environment (called also a *generalized reservoir*) is specified by the set of its intensities  $P_1^0, P_2^0, \dots$ . This description is quite schematic; it ignores the detailed cell structure of the environment that may be quite complex. The specification is adequate, nevertheless, for deciding whether or not a system is in equilibrium when coupled to this environment. The condition for this is that the intensities of the system should equal those of the environment:  $P_k = P_k^0$ .

In general, for a given set of  $P_k$  the system will have a uniquely determined set of values for the conjugate  $X_k$ , and vice versa. The condition for this is

$$\frac{\partial(P_1, P_2, \dots)}{\partial(X_1, X_2, \dots)} \neq 0, \infty. \quad (4.9)$$

In the so-called regular points of Gibbs space where conditions (4.9) are satisfied the principle of thermostatic determinism takes on a very simple form: For a system in equilibrium with a reservoir  $R(P_k^0)$  the free variables take on a unique set of values  $X_k^0$  and vice versa. We shall say that the sets  $P_k$  and  $X_k$  are *matched* with each other.

This mutual determination of the invariants of a system and the intensities of a reservoir is confirmed by experiment. Nevertheless, the limitations imposed by conditions (4.9) are significant. The Jacobian in question vanishes at critical points and is infinite at absolute zero.

In the first case the initial intensities are inadequate for determining the values of the free variables (e.g., mole numbers per given volume) because of the huge critical fluctuations. Near absolute zero the

responses  $X_k$  of the system become temperature independent and therefore are poor indicators of the temperature.

Thus the singularity of the formalism of MTE at critical points and at absolute zero has its counterpart in the experimental situation. Consequently, the limitation of MTE is rather different from the breakdown of, say  $\text{CMP}(\mu)$ . The information provided by the theory is incomplete rather than incorrect.

It is easy to point out the oversimplification in MTE that is responsible for its lack of detail, and to formulate a heuristic idea that guides us towards the deepening of its foundations. Whereas in MTE the virtual states have but a formal role, in the new theory they are assigned physical reality as fluctuations states. The free variables of a thermodynamic system are considered as random variables and the principle of thermostatic determinism is weakened to the extent that instead of the *values* of these variables, only their *probability distribution functions* (d.f.) are assumed to be fixed in equilibrium.

The injection of statistical ideas into the theory calls for an extension of the conceptual structure. First, we have to consider ensembles of systems  $e(x_k|x_\lambda)$ . An ensemble is defined as an unlimited set of systems describable in terms of the same selection of variables  $X$ ; moreover the fixed quantities  $X_\lambda$  have the same value  $x_\lambda$  in each system, while the values of the free variables  $X_k$  take on random values  $x_k$ .

Generally speaking, the variation of the free variables will display a complex interplay of randomness with correlations stemming from molecular dynamics. One arrives at the simplest theory by considering independent random variables in which correlations are ignored.<sup>38</sup> In the theory of pure randomness the coupling between systems brings about a total loss of the "memory" of the state existing before the coupling was brought about. This point of departure leads to the theory of the statistical effects that take place in thermodynamic equilibrium. Accordingly, the theory obtained is called the statistical thermodynamics of equilibrium, briefly STE.

If an ensemble  $e(x_k|x_\lambda)$  is in equilibrium with a reservoir  $R(\pi_k)$  to which it is coupled by  $X_k$  exchange, the probabilities of the free variables are provided by the generalized canonical d.f.<sup>39</sup>

<sup>38</sup> To be more precise, the theory does not deal explicitly with correlations, but these are implicit in the set of fixed variables.

<sup>39</sup> This result is of course well known and can be safely made the point of departure for the following argument. However, we wish to give a few hints concerning a proof that has been given.<sup>3</sup> The derivation in question is based only on qualitative postulates concerning the existence of a d.f. conditioned by



$$dF(x_k, x_\lambda, \pi_k) = dG(x_k, x_\lambda) \exp \left[ - \sum \pi_k x_k \right] Z^{-1}(\pi_k, x_\lambda) \quad (4.10)$$

The normalization of probabilities leads to

$$Z(\pi_k, x_\lambda) = \int_{x_k} \exp \left[ - \sum \pi_k x_k \right] dG(x_k, x_\lambda). \quad (4.11)$$

Here,  $G(x_k, x_\lambda)$  is the *structure function* of the system and  $dG$  denotes the number of microstates within the range  $x_k$  and  $x_k + dx_k$  of the free variables.<sup>40</sup> Its Laplace transform  $Z$  is the *partition function*, or *generating function*.

Although the formalism based on (4.10) and (4.11) is well known, we have some new angles to emphasize which arise within a systematic discussion of the three types of measurements that can be interpreted and evaluated in terms of this formalism:

(A) Coupling of a known system ( $x_\lambda$ ) with a known environment  $R(\pi_k)$ . The predicted response of the system is the d.f. of  $X_k$ , in particular the canonical average  $\bar{x}_k$ ,

(B) Measuring the response  $x_k$  of a known system ( $x_\lambda$ ) and inferring the intensities  $\pi_k$  of the environment,

(C) Inferring the nature of an unknown system ( $x_\lambda$ ) from its response  $x_k$  when coupled to a known environment  $R(\pi_k)$ .

Case (A) corresponds to the standard interpretation of the formalism. It leads at once to the f.e. of MTE if

$$\bar{x}_k = - \partial \ln Z / \partial \pi_k \quad (4.12)$$

is identified with the corresponding  $X_k$ , and the entropy is defined as

$$S = s(\bar{x}_k), \quad (4.13)$$

where the random entropy function is

$$s = \ln Z + \sum \pi_k x_k. \quad (4.14)$$

Boltzmann's constant is chosen as unity. Thus relation (4.7) is now replaced by

$$\partial s(\bar{x}_k) / \partial \bar{x}_k = \pi_k. \quad (4.15)$$

the relevant parameters and uninfluenced by previous history. It is an important point in the present context that the system that is coupled with the infinite reservoir is not assumed to have many degrees of freedom and may consist even of a single particle. The essential idea of the method which is due to L. Szilard, *Z. Physik* **32**, 735 (1925), is quite out of line with the usual techniques of statistical mechanics. However, as shown by B. Mandelbrot, *IRE Trans. on Inform. Theory* **IT-2**, 190, (1956); *Ann. Math. Stat.* **33**, 1021 (1962), it can be considered as an instance of standard procedures of mathematical statistics.

<sup>40</sup> This is a slight modification of terminology introduced by A. I. Khinchin, *Mathematical Foundations of Statistical Mechanics*, translated by G. Gamow (Dover Publications, New York, 1949).

The measurement of the  $\bar{x}_k$  as a function of the  $\pi_k$  allows us to arrive, through integration, at the f.e.

This procedure leaves an integration constant in the entropy undetermined. This constant is far from irrelevant and its handling warrants a brief comment. The determination of the constant by the use of Nernst's law ( $\lim S = 0$  for  $T \rightarrow 0$ ) is objectionable because one cannot be sure (i) whether the temperature is low enough for the entropy to vanish, and (ii) whether the system is actually in equilibrium. The correct procedure is to calculate the entropy constant in the ideal gas (low density) limit with the help of QS. If the results of this very reliable calculation are combined with the experimental values of the specific heat one obtains  $S(T_0)$ , where  $T_0$  is lowest temperature actually reached. If this value is practically zero, we have a positive proof that equilibrium is established. Otherwise, one of the conditions (i) or (ii) is not satisfied and the case requires further study.<sup>41</sup>

We turn now to the experimental situation listed under (B). It was recently recognized by Mandelbrot<sup>39</sup> that the inversion of the conventional probabilistic problem (A) has an interesting physical interpretation. Suppose we make a finite number of measurements of the random variable  $X_k$ , say, the energy. We may use this information to arrive at a guess concerning the parameters  $\pi_k$ , in particular, the temperature of the reservoir with which the system has been in contact before the measurement of its energy. This, Mandelbrot points out, is precisely the problem of thermometry. Although one usually measures some convenient thermometric property, this is easily calibrated in terms of the

<sup>41</sup> Although the procedure outlined above is well known, the meaning of Nernst's law as an essential ingredient for the operational definition of equilibrium does not seem to be generally appreciated. In fact, the third law has been the subject of an extensive discussion which may have been complicated by a semantic ambiguity surrounding the term "absolute entropy." On the one hand, the entropy is "absolute," in the sense that it involves the *entropy constant* provided by quantum statistics and not only the empirical *entropy differences*. On the other hand, the entropy is *relative* to the choice of independent components. Far from causing difficulties, this circumstance renders the use of the entropy concept particularly effective in providing subtle structural information about the level of equilibrium, whether it is extended to the distribution of spins, isotopes, molecular orientation, and the like. See F. Simon, *Ergeb. exak. Naturw.* **9**, 222 (1930); L. Pauling, *J. Am. Chem. Soc.* **57**, 2680 (1935); K. Clusius, L. Popp, and A. Frank, *Physica* **4**, 1105 (1937); J. O. Clayton and W. F. Giaque, *J. Am. Chem. Soc.* **54**, 2610 (1932); F. E. Simon, "40th Guthrie Lecture," in *Year Book of the Physical Society, 1956* (The Physical Society, London, 1957). Of course, an exclusively macroscopic thermodynamics can deal only with entropy differences. However, such a theory has to accept the awkward fact that its basic concept, equilibrium, cannot be put on an operational basis—an impressive case to show that a theory such as MTE calls for a deeper theory to solve some of its main problems.



energy. We note that this formal conception of thermometry covers also those striking instances of "measurements" in which, say, the composition of fossils is used to infer the temperature of the ocean in early geological times.<sup>42</sup>

From the formal point of view, the inference from an observed value of a random variable to the parameter of the d.f. is a problem of parameter estimation which is dealt with in mathematical statistics, sometimes called also *retrodiction*.<sup>43</sup> It is a standard technique in the evaluation of experiments and will prove to be an essential ingredient of a realistic theory of measurement. The suggestion that the methods of mathematical statistics be used within the context of basic theory might produce at first blush some apprehension. The inversion of probability calculus is by no means as unique as, say, the inversion of differentiation. Hence, the problem of retrodiction is beset by ambiguities and disputes, involving not only the choice of mathematical techniques, but also methodological difficulties centering around the nature of induction. We hasten to point out that the uses that we wish to make of estimation theory are not affected by these difficulties. In fact, our analysis of situation (C) will lead to a considerable clarification of the problem of induction.

Meanwhile we return to the problem of the estimation of the intensities, as it arises, for instance, in thermometry. The formal aspects of this problem are very simple. It is satisfactory for our purposes to consider a single method that is plausible enough on its own right without requiring for its justification the technicalities of mathematical statistics and that yields an intuitive interpretation of known formulas of statistical mechanics. At the same time, as Mandelbrot points out, this method is a standard one in mathematical statistics and is called the *maximization of likelihood*.<sup>44</sup>

Suppose that in a single measurement the free variables  $X_k$  of a system ( $x_\lambda$ ) are observed to have the values  $x_k$ . (For instance, in the case of thermometry the energy  $U$  of the small system, the thermometer, is found to have the value  $u$ .) We define the estimate  $\hat{\pi}_k$  of the unknown intensities  $\pi_k$  by the requirement that this choice should maximize

the probability of the event that has been actually measured, namely, that the variables  $X_k$  of the system exhibit the values  $x_k$ . This is achieved by maximizing the logarithm of the probability (10) with respect to  $\pi_k$ . The expression  $\ln dF$ , taken as a function of the  $\pi_k$ , is usually called the *likelihood function*. This term is meant to be reminiscent of "probability" without implying that (4.10) is, in the technical sense, a probability for the parameters  $\pi_k$ . For such an assertion there is no basis and  $dF$  need not even be normalizable in the  $\pi_k$ .

We see from (4.10) and (4.14) that the maximization of the likelihood function is equivalent to the minimization of the random entropy  $s(\pi_k, x_k)$  with respect to  $\pi_k$ . Hence,

$$[\partial s(\pi_k, x_k)/\partial \pi_k]_{\pi_k = \hat{\pi}_k} = 0 \quad (4.16)$$

or

$$-(\partial \ln Z/\partial \pi_k)_{\pi_k = \hat{\pi}_k} = x_k. \quad (4.16a)$$

The left-hand side of this equation is the average  $\bar{x}_k$  computed with the canonical d.f. belonging to the intensities  $\hat{\pi}_k$ . This result is eminently plausible. We select those values  $\hat{\pi}_k$  which produce a canonical d.f., with the average  $\bar{x}_k(\hat{\pi}_k)$  being equal to the single observed value  $x_k$ . This procedure leads to consistent results if the observation is the average of a finite number of measurements.

The extremal value of the likelihood is a maximum, the quadratic form, with the matrix elements

$$\frac{\partial^2 s}{\partial \pi_i \partial \pi_k} = -\frac{\partial \bar{x}_i}{\partial \pi_k} \quad (4.17)$$

evaluated for the estimated intensity values  $\hat{\pi}_k$ , is positive definite. It can be shown that this condition is identical to the condition of thermostatic stability in MTE.

We define now the "estimated entropy"

$$\hat{s}(x_k) = \min (\ln Z + \sum \pi_k x_k) \quad (4.18)$$

and obtain from (4.14), (4.16), and (4.17)

$$\partial \hat{s}/\partial x_k = \pi_k. \quad (4.19)$$

It can be shown that (4.18) and (4.19) form the basis of a complete formalism of MTE which is an alternative to (4.14) and (4.15). Moreover, the functional form of  $\hat{s}(\bar{x}_k)$  is the same as that of  $\hat{s}(x_k)$ .

Relation (18) has been used to great advantage by Fowler<sup>45</sup> and Khinchin.<sup>40</sup> But the formal relation gains an intuitive interpretation as a maximization of likelihood.

We see now that the transition from MTE to the

<sup>42</sup> H. C. Urey, H. A. Lowenstam, S. Epstein, and C. R. McKinney, *Bull. Geol. Soc. Am.* **62**, 399 (1951); S. Epstein, R. Buschbaum, H. A. Lowenstam, and H. C. Urey, *ibid.* **64**, 1315 (1953).

<sup>43</sup> This term was used by S. Watanabe, *Rev. Mod. Phys.* **27**, 179 (1955), however, in a sense that is essentially different from the above interpretation: Present observations are used to retrodict past observations.

<sup>44</sup> R. A. Fisher, *Phil. Trans. Roy. Soc.* **222**, 309 (1921); R. A. Fisher, *Contributions to Mathematical Statistics*, (J. Wiley & Sons, Inc., New York, 1950).

<sup>45</sup> R. H. Fowler, *Statistical Mechanics* (Cambridge University Press, New York, 1936).

dominant STE is remarkably simple. The f.e. and the resulting formalism remain valid, but there is a change in the conceptual interpretation. More precisely, we have two conceptual interpretations corresponding to the basic experimental situations (A) and (B). In the first case we have an ensemble with definite intensities  $\pi_k$  and canonically distributed  $x_k$ . In the second case we have  $X_k$  fixed and estimated intensities  $\hat{\pi}_k$ . When Boltzmann's constant goes to zero (or Avogadro's number to infinity) the two versions of the f.e. degenerate into the single f.e. of MTE. We have  $\bar{x}_k = X_k$  and  $\pi_k = \hat{\pi}_k$ . Moreover the requirement for the maximization of likelihood provides an intuitive interpretation for the basic extremum postulate of MTE.

We turn now to the third experimental situation listed above under (C), in which we attempt to identify an object specified in terms of its fixed variables  $x_\lambda$ , assuming that the response  $x_k$  in the known environment  $R(\pi_k)$  has been measured. In this wording the problem greatly exceeds the scope of the formula (4.10) and it is in this wider sense that we shall discuss it. We are confronted with the "problem of object" that is of great practical importance for every experimental science. Nevertheless, one might doubt the wisdom of injecting it into basic theoretical physics, and indeed, this has not been done up to the present time. The point is that there is no satisfactory method for estimating the nature of an object from its observed responses without prior knowledge of the possible set of objects available for selection. In practice, such prior taxonomical information on possible objects is available by induction from past experience. However, neither the justification of induction nor an insight into its limitation was provided by classical physics. Attempts at discussing this problem within the classical context were abstruse and devoid of interesting results. The whole question gradually lost respectability and it seemed to have escaped notice that the solution of the problem of the existence and observability of definite objects is implicit in the practical procedures of quantum physics. We shall attempt to identify and to formulate explicitly the conceptual aspects of the theory that are responsible for this success. We note that this view is the opposite of the accepted opinion according to which the concept of *object* "breaks down" in QM.

The scope of quantum physics is extremely wide. In keeping with our program of logical differentiation we ought to subdivide the field into precisely formulated deductive systems. However, this we are not yet prepared to do. Instead, we shall start by con-

sidering at first a restricted and well-understood part of the theory and proceed by introducing additional conceptual elements.

The simplest part of quantum physics that serves as our point of departure deals with the discrete stationary states of stable structures of particles only. We shall refer to this theory briefly as QS. This symbol can be read also as "quantum statics" and should remind one of "thermostatistics" rather than of "mechanical statics." In fact, QS can be conceived as the deepening of STE. The concept of "time" plays a similar, and somewhat rudimentary role in both of these theories. We shall consider the generalizations of QS that involve the concept of time in a more elaborate manner in Sec. IV.D.

We shall list now the features of QS that are essential for our argument.

(i) QS is a theory of objects, or structures, constructed of distinct classes of identical particles. Within the domain of molecular and low-energy nuclear chemistry (with the exclusion of  $\beta$  decay), we have only the three classes of electrons, protons, and neutrons.

(ii) Both particles and their structures are capable of existing in *pure states* represented by state vectors in Hilbert space, or wave functions specified by a set of quantum numbers. The pure states represent *potential* forms for the existence of objects. If such a state *actually* exists, we say the state is occupied, or realized. *The realizations of the same pure state* in different regions of space time form a class of absolutely identical objects.

(iii) Changes in occupation are called *transitions*, in the course of which a formerly occupied state is *annihilated* while another one is *created*. Transitions give rise to observable effects, the calculation of which belongs into the time-dependent theory. However, we anticipate that the predictions of observable effects are of a statistical nature, and that the probabilities of the random variables which constitute the measured signal depend parametrically on the quantum numbers of the initial and the final states.

(iv) The time-independent Schrödinger equation allows one to compute all pure states that can be constructed from a given assembly of particles.

(v) Sets of pure states provide so-called mixtures that can be identified with the ensembles of STE and hence with the equilibrium states of the systems of MTE.

Item (v) is parallel to the similar situation in statistical mechanics, provided that the pure states are considered as the analogies of the points of  $\Gamma$  phase space. However, here the similarity ends, since

items (i) through (iv) are entirely without classical analog. These are precisely the features that allow us to put the problem of object on a new firm foundation.

From the philosophical point of view item (iv) is of the greatest interest. It means that, in principle, all of the pure states of structures built from a given set of particles can be computed on theoretical grounds without any recourse to experiment! Whenever this calculation has been actually carried out, the results have been verified by experiment to a high accuracy. There are undoubtedly huge classes of cases in which the same agreement could be achieved, provided that one overcomes the mathematical difficulties that increase enormously with the complexity of the systems. We may at this point leave open the question whether or not the scope of QS extends to systems of all degrees of complexity.

Although the calculation of the properties of pure states by exclusively theoretical means is of the greatest interest, it is no less important from the practical point of view that the taxonomical task of listing and specifying the set of pure states can be undertaken by judicious combination of theory and experiment. In fact, we state: *The retrodiction of the discrete quantum numbers specifying pure states from the statistical evaluation of actual signals can be carried out in principle, and very often in practice, with absolute certainty.*

The feasibility of this task hinges on items (i) through (iii). In the first place, the fact that different representatives of the same pure state are absolutely identical allows us to repeat the "same" experiment an unlimited number of times. [Items (i) and (ii).] Therefore, the statistics of the observed signal [item (iii)] can be made sufficiently good to resolve the predictions corresponding to different discrete values of the parameters to be estimated.

An example is the spectroscopy of a system emitting a line spectrum. Many emission processes take place between the "same" initial and final states and yield the "same" emission within the limits of the line width. The selection rules, particularly in a magnetic field (Zeeman effect) enable one to analyze the experimental data to yield the quantum numbers of the atomic states.

In spectroscopy the statistical element of the procedure plays a somewhat subordinate role. Therefore, we mention another case, although it is, strictly speaking, outside the scope of QS and should be taken up only in the next section; the problem of determining the spin, or some other discrete intrinsic property of a particle from scattering experiments. The tenta-

tive assumptions of different discrete spin values lead to different theoretical predictions of an observable signal, say, the angular distribution of scattering. Since the "same" experiment can be repeated an indefinite number of times on identical replicas of the same class, it is, in general, possible to resolve the different predictions and eliminate all but one of the competing possibilities.

It is interesting to compare these considerations with the well-known Bohr-Heisenberg theory of measurement<sup>46</sup> which insists that the space-time specification required by  $\text{CMP}(\mu)$  cannot be achieved even under ideal conditions in the total absence of noise, and is limited by the uncertainty principle. In this context the term "measurement" is not supposed to refer to real measurements, but constitutes an ingenious conceptual device to clarify the limitations of mechanical models. These considerations are indispensable whenever such models are used, either for heuristic purposes or for the intuitive visualization of a situation.

In contrast, the present reasoning proposes to sort out the factors that brought about the extension of actual experimentation in the microscopic domain. The performance even of qualitative experiments is remarkable in view of the fact that this was held to be impossible as recently as the beginning of this century. This pessimistic forecast was by no means unreasonable from the point of view of classical continuum physics.<sup>47</sup> The factors that allow us to make error-free retrodiction from noisy measurements are precisely those discontinuous features of quantum physics that have no classical analog and that appeared disruptive within the fabric of continuum physics.

The essential point is the discovery of the concept of *absolute identity* of different replicas realizing the same *pure state*. This is in strong contrast with the concept of identity in common experience. Macroscopic objects are never exactly identical. However, we accept two objects as "identical" in a vague sort of way if we cannot discern any difference between them, or if their differences are within specifications. Hence the "identity" of common experience is a concept that is only meaningful relative to the precision of measurement or to conventional specification. Alleging the identity of two objects within

<sup>46</sup> Niels Bohr, *Atomic Theory and the Description of Nature*, (Cambridge University Press, New York, 1934).

<sup>47</sup> If the apparent continuity of the laws governing the behavior of macroscopic objects would extend to the microscopic domain, we could infer nothing about the properties of single atoms by coupling them to macroscopic measuring devices.

continuum physics would seem merely to admit one's inability to discern the existing differences.

We may sum up the situation by saying that QS contains rigorous results of a taxonomical character concerning the existence of classes and their properties which are entirely foreign to classical physics. Remembering from Sec. II that dominant systems have their characteristic invariance property, we say that the absolute identity of any realization of the same pure state is the dominant invariance of QS, to be referred to as *morphic invariance*. It is the morphic invariance that brings it about that complex systems of well-defined identity can be built in nature through the mechanism of random processes.

Up to this point we have referred to the quantum numbers only as identifying tags. We now give a short summary of their physical meaning. The first step in describing a finite stable structure is the establishment of an orthogonal set of energy eigenstates. If macroscopic translation is separated off, this spectrum is discrete, and falls within our definition of QS. The knowledge of the number of states  $g_i$ , having the energy eigenvalue  $E_i$ , provides us with the structure function and leads to the general formalism of STE.

The actual calculation of  $g_i$  is based on a specification of the additional quantum numbers. First we consider the quantum numbers associated with the total angular momentum and one of its components. The dynamic interpretation suggested by this designation establishes a connection with CMP. It is important to realize however, that these quantum numbers admit also an intuitive geometrical interpretation in terms of the shape of the wave function. The idea of this geometrical interpretation ties in with the "morphic" aspect of QS emphasized above. The geometrical representation of the shape of the wave function<sup>48</sup> is more realistic and is also a more intuitive picture of stationary atomic states than the historically motivated tracing of planetary orbits.

The morphic effects associated with angular momentum are geometrically represented in terms of the spherical harmonics. The same functions arise also in the classical vibration of macroscopic objects. It should be emphasized, therefore, that morphic invariance does not extend to macroscopic vibration. The difference becomes evident in terms of the radial functions. In the case of the hydrogen atom the scale of the radial function, say, the location of its first maximum, is expressed in terms of universal con-

stants; it constitutes a significant scientific statement concerning the class of all hydrogen atoms. In contrast, the scale of the radial wave function of a macroscopic object specifies only one individual object, it is not a significant scientific statement.

The importance of the morphic interpretation of the angular momentum is further underlined by the existence of such nonclassical integrals as parity and statistics,<sup>49</sup> which have no classical dynamic analog, but which admit a morphic interpretation in a fashion quite similar to angular momentum.

Finally, we turn to the discussion of the parameters that specify the configurations of molecules. The last term is meant here in a generic sense, it includes macromolecules and macroscopic objects also. These parameters specifying configuration are often accepted as classical ones, since they can be visualized in terms of localized potentials. However, these potentials have a phenomenological character (PhCM of Sec. IV.B) and cannot be classified among the dynamical integrals of CMP( $\mu$ ). We claim that the parameters describing localization are expressions of the morphic aspects of QS on a molecular and macroscopic level. In fact, the quantum effects involved in these discussions can become quite subtle and are still incompletely understood in some marginal, but presumably not unimportant, cases.

The problem of molecular configurations was first solved in great generality by Born and Oppenheimer,<sup>50</sup> who initiated the method usually referred to as the adiabatic approximation. Consider an assembly of electrons and invariant nuclei. The Schrödinger equation of the system is derived, as usual, from the Hamiltonian; we shall call it more specifically the *particle Hamiltonian*, a function of the coordinates and momenta of the particles:

$$H = T_n + T_e + V(x, X), \quad (4.20)$$

where  $T_n$  and  $T_e$  are the nuclear and the electronic kinetic energy, and  $V$  the total potential energy;  $x$  and  $X$  represent all of the electronic and nuclear coordinates, respectively.

The method exploits the large mass ratio of nuclei

<sup>49</sup> The term "statistics" is a misnomer. It would be more logical to say that bosons and fermions have an even and odd *permutational parity*, respectively, thus emphasizing the obvious analogy with the conventional *inversion parity*, a symmetry property. To be sure, permutational parity affects the statistical properties of many-particle systems. However, this effect is largest at absolute zero where the system is in a single state and there is no statistical situation in the proper sense of the word. The distinction between even and odd permutational parity disappears in the high-temperature, low-density limit, where the important effect is statistics.

<sup>50</sup> M. Born and J. R. Oppenheimer, *Ann. Physik* **84**, 457 (1927).

<sup>48</sup> H. E. White, *Introduction to Atomic Spectra* (McGraw-Hill Book Company, Inc., New York, 1934), pp. 143 and 146.

and electrons. As a first step we solve the electronic problem at fixed nuclear positions. We can think of situation as being brought about by letting the nuclear masses tend to infinity implying that  $T_n$  tends to zero. The Schrödinger equation in this case is

$$(T_n + V)\phi(x, X) = W(X)\phi(x, X), \quad (4.21)$$

where the eigenvalue  $W$  and the eigenfunction  $\phi$  depend parametrically on the fixed nuclear configuration  $X$ . We confine our attention to the neighborhood of the configuration  $X^0$  for which the lowest eigenvalue has a stable minimum. Further, we assume that in this neighborhood the lowest eigenvalue  $W^0(X^0)$  is nondegenerate.<sup>51</sup> We return to the justification and limitation of this assumption below.

The solutions of the original problem of finite nuclear masses is sought in the form

$$H\phi(x, X)\psi_n(X) = E_n\phi(x, X)\psi_n(X), \quad (4.22)$$

where the eigenfunctions  $\psi_n$  of the nuclear motion satisfy to a good approximation the equation

$$\mathcal{H}\psi_n = E_n\psi_n \quad (4.23)$$

with

$$\mathcal{H} = T_n + W^0(X). \quad (4.24)$$

Evidently (23) has the form of a Schrödinger equation for the nuclear motion alone. The electrons that convey the binding appear only implicitly in the "potential"  $W^0(X)$ . We shall refer to  $\mathcal{H}$  as the quasi-Hamiltonian. In spite of its formal analogy with the particle Hamiltonian  $H$ , there are differences that are fundamental for the present argument. Although the transition from  $H$  to  $\mathcal{H}$  involve a number of approximations, a matter to which we shall return, it would be nevertheless misleading to conceive of this transition merely as the substitution of a rigorous formalism by an approximate one. Instead, we propose to think of the procedure as<sup>52</sup> a transformation between formalisms of different types. While the particle Hamiltonian is firmly rooted in mechanics, the quasi-Hamiltonian has direct ties with the thermodynamic description of the system.<sup>53</sup>  $H$  is a mechanical concept inherited from CMP, it is ex-

pressed in terms of the coordinates of all of the particles. This is no longer true of  $\mathcal{H}$ . Not only have the electronic coordinates been eliminated, but the nuclear coordinates appear in such collective terms as Eulerian angles and normal coordinates of the vibration around an equilibrium. The existence of an equilibrium configuration brings it about that  $\mathcal{H}$  has geometrical symmetries; a point group for molecules and a space group for crystals, whereas the particle Hamiltonian has only the permutational symmetry, if we ignore the translation and rotation of the system as a whole. A single-particle Hamiltonian may generate a huge number of quasi-Hamiltonians. Consider, say, an assembly of a large number of carbon and hydrogen atoms. There are thousands of ways of combining these into molecules, each of which is described by its own quasi-Hamiltonian. It is the Schrödinger equation based on  $\mathcal{H}$  that leads to the relevant structure function and to the fundamental equation of STE and MTE. In particular, the configurational symmetry of the quasi-Hamiltonian is essential for the derivation of the phase rules.<sup>2</sup>

A final statement to round out the usefulness of the adiabatic method is that the quasi-Hamiltonian and its energy spectrum can be empirically determined from spectroscopic data.

We turn now to a critical discussion of our assumption that the lowest electronic state associated with equilibrium configuration  $X^0$  is nondegenerate. A systematic reason for degeneracy would arise only for symmetric configurations. However, the Jahn-Teller theorem<sup>54</sup> assures us that degenerate states of nonlinear polyatomic molecules are unstable with respect to deformation of the symmetric configuration that removes the degeneracy. For this reason, the assumption of the absence of degeneracy in the adiabatic approximation would seem to be generally justified. There are nevertheless exceptional situations that require an essential deepening of the theory. It may happen that an unstable symmetric configuration splits into, say, two configurations of lower symmetry which are separated only by a potential barrier that is sufficiently low to permit a quantum-mechanical resonance between these states. Thus we are led to the entirely novel situation of having a resonance between two quasi-Hamiltonians, the so-called dynamic Jahn-Teller effect.<sup>55</sup> Even though the

<sup>51</sup> We exclude even an approximate degeneracy, i.e., the lowest excited level  $W'(X)$  should be much higher than the nuclear energies  $E_n$  of (4.22).

<sup>52</sup> The existence of spin casts doubt on the point of view that would consider the Schrödinger equation derived from (4.20) as the absolutely correct statement of the problem. The correct account of the spin requires a relativistic treatment, and it would seem to be impossible to keep out the complications of relativistic field theory.

<sup>53</sup> In Sec. IV.A we formulated the program of finding the

qualitative differences between the mechanical and the thermodynamic viewpoints. A partial answer to this question is implicit in the relation of  $H$  and  $\mathcal{H}$ .

<sup>54</sup> H. A. Jahn and E. Teller, Proc. Roy. Soc. (London) **A164** 117 (1938).

<sup>55</sup> See W. Moffitt and A. D. Liehr, Phys. Rev. **106**, 1195 (1957); W. Moffitt and W. Thorson, *ibid.* **108**, 1251 (1957);

occurrence of this phenomenon is rather exceptional, it indicates that the existence of the quasi-Hamiltonian (4.24), and the corresponding Schrödinger equation for nuclear motion must not be taken for granted.

#### D. Dynamics of Structures

The "static" theories MTE, STE, and QS that deal with problems of structure have their "dynamic," or "kinetic" counterparts MTD, STD, and QD. In the block diagram (Fig. 1) the symbols of these systems are in broken rectangles to indicate that they are still essentially incomplete. In particular, QD is supposed to be a dominant theory in which the conceptual aspects of QS and of RM are brought in harmony with each other. The value of the present method will be ultimately judged by its success, or the lack of it, in bringing about such a dominant theory. Meanwhile we shall merely sketch a few ideas that can be discussed at the present status of the theory.

It is indicative of the difficulties of the dynamics of structures that even the traditional dichotomy between statics and dynamics is an oversimplification. The static theories have significant temporal aspects and the transition to dynamics requires a number of distinct steps, each of which leads to a deepening of the existing theories. The eventual situation will be presumably analogous to, even though more complicated than, the logical fine structure of CED represented in Fig. 2. Mechanistic analogies are of little help in disentangling this situation. In the first place, CMP has no significant static limit, since time-independent conditions can be maintained only in the trivial case of systems consisting of noninteracting particles.<sup>56</sup> Second, the concept of time in CMP plays the same standard role in all conceivable problems, a deceptive simplicity that is in strong contrast with the multiplicity of roles played by the concept of time in thermodynamics and quantum mechanics. We shall occasionally refer to these theories by the generic name *quantum thermodynamics*. This term is to denote a whole cluster of deductive systems, the most important of which are still in-

complete. The diversity of the temporal processes in these theories leads to a greatly increased flexibility in the representation of reality, the ramifications of which are far from being fully explored.

We shall concentrate on two closely related issues and emphasize a duality that is characteristic of quantum thermodynamics and is in contrast with mechanistic monism. This means that we claim an independent status for pairs of concepts when the mechanistic philosophy calls for a reduction of one to the other. The first duality is that of two principles of causality, while the second contrasts energetic and entropic processes.

The great predictive success of CMP and of CED has led to the conviction that all causal chains in nature are accounted for by differential equations and rely on the *complete specification* of the initial state of the system. Actually in thermodynamics we encounter another situation in which causal chains are determined by a *selective* specification of the initial conditions. We shall speak of a *second principle of causality* based on *selective memory*, that is to be distinguished from the *first principle of causality* based on *exhaustive memory*.<sup>57</sup>

As a convenient point of departure we consider the composite systems of MTE. We have seen in Sec. IV.C that the concept of thermodynamic operations, followed by entropic processes triggered by these operations, implicitly contains an element of temporal sequence. Such sequences can be repeated to form what we shall call *composite (entropic) processes*. Due to the fact that the principle of thermostatic determinism assures us of the uniqueness of the final state of each step, the entire composite process assumes a deterministic character, provided that the operations are preset by some automatic device. Alternatively, if the operations are governed by the terminal states through feedback, the composite process becomes goal directed. Of course, while composite processes consist of temporally ordered sequences, they lack a definite time scale as long as one is confined to using MTE. An important step toward providing a time scale is achieved in MTD in which the approach to equilibrium appears as a relaxation process characterized by definite relaxation times. However, in a purely macroscopic theory the completion of a relaxation process requires an infinite amount of time. This

H. C. Longuet-Higgins and K. L. McEwen, J. Chem. Phys. 26, 719 (1957); H. C. Longuet-Higgins, U. Opik, M. H. L. Pryce, and R. A. Sack, Proc. Roy. Soc. (London) A244, 1 (1958); A. D. Pierce, "Electron Lattice Interaction and Generalized Born-Oppenheimer Approximation," Ph.D. Thesis Massachusetts Institute of Technology, January 1962 (unpublished).

<sup>56</sup> This statement is not inconsistent with the existence of mechanical statics but points once more to the semantic confusion surrounding the term "mechanics." The statics in question belongs to PhCM rather than to CMP (see Sec. IV.B).

<sup>57</sup> This terminology would be ambiguous in the case of the systems with "real" memory, that is, for computers and organisms. These have been, of course, tacitly excluded thus far, but we shall briefly discuss them in the next section.

difficulty is finally removed in STD. In this theory equilibrium includes thermal noise and a process terminates in a finite stretch of time as the static equilibrium is approached within the average noise level.

The composite entropic processes provide examples for the second principle of causality and we shall describe in some detail the distinction between selective and exhaustive memory. The first aspect of selectivity is that a system may be coupled to its environment by the exchange of energy and matter, and yet it suffices to specify the environment in terms of a few intensity parameters. This specification is adequate to determine the effect of the environment on the state of the system, although it would have to be enormously increased to satisfy mechanical requirements according to CMP( $\mu$ ) or even QM. However, this additional detail is irrelevant in the sense that it has no effect on the observed behavior of the system. The second aspect of selectivity is that the variables of the system are classified into free and fixed variables. Simple as this idea is, it is highly nonmechanical, since in CMP( $\mu$ ) the energy of an isolated system in rest is the only invariant, apart from the particles the invariance of which has been postulated. The role of the fixed variables is to identify the system. In particular, the fixed variables along with the intensities of the environment determine the probability distribution function of the free variables. If some of the constraints imposed on the system are relaxed, the entropic process triggered by this operation brings about the loss of the memory of the formerly fixed variables. This loss of memory is a prerequisite for the uniqueness of the final equilibrium.

Whereas the first two aspects of selectivity emphasize the constructive role of "forgetting," the third aspect deals with the *persistence* of the values of the fixed variables. We emphasize that the actual preservation of the fixed variables under realistic "noisy" conditions, as a result of quantum-mechanical stability, is physically meaningful. This is in contrast with the exhaustive but fragile memory of the initial state in CMP( $\mu$ ) that is so often erased by the slightest perturbation and is denied physical meaning by the principle of regularity. It takes only some reflection to realize that the existence of identifiable objects, which respond in a predictable fashion under "identical" conditions, depends on the second principle of causality; the object is permanent within its lifetime and the conditions are identical only because the relevant specification is selective.

We are now in a position to clarify the relation of

causality and determinism. In common parlance these terms suggest different meanings, and indeed we can provide distinct interpretations for them in the thermodynamic theory. The choice of thermodynamic operations that govern the composite process may, or may not, depend on our decision, and accordingly we may speak either of causal or deterministic chains of events. The former would arise in experiments, the latter, say, in the astronomical setting, or in the evolution of an organism determined by the genetic code. Of course, the delimitation of the two situations is by no means fixed, but shifts with the advances of experimental techniques.

In order to complete the description of real situations, we have to supplement entropic composite processes with energetic ones. Since unbalanced forces produce accelerations, these processes can be treated in MTE or STE only in the limiting case for which the accelerations are negligible. It is interesting that entropic processes are not subject to such a restriction, their treatment is perfectly germane to the equilibrium theories.<sup>58</sup> As soon as accelerations are admitted, we have to use a dynamic theory. The problem is complicated by the fact that energetic processes are almost always tied up with entropic processes, and it is, in fact, the interplay of the two that is our main concern in the present context. This problem presents itself in the sharpest form within quantum mechanics and this is the only approach that we wish to consider here.<sup>59</sup>

In quantum mechanics energetic processes are described in terms of the time-dependent Schrödinger equation that implies the temporal evolution of the

<sup>58</sup> This is in contrast with the usual contention that thermostatics deals with reversible processes and irreversible thermodynamics with irreversible ones.

<sup>59</sup> A few parenthetical remarks concerning the role of energetic and entropic processes in MTE and STE are meant only to outline the meaning of some of our terms by linking them with traditional designations. The hydrodynamics of ideal fluids and the phenomenological theory of relaxation processes are limiting cases of MTD which deal with energetic and entropic processes, respectively. The theory of Markov chains is a limiting case of STD dealing with entropic processes. This is essentially an instance of mathematical probability theory in which the postulated probabilities for elementary events allow us to compute probabilities of complex events (that is, sets of chains of elementary events). There are many phenomenological theories, such as the hydrodynamics of viscous fluids and thermohydrodynamics, that deal with the joint effects of energetic and entropic processes. These theories are important from the practical point of view but provide little fundamental insight. A much more detailed description of the interplay of energetic and entropic processes for a particularly simple type of system is provided by the Boltzmann equation of the kinetic theory of gases. The achievement of this theory is somewhat obscured by the fact that, according to the tradition set by Boltzmann the aim is a rigorous derivation of this equation from Liouville's equation. In other words, in conformity with the mechanistic program one proposes to reduce entropic processes to energetic ones (Boltzmann's problem).



wave function in terms of a unitary transformation

$$\psi(t) = U(t - t_0)\psi(t_0). \quad (4.25)$$

The conservation of entropy appears as the unitary invariance of the number of dimensions of the subspaces of Hilbert space spanned by the state function or, more generally, by the density matrix. Another aspect of the entropy conservation is the maintenance of strict phase relations, a characteristic property of wave propagation in continuous media. Accordingly, we shall briefly refer to energetic processes as *propagations*. Of course, in the case of stationary states the phase does not propagate, but varies synchronously over all space.

We introduce now the concept of *events* to denote: (i) transitions between stationary discrete quantum states, (ii) interaction processes described in terms of the *S*-matrix formalism, including the events of high-energy physics. In all of these cases we have the same type of situation as in a chemical reaction.<sup>60</sup> An initially existing state disappears, whereas another state appears. This is described formally in terms of annihilation and creation operators. The difference between quantum events and chemical reactions is that the former are the elementary indivisible constituents out of which chemical reactions and, more generally, entropic processes, are constructed. Quantum events exhibit in a particularly clean-cut fashion the characteristic features (selective memory) of entropic processes that we have summed up under the designation of the second principle of causality. First, there is the peculiar persistency of quantum states. As long as the system is in a particular pure state, the corresponding quantum numbers have the character of fixed variables. Also the negative aspect of the selectivity of memory is very significant. A system in a pure state does not "remember" where it came from, nor the instant when the transition into the state occurred; pure states do not "age," although they have a definite lifetime. All of these factors are essential prerequisites of the morphic invariance of the pure state which, in turn, ensures error-free retrodiction, as we have already seen.

Events bring about a measure of randomization of the phase relations. The random aspect of events stems from the unpredictability of the instant at which an individual event is initiated. Otherwise, of course, events are by no means so unstructured as, say, the steps of the "random-walk" problem. Since their description consists in the specification of the initial and final states, events have their individual

characteristics just as the states involved have.

The instant of an event is in some respects analogous to the instant of an operation that triggers an entropic process, although without any subject or even a molecular device as a catalyst, to perform the operation. At the same time genuine operations involving manipulations of the boundary conditions also have their legitimate role in quantum mechanics. In particular, relaxation of an internal constraint in a composite system changes the basic set of eigenfunctions of the system. Therefore, even while the wave function is instantaneously unchanged, the result is the creation of a huge number of phase relations. Subsequently these are destroyed in a series of events that constantly interrupt the propagations. This is the mechanism by which the entropy increases.

It is obvious that both propagations and events are indispensable for a descriptive account of quantum phenomena, and both concepts are essential ingredients of the formalism. This is particularly evident in the perturbation expansion in which propagations and events appear intertwined. From the formal point of view, this technique can be considered as the generalization of the basic problem of mathematical probability theory. Again the probability of complex events is computed from that of elementary events. However, the theory operates in terms of probability amplitudes rather than in terms of probabilities. This conceptual shift is comparable to the one that is instrumental in effecting the transition from MTE to STE. Once more the theory is deepened, our probabilities are now capable of interference, in other words, stochastic events can be combined with propagations expressed in terms of differential equations. Whereas entropic processes cannot be joined to CMP without disrupting the formalism, energetic processes can be joined to this modified probability theory.

Potentially we have a most harmonious correspondence between theory and experiment. However, these potentialities are only incompletely realized in the existing presentations of quantum mechanics. There are two major reasons for this situation. First, there is the more or less accidental historical link between quantum mechanics and CMP( $\mu$ ) which induces us to assign a privileged status to propagations over events. The rule that requires the reduction of events to propagations has been transferred from CMP( $\mu$ ) to quantum mechanics, even though the reasons for this program that were imperative in the mechanistic scheme do not prevail in quantum thermodynamics. The fact that the rule is often

<sup>60</sup> A. Einstein, *Verhandl. deut. Physik Ges.* **16**, 820 (1914).



broken or circumvented does not reestablish logical clarity. The second, and deeper reason is that the theory in which events and propagations are freely compounded for the construction of complex events is, in spite of important achievements, still in an incomplete state. This is particularly true of that part of quantum thermodynamics which we have called QD in the block diagram. The present method of analysis enables us to dispose of the first of these difficulties and, by sorting out the elements of the situation, we hope to prepare the ground for attacking the second.

It is well known that the propagations (4.25) are insufficient to account for all of the coupling effects of quantum mechanics, and the processes of measurement have to be joined as independent conceptual entities, a point expressed with particular precision by von Neumann.<sup>61</sup> We claim that the present suggestion of supplementing propagations by events as irreducible primitive concepts is the generalization of the traditional view. The crucial point is that many events are measurable. Atomic physics became possible because of the discovery of a long line of devices, from scintillation counters to bubble chambers, that enable us to retrodict events from observed signals. However, events occur whether or not we observe them. Therefore, the supplementation of propagations cannot be relegated to a special class of studies devoted to the theory of measurement, but such additional elements have to be standard parts of the formalism. This point of view enables us to avoid some of the paradoxes that arise from the overemphasis of the subjective elements in the quantum formalism. As an example of this sort we consider, with von Neumann, the transformation of a pure state into a mixture of increased entropy because of the coupling with a measuring device. A typical apparatus would be a screen with a number of slits and a counting device in the path of the beam of particles. In our language, we consider the coupling with the measuring device a thermodynamic operation in which certain constraints are enforced.<sup>62</sup> In this procedure the splitting of the beam is a propagation, the absorption or scattering in the counter at a location corresponding to a particular split beam is an event in which one state is actualized to the exclusion of other potentialities.<sup>63</sup>

<sup>61</sup> J. von Neumann, *Mathematische Grundlagen der Quantenmechanik*, (Verlag Julius Springer, Berlin, 1932), Chap. V.

<sup>62</sup> Note that in systems in equilibrium considered in MTE the enforcement of a constraint produces no entropy increase. The present case is different, since we start from a pure state, a nonequilibrium situation.

<sup>63</sup> This collapse of the wave function is a standard occurrence and is the inevitable consequence of the fact that the

In the course of this process the assembly of particles making up the beam is transformed from a pure state into a mixture with a corresponding increase of entropy. We have said nothing, thus far, of measurement. However, if the events are observed and recorded, we have gained information, this gain can be considered as partially balancing the increase of entropy.<sup>64</sup> Thus measurement is associated with an increase of information, whereas the parallel increase in entropy takes place independently of any subjective act of measurement. We add that the typical entropy increases of MTE arise in the course of relaxations rather than of enforcement of constraints.

The suggested new relation between propagations and events raises a number of problems that have to be solved before the theory can be reconstructed along the lines indicated. A problem of paramount importance concerns the validity of the Schrödinger equation. In the traditional theory it is often taken for granted that the Schrödinger equation is entirely correct and contains all legitimate quantum-mechanical information about systems of any complexity.<sup>65</sup> How is this statement modified by the fact that events are accorded an independent status? We propose the tentative rule that the results deduced from the Schrödinger equation are correct whenever they satisfy the principle of regularity (see Sec. II). This principle infringes sufficiently on the validity of (4.25) to allow us to join entropic processes to the formalism without in any way impairing its consistency. We shall apply the principle of regularity to both of the abovementioned criteria of entropy conservation.

The most obvious infringement of the definiteness of results of (4.25) arises in case of degeneracy. Consider, for instance, a time-independent Hamiltonian. The eigenfunctions of this operator should be constant for eigenfunctions associated with nondegener-

wave function has a dual reference to classes and to individual systems. Events refer to an individual "choice" out of the set of possibilities determined by the evolution of the wave function of the class. This duality is foreshadowed in MTE, the formalism of which deals with the state of *normal* equilibrium to which an *actual* system may, or may not, conform. The widespread reluctance to make full use of the collapse of the wave function is sufficiently explained by the fact that this phenomenon seems paradoxical in terms of the classical framework of CMP and CED or if one attempts to interpret the Schrödinger equation as a classical wave equation.

<sup>64</sup> L. Szilard, *Z. Physik* **53**, 840 (1929); L. Brillouin, reference 10, Chap. 13.

<sup>65</sup> The attitude reflected in this assumption is obviously the same one that generated similarly sweeping claims for the formalism of CMP( $\mu$ ). It would be tempting to subject this claim to critical analysis that could center around the uncertainties in the choice of the appropriate Hamiltonian discussed at the end of Sec. IV.C. However, the line of thought pursued above is more constructive at this juncture.

ate eigenvalues. However, in the case of degeneracy this result is upset even by the smallest perturbation. Hence, the principle of regularity requires that the implications of the strictly deterministic conclusions of (4.25) should not be considered physically meaningful in this case. Thus there arises a gap that is filled by the random events resulting in entropic processes.

We consider now the entropy conservation of energetic processes in terms of the criterion of coherent phase relations. If Eq. (4.25) is taken seriously as an entirely rigorous description of the system, such coherent phase relations would extend over infinite space-time. In reality, however, coherence can be expected to prevail only in a finite space-time domain. In many simple problems involving, say, a single collision, this artificial extension of the range of coherence is a harmless idealization. Not so in composite processes, for which the extent of coherence is often significant and should not be summarily decided by postulate without specific examination. In composite systems, the interruption of coherence occurs at the walls constituting the cell boundaries. However, just as phase boundaries play the role of "natural" walls, it seems that wave functions corresponding to pure states have their "natural" space-time extension of coherence. Such intrinsically coherent units should become basic entities of the suggested theory. They are to be joined to each other either incoherently or coherently.

We turn now to the discussion of the well-known controversy between Einstein and Bohr<sup>5</sup> concerning the desirable and attainable features of quantum mechanics. The essence of this argument is the compatibility of causality with a complete space-time description of systems. Bohr emphasized the complementarity of the two descriptions, whereas Einstein held up CMP( $\mu$ ) and CED as ideal theories in which the two requirements are entirely compatible. Accordingly, the argument always turned around the point, whether or not quantum mechanics could be cast into a form that agrees more closely with the structure of the classical theory.

This argument has been deadlocked for a long time. We propose that the reason for this impasse is that both participants tacitly assumed that there is only one type of causality depending on the exhaustive specification of the initial conditions. In contrast, we have argued that most of the causal chains expressing the regularities in nature are of a second kind and are based on the selective specification of composite processes in composite systems. Although the quantum thermodynamics of these systems is still

to be developed in a systematic manner, there seems to be no incompatibility between the piecewise continuous space-time description of these systems and the existence of causal chains depending on selective specification. An exacting test for such a view is the development of theoretical constructs that are to represent the behavior of living organisms.

### E. Physics of Organisms

Living organisms exhibit complex morphological and functional properties that are very different from the properties of systems investigated in physics. Nevertheless, physics is supposed to have a fundamental character and it is a widely entertained hope that in some sense, still to be clarified, biology is reducible to physics. Let us assume that physics reaches a degree of development in which the principles governing the building of complex structures from elementary entities is well-enough understood. In this not unlikely situation we should be able to synthesize also the conceptual material that is necessary for the understanding of the properties of structures of increasing complexity. For nuclei, atoms, and molecules this has already been achieved to a not inconsiderable degree. According to the point of view that is optimistic with respect to the reducibility of biology, this gradual extension of our understanding need not stop at any sharp boundary separating inanimate and living objects. We may set aside the more speculative aspects of this question by appraising the scope and limitations of the reducibility program at three stages of development of the physics of structures: (i) mechanistic physics based on CMP( $\mu$ ), (ii) traditional quantum mechanics, and (iii) the quantum thermodynamics of composite systems outlined in Sec. IV.E.

The discussion based on CMP( $\mu$ ) is only of historical interest. The obvious failure of this discipline to account for anything resembling an organism produced a strong case for vitalism, a doctrine that postulates *ad hoc*, irreducible, vital forces to fill the gap left by mechanistic physics. This argument can now be dismissed as inconclusive, since not even phenomenological mechanics is "mechanistic" in this technical sense of the word (see Sec. IV.B). This state of affairs changed radically with the development of quantum mechanics and the subsequent clarification of chemical stability and reactivity. In the terminology of Sec. IV.C we may say that the morphic invariance of QS provides at least the prerequisites for the explanation of the morphological aspects of biology. If, in addition, we remember the recent spectacular advances of molecular biology it

seems hard to maintain an attitude that would hold any specific aspect of biology as out of bounds for physical-chemical investigations. At the same time, we are still far from a satisfactory solution of the reduction problems, the scope and limitations of which we shall attempt to spell out as follows. Reduction seems to proceed most satisfactorily with respect to problems "in the small," whereas it has not even started for problems "in the large." This contrast between the "atomistic" and "holistic" attitudes of physics and biology is well known, it is the real stumbling block of the reduction program. It is our contention that this inability to cope with problems of organization is only a property of mechanistic physics, rather than of physics in general. In particular, this limitation, still present in traditional quantum mechanics, stems from the historical link with  $CMP(\mu)$  (see Secs. IV.C and IV.D). While a huge amount of detail remains to be worked out, it seems that the quantum thermodynamics of composite systems has the necessary flexibility to account for the holistic problems of organisms.

We note that this theory incorporates a number of concepts that are evidently indispensable for any theory of organisms. We have the distinction between free and fixed variables, processes and operations; processes are controlled by fixed variables, whereas the fixed variables are changed by operations or parametric processes. The combination of processes and operations leads to the concept of composite processes and to the second principle of causality, which depend on selective specification of the initial conditions. In MTE one usually considers composite systems consisting of two subsystems. However, the complexity of composite systems can be increased in a variety of ways. The first step is to increase the number of subsystems, then, by appropriate connections, couplings may be introduced between any two of them, not necessarily adjacent in space. The result may be an entity with complex topological properties. The restrictivity of these connections may be regulated, just as chemical reactions are catalyzed, or poisoned. The system reaches a measure of autonomy if the entire control system is operated automatically by feedback from the environment and/or the state of the system. The second principle of causality ensures a mixed causal, stochastic response of the system. For systems of a certain complexity the code containing the instructions for its response may become rather complex and be in need of logical organization to ensure a reasonably unique operation. The logical structure of the block diagram

(Fig. 1) exhibits one possibility of a consistent organization of a complex logical structure in which potential inconsistencies among different sets of instructions are kept under control. A further step leading toward complexity is that composite systems are united into a supersystem. The coupling may involve the exchange of additive invariant and/or the exchange of information. All this can be repeated to yield a complicated hierarchy of structures.

Beyond a certain complexity the code of instructions plays the role of a rudimentary "mind." Moreover, the logical structure of this mind and the physical structure of the system attuned to each other for smooth functioning are expressions of a psychophysical parallelism.

Summing up, we may say that the basic problem of the physics of organism is to establish the connection between the built-in patterns of constraint and freedom on the one hand, and the functioning of the organism on the other. This concept of constraint and freedom is entirely foreign to  $CMP(\mu)$ , but is present in all aspects of quantum thermodynamics. In fact, these concepts are present even in PhCM. This is the conceptual basis of the fact that machines such as automata and computers can simulate certain functions of organisms. By providing standardized interchangeable parts, the makers of the machines imitate the morphic invariance of nature. This imitation can never reach the perfection of the original, and jamming and overheating certainly set a limit to the complexity of devices made out of macromechanical elements.

## V. PHILOSOPHICAL REFLECTIONS

The method of analysis of this paper is, I believe, in agreement with the spirit and the underlying goals of the philosophical school that is alternately called analytic, positivist, or empirical. I hope not to be too far off the mark in using these terms as synonyms.

The concepts of logical differentiation and integration arose within the examination of the language of physics, which is a legitimate pursuit in this school of thought.

A point of agreement is the close attention paid to empirical requirements; more specifically, the approach to quantum physics as described in Sec. IV is quite in line with the positivist program of developing the theory of the structure of matter in close parallel with experiment.

Moreover, the principle of regularity (Sec. II) is a methodological rule that serves as a safeguard against

taking theoretical systems more seriously than their empirical support warrants.

At the same time, the present paper and its implications are at variance with some of the current practices of positivism. The clarification of these issues can be achieved as a by-product of the present analysis.

Let us consider first the so-called *operational character* of the theoretical concepts. It goes without saying that the deductive systems of physics have to have a range of concordance with experience.

Yet, there is a growing awareness of the fact that there is something wrong, or at least lopsided, about the great emphasis on "operationalism" which for several decades has dominated empirical philosophy.

We could do hardly better than quote from Bridgman's<sup>66</sup> penetrating reappraisal of the early ideas of operationalism. "If I were writing the 'Logic' today I would change the emphasis so as to try to avoid what I regard as the one most serious misunderstanding. That is, I would emphasize more that the operations in terms of which a physical concept receives its meaning need not be, and as a matter of fact are not, exclusively the physical operations of the laboratory. The mistaken idea that the operations have to be physical or instrumental, combined with the dictum . . . , 'The concept is synonymous with the corresponding set of operations,' has in some cases led to disastrous misunderstanding. If I were writing, again I would try to emphasize more the importance of the mental or paper-and-pencil operations. Among the very most important of the mental operations are the verbal operations. These play a much greater role than I realized at the time. . . ."

The analytic definitions of the present approach are of course "paper-and-pencil" operations. Apart from being of equal importance with the instrumental operations, the two are related to each other in a well-structured manner. In the absence of precise analytic definitions the meaning of the instrumental operations cannot even be properly evaluated.

The operational point of view considered as a sole criterion would always favor the low-level abstractions. However, the most spectacular advances in theory are connected with the discovery of abstractions of a very high level.

The constructive aspect of operationalism is appreciated particularly in the process of logical integration. If we have two theoretical systems, both of them confirmed by experiment but inconsistent with

each other, we usually find that the inconsistencies are produced by nonoperational assumptions that can be dropped without losing the measure of experimental agreement already achieved. In fact, subsequent developments often result in an extraordinary expansion of the range of concordance.

This is what happened as CMP was generalized into the dominant RM. Einstein's operational analysis of the concept of simultaneity was a means to an end, it made the integration of CMP and CED possible. The concept of absolute simultaneity was abandoned because it blocked integration. The fact that it was not operational showed that this change in the foundation could be undertaken without damage.

However, "logical integration" has been, thus far, not in the vocabulary and the *purpose* of operationalism was not sufficiently appreciated. Erroneously it was taken for an end in itself, or, an ironical perversion of its real role, a means to forestall another "catastrophe" that would force us to re-examine our basic assumptions.

Although an occasional reappraisal of the foundations may seem a not entirely welcome interruption of the routine of research work, it is now recognized to be the unavoidable price to be paid for the continued use of new high-level abstractions. We again quote Bridgman: "To me now it seems incomprehensible that I should ever have thought it within my powers, or within the powers of the human race for that matter, to analyze so thoroughly the functioning of our thinking apparatus that I could confidently expect to exhaust the subject and eliminate the possibility of a bright new idea against which I would be defenseless."

We turn now to another difficulty of positivism, namely, its predominantly restrictive character which bids us to dismiss most problems of traditional philosophy as "meaningless." Granted that the traditional methods are lacking in precision, we are faced with the unhappy choice of dealing with significant problems in an unsatisfactory manner or bringing to bear a precise method on problems the wider import of which is not immediately apparent.

There are at least two ways of breaking this deadlock. One could make a case for applying less rigid standards in appraising intuitive methods, or to extend the scope of analytic philosophy to more significant problems. It is only the second path that will be followed up at this point.

In order to understand the origin of the restrictiveness of positivism, we have to go back to the beginnings of mechanistic physics. With the brilliant suc-

<sup>66</sup> P. W. Bridgman, *Daedalus* 88, 518 (1959).

cess of Newtonian mechanics, it seemed tempting to brush away the complex and eroded conceptual system of scholastic philosophy. The proposition of temporarily restricting oneself to the conceptual framework of the new mechanics seems entirely sound, even in retrospect. However, the contention that this conceptual framework would be satisfactory at all times was unwarranted, and turned out to be actually incorrect.

During the mechanistic era it became customary to dismiss types of questions that did not fit into mechanistic systems as unscientific.

As the crisis of classical physics revealed the limitation of the mechanistic conceptual scheme, the first inference was that the range of *legitimate scientific questions is even further limited*, since not even the mechanistic questions are admissible.

The pluralistic character of the present approach brings two new elements into this picture. In the first place, each deductive system implies a characteristic set of precise questions. The number of interesting questions that become "meaningful" is particu-

larly extensive in thermodynamics and quantum mechanics.

It is often stated that the concept of object breaks down in quantum mechanics. Actually, however, the opposite is true. As we have seen in Sec. IV, for the first time in QM we are in a position to give a formal representation of an object with many subtle ramifications and we can now solve the related philosophical puzzles that have been unresolved since their discovery by the Eleatic philosophers. It seems that the new object concept is flexible enough to include living organisms that are entirely outside the mechanistic scheme.

The extension of meaningful conceptual problems in the present context proceeds in still another dimension. Not only do we have the concepts within each deductive system, but the deductive systems themselves are conceptual entities of distinct individual characteristics related to each other in quite specific fashion. These entities are of a logical type that is markedly different from that of the primitive concepts within the deductive systems.

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