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AERODYNAMIC STUDIES: The Forces Acting On An Air Vehicle A Review of the Literature

M. Z. KRZYWOBLOCKI

INSTITUTE FOR SYSTEM RESEARCH THE UNIVERSITY OF CHICAGO

JANUARY 1959



WRIGHT AIR DEVELOPMENT CENTER



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AERODYNAMIC STUDIES:

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M. Z. KRZYWOBLOCKI

INSTITUTE FOR SYSTEM RESEARCH THE UNIVERSITY OF CHICAGO

JANUARY 1959

Aeronautical Research Laboratory Contract No. AF 33(616)-2797 Project 7060

WRIGHT AIR DEVELOPMENT CENTER AIR RESEARCH AND DEVELOPMENT COMMAND UNITED STATES AIR FORCE WRIGHT-PATTERSON AIR FORCE BASE, OHIO

FOREWORD

Contract AF 33(616)-5689, Project 7060, (unclassified title) "Scientific and Engineering Research Investigations in Flight Dynamics," effective 1 May 1958 between the United States Air Force and the University of Chicago provides for scientific and engineering research investigations in flight dynamics. The contract is monitored by Wright Air Development Center, Aeronautical Research Laboratory, Engineering Analysis Division, Lt. Col. Edwin H. Nowak, Chief, and Mr. Paul W. Nosker, Assistant Chief. The work at the University is conducted under the general jurisdiction of Dr. Warren C. Johnson, Vice President in Charge of Special Scientific Programs, and Dr. Francis E. Bothwell, Director of the Laboratories for Applied Sciences. The work under this contract is performed by the staff of the Institute for System Research under the supervision of Dr. B. E. Howard, Associate Director of the Institute for System Research.

Study 10, entitled "Aerodynamic Forces and Moments," under the above contract pertains to the determination of aerodynamic forces and moments that will be exerted on a given airframe under various flight conditions. Phase One of this study calls for regular review of the scientific and technical literature relating to this subject. Phase One is being conducted by Dr. M. Z. Krzywoblocki, professor of gasdynamics and theoretical aerodynamics at the University of Illinois, under a consulting agreement with the University of Chicago. It is a continuation of similar work begun in 1951 under Contract AF 33(038)-15068, Supplement No. 2, between the United States Air Force and the University of Chicago as part of the program of the Advisory Board on Simulation, and continued under Contract AF 33(616)-2797.

The earlier work by Dr. Krzywoblocki was published by the University of Chicago in two volumes and 12 supplements entitled: AERODYNAMIC STUDIES: The Forces Acting on an Air Vehicle--A Review of the Literature and a third volume entitled AERODYNAMIC STUDIES: Possible Trends in Fluid Dynamics. To meet the persistent demand for these earlier reports issued by the Advisory Board on Simulation, they are being reissued as individual parts of a WADC Technical Note under the present program in combination with those generated under the present contract and under Contract AF 33(616)-2797. Thus, the present portion, which was first issued by the Advisory Board on Simulation as Volume III of the Aerodynamic Studies, becomes Part XV of WADC TN 56-360. [Note: In order to minimize the cost of republishing these earlier reports and to hasten their availability, the ABS volumes are being reproduced with the least possible editorial and typographical changes. Consequently, certain differences and non-uniformities of style and make-up will be apparent between these earlier parts and those parts of the series generated under the present contract. Acknowledgement is due to the Technological Press of Massachusetts Institute of Technology and John Wiley and Sons, Inc., for permission to Dr. Krzywoblocki to present a condensation of Chapter II, Cybernetics, by Norbert Wiener, and to Interscience Publishers, Inc., for their similar kindness regarding the use of the material appearing in the first eight pages of Quantum Theory of Fields, by Gregor Wentzel.

This Technical Note is expected to be a continuing series, and as additional material which has significant bearing on the problems under consideration is reviewed it will be referenced in successive parts of WADC TN 56-360.

A discussion of the administrative history of the Advisory Board on Simulation and the purpose of the Air Force in sponsoring it, together with a roster of the eminent specialists from industry, government, and other universities who served on it, is to be found in the Foreword of Part I of this Technical

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Note and in the final report of the Advisory Board, published as WADC Technical Report 54-250, <u>Dynamic</u> <u>System Studies</u>. A survey of the literature dealing with the forces acting on air vehicles is one of the lines of investigation initiated by the Advisory Board.

In order to obtain the most effective aerial weapons in the shortest time at the least cost, it is necessary to employ dynamic systems engineering, a principal tool of which is simulation. Since the object of simulation is to predict or to reproduce in the laboratory the true behavior of air vehicles in flight, it is necessary either to physically simulate or to mathematically calculate all of the forces acting on various parts of an air vehicle and to combine them in some manner to determine the force on the vehicle as a whole.

Naturally, then, an understanding of the nature of the aerodynamic forces acting on an air vehicle is fundamental; to simulate the motion of the air vehicle it is necessary to be able to calculate the forces. Unhappily, the state of the art is such that exact mathematical expressions for the forces are not known. Aerodynamicists therefore rely on such tools as wind tunnels, and make use of a vast amount of empirical data

The ultimate goal of exact expressions for those forces involves theoretical investigations outside the scope of the Advisory Board's initial study. Nevertheless, the planning of a simulation facility demanded practical answers to the following questions: (1) What are the most general and most reliable expressions used today for the aerodynamic forces on air vehicles? (2) What are the fundamental hypotheses behind these expressions and the limitations inherent in them? (3) What are the boundaries of accuracy for calculating forces by present methods? (4) In what areas and in what directions can significant advances in understanding aerodynamic forces be expected in the immediate future? (5) In what areas are the problems of such a profound nature that significant advances cannot be expected in the foreseeable future?

As an attempt to systemize the knowledge needed to answer these five questions, these Aerodynamic Studies were undertaken. In addition, it was expected the studies would prove valuable beyond the limits of this goal.

Burton P. Sauer Technical Editor Institute for System Research

ABSTRACT

This work is an annotated bibliography of the scientific literature pertaining to methods of calculating the aerodynamic forces acting on an air vehicle in flight. The present segment of the work includes material reviewed by the author in the period July 1955 through September 1955. The more interesting papers and reports (from the viewpoint of the aerodynamicist) are discussed briefly; others are listed without comment.

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1. SOME FUNDAMENTAL CONCEPTS OF MECHANICS AND THE QUANTUM THEORY OF FIELDS

1.1 Classical Mechanics

The formulation below is based principally on Chapter VI of Joos' Theoretical Physics (Reference 64).

Classical Newtonian mechanics is based on extrapolation of macroscopic physical occurrences, and in its application to an assemblage of particles the results are rigorous only when the latter are macroscopically defined. Classical mechanics of a system of N particles based on Newton's second law can be expressed by the following formula for the kth particle:

$$\mathbf{m}_{\mathbf{k}} \, \mathbf{d}^2 \vec{\mathbf{r}}_{\mathbf{k}} / \mathbf{d} t^2 = \vec{\mathbf{F}}_{\mathbf{k}} + \sum_{\mathbf{i}} \vec{\mathbf{F}}_{\mathbf{i} \mathbf{k}}, \qquad (1)$$

where $m_k = mass$ of kth particle (assumed to be constant);

 \vec{r}_{k} = displacement vector;

 $\vec{F}_{l_{r}}$ = external forces acting on kth particle;

 \vec{F}_{ik} = internal molecular forces on kth particle.

The usual assumption for internal forces is $\vec{F}_{ik} = -\vec{F}_{ki}$. The total energy of the system can be derived from eq. (1) by integrating with respect to time its product with the velocity:

$$\frac{1}{2} \left\{ \sum_{\mathbf{k}} m_{\mathbf{k}} \left[(d\vec{\mathbf{r}}_{\mathbf{k}}/dt)_{t}^{2} - (d\vec{\mathbf{r}}_{\mathbf{k}}/dt)_{t_{0}}^{2} \right] \right\} = \int_{\mathbf{r}_{\mathbf{k}}(t_{0})}^{\mathbf{r}_{\mathbf{k}}(t)} \sum_{\mathbf{k}} \vec{\mathbf{r}}_{\mathbf{k}} \cdot d\vec{\mathbf{r}}_{\mathbf{k}} + \int_{\mathbf{r}_{\mathbf{k}}(t_{0})}^{\mathbf{r}_{\mathbf{k}}(t)} \sum_{\mathbf{k}} \sum_{\mathbf{j}} \vec{\mathbf{r}}_{\mathbf{j}\mathbf{k}} \cdot d\vec{\mathbf{r}}_{\mathbf{k}}.$$

$$(2)$$

This expression may be simplified for conservative forces, i.e., for which curl $\vec{F}_{ik} = 0$. These forces have the following property:

$$\vec{F}_{jk} = -\operatorname{grad}_{k} U_{jk}; \quad \vec{F}_{kj} = -\operatorname{grad}_{j} U_{jk} = -\vec{F}_{jk}. \quad (3)$$

Introducing this notion of potential, eq. (3), referred to both the external and internal forces, into eq. (2), one obtains the expression for the total energy for a system of N particles:

$$\mathbf{T} + \sum_{\mathbf{k}}^{n} \mathbf{U}_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}}^{n} \sum_{\mathbf{j}}^{n} \mathbf{U}_{\mathbf{j}\mathbf{k}} = \text{const.}, \qquad (4)$$

where the kinetic energy is given by:

$$T = \frac{1}{2} \sum_{k} m_{k} (d\vec{r}_{k}/dt)_{t}^{2},$$
 (4a)

and the constant may be referred to the initial conditions at $t = t_0$.

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Consider the case when all the internal molecular forces are in equilibrium:

$$m_k (d^2 \vec{r}_k/dt^2) - \vec{F}_k = 0.$$
 (5)

Now, if a system of free particles is in equilibrium, the total work done by all forces, including inertia, in a small virtual displacement is zero:

$$\sum_{\mathbf{k}} \left[\vec{\mathbf{F}}_{\mathbf{k}} - \mathbf{m}_{\mathbf{k}} \left(d^2 \vec{\mathbf{r}}_{\mathbf{k}} / dt^2 \right) \right] \cdot \delta \vec{\mathbf{r}}_{\mathbf{k}} = 0, \qquad (6)$$

and labelling each coordinate separately and consecutively in reference to all N particles:

$$\sum_{i} (\mathbf{F}_{i} - \mathbf{m}_{i} \ddot{\mathbf{x}}_{i}) \cdot \delta \mathbf{x}_{i} = 0; \ \ddot{\mathbf{x}}_{i} = d^{2} \mathbf{x}_{i} / dt^{2}.$$
(6a)

Introduce generalized coordinates q_f and assume that each Cartesian coordinate is a function of them, i.e., $x_i = x_i (q_1, \ldots, q_f)$; there are in general f = 3N independent degrees of freedom for a system of N free particles. In the case of "*t*" constraints on the system, the magnitude "f" is equal to (3N-t). By simple calculation one gets with $\dot{q}_i = d q_i/dt$:

$$\mathbf{m}_{i} \mathbf{x}_{i} \delta \ddot{\mathbf{x}}_{i} = \sum_{k} \left[\frac{d}{dt} \frac{\partial}{\partial \dot{q}_{k}} (1/2 \mathbf{m}_{i} \dot{\mathbf{x}}_{i}^{2}) - \frac{\partial}{\partial q_{k}} (1/2 \mathbf{m}_{i} \mathbf{x}_{i}^{2}) \right] \delta q_{k};$$
(7)

and

$$\mathbf{F}_{i} \delta \mathbf{x}_{i} = -\delta \mathbf{U}_{i} = -(\mathbf{U}_{i, q1} \delta \mathbf{q}_{1} + \ldots + \mathbf{U}_{i, qf} \delta \mathbf{q}_{f}), \qquad (7a)$$

so that:

$$\sum_{k} \left[\frac{d}{dt} \sum_{i} \frac{\partial}{\partial \dot{q}_{k}} (1/2 m_{i} \dot{x}_{i}^{2}) - \sum_{i} \frac{\partial}{\partial q_{k}} (1/2 m_{i} \dot{x}_{i}^{2}) + \sum_{i} \frac{\partial}{\partial q_{k}} \right] \delta q_{k} = 0.$$
(8)

Since δq_k are independent, the bracketed expression vanishes identically, individually for each k, and since U is not a function of \dot{q}_k but only of q_k , i.e., U, $\dot{q}_k = 0$, one has:

$$\frac{d}{dt}(T-U), \quad \dot{q}k = (T-U), \quad qk = 0; \quad T = \sum_{k} 1/2 \ m_{k} \dot{x}_{k}^{2}. \quad (9)$$

If non-conservative forces \mathbf{F}'_i are considered in addition, the work done is:

$$\sum_{i} \mathbf{F}'_{i} \ \delta \mathbf{x}_{i} = \left(\sum_{i} \mathbf{F}'_{i} \ \frac{\partial \mathbf{x}_{i}}{\partial \mathbf{q}_{1}}\right) \ \partial \mathbf{q}_{1} + \ldots + \left(\sum_{i} \mathbf{F}'_{i} \ \frac{\partial \mathbf{x}_{i}}{\partial \mathbf{q}_{f}}\right) \ \delta \mathbf{q}_{f}. \tag{10}$$

Let:

$$\sum_{i} \mathbf{F}'_{i} \frac{\partial \mathbf{x}_{i}}{\partial \mathbf{q}_{k}} = \mathbf{F}'_{\mathbf{q}k};$$
(10a)

then eq. (9) becomes:

 $\frac{d}{dt}\mathbf{L}, \ \dot{\mathbf{q}}\mathbf{k} - \mathbf{L}, \ \mathbf{q}\mathbf{k} = \mathbf{F}'_{\mathbf{q}\mathbf{k}}; \ \mathbf{L} = \mathbf{T} - \mathbf{U}, \tag{11}$

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the function L being called the Lagrangian function. Eqs. (11) are known as the Lagrangian equations of the second kind. Let:

$$T = 1/2 \sum_{i} m_{i} (x_{i,q1} \dot{q}_{1} + ... + x_{i,qf} \dot{q}_{f})^{2}, \qquad (12)$$

or

$$T = 1/2 \left(P_{11} \dot{q}_1^2 + P_{22} \dot{q}_2^2 + \dots + 2 P_{12} \dot{q}_1 \dot{q}_2 + \dots \right),$$
(12a)

where the coefficients P_{jk} in this expression in q_i 's can be easily determined from eqs. (12) and (12a). In a Cartesian coordinate system the momentum components are:

$$\mathbf{p}_{i} = \mathbf{m}_{i} \dot{\mathbf{x}}_{i} = d(1/2 \mathbf{m}_{i} \dot{\mathbf{x}}_{i}^{2})/d \dot{\mathbf{x}}_{i} = \mathbf{T}, \dot{\mathbf{x}}_{i}.$$
 (13)

By analogy:

$$P_{k} = T, \dot{q}_{k} = (P_{lk}\dot{q}_{l} + ... + P_{fk}\dot{q}_{f}).$$
 (14)

Introduction of eq. (14) into eq. (9) gives:

$$d p_{k}^{\prime} / dt = \partial L (q_{k}^{\prime}, \dot{q}_{k}^{\prime}) / \partial q_{k}^{\prime}.$$
(15)

Introduce the Hamiltonian, defined as:

$$H(p_{k}, q_{k}) = \sum_{k} p_{k} \dot{q}_{k} - L(q_{k}, \dot{q}_{k}), \qquad (16)$$

and since

$$L_{,\dot{q}k} = T_{,\dot{q}k} = p_k; T = T(q_k, \dot{q}_k); U_{,\dot{q}k} = 0,$$
 (17)

then:

$$d H = \sum_{k} (H_{pk} d_{pk} + H_{qk} d_{qk}) = \sum_{k} (\dot{q}_{k} dp_{k} + p_{k} d\dot{q}_{k})$$
(18)

$$-\sum_{\mathbf{k}} (\mathbf{L}, \mathbf{q}_{\mathbf{k}} d\mathbf{q}_{\mathbf{k}} + \mathbf{L}, \mathbf{\dot{q}}_{\mathbf{k}} d\dot{\mathbf{q}}_{\mathbf{k}}) = \sum_{\mathbf{k}} (\dot{\mathbf{q}}_{\mathbf{k}} d\mathbf{p}_{\mathbf{k}} - \dot{\mathbf{p}}_{\mathbf{k}} d\mathbf{q}_{\mathbf{k}}).$$

Comparison of coefficients in eq. (18) yields:

$$H_{, nk} = \dot{q}_{k}; H_{, nk} = -\dot{p}_{k}.$$
 (19)

These are Hamiltonian canonical equations. The Hamiltonian L may be identified with the total energy, for a conservative system, as the following analysis shows: Since T is a homogeneous quadratic function of \dot{q}_k , eq. (12a), then from here and eq. (14) one has:

$$\sum_{\mathbf{k}} \dot{\mathbf{q}}_{\mathbf{k}} \mathbf{T}, \dot{\mathbf{q}}_{\mathbf{k}} = 2\mathbf{T} = \sum_{\mathbf{k}} p_{\mathbf{k}} \dot{\mathbf{q}}_{\mathbf{k}}, \qquad (20)$$

and since by definition L = T - U, eq. (16) becomes:

$$H(p_{t_{r}}, q_{t_{r}}) = 2T - (T - U) = T + U = E = Total Energy.$$
 (21)

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This total energy of the system is constant in time since substitution of eq. (19) in the time derivative of H gives zero as the result:

$$\frac{dH}{dt} = \sum_{k} (H, \frac{dp_{k}}{pk} + H, \frac{dq_{k}}{dt} = 0.$$
 (22)

In classical mechanics a system is described by a statement of the coordinates and velocities of all its particles. Here it proves more desirable to use the momenta rather than the velocities. If there are N coordinates and N momenta, we can then visualize the situation by setting up a 2N dimensional space, called a phase space, in which the coordinates and the momenta are plotted as variables; here a single point, called a representative point, gives complete information about the system. An assembly of systems corresponds to a collection of representative points and it is generally assumed that there are so many systems in the assembly that the distribution of representative points is practically continuous in the phase space.

1.2 Quantum Mechanics

Before the advent of quantum theory, nature's apparent continuity had been appealed to in applying the scheme of classical mechanics to the formulation of a theory of the mechanics of an assemblage of microscopically defined particles. But the necessity for a departure from classical mechanics is clearly shown by experimental results. With the recognition that there is no logical reason why Newtonian and other classical principles should be valid outside the domain in which they have been experimentally verified has come the modern point of view that departures from these principles are indeed necessary. Simply, the classical mechanics fails to explain some microscopic phenomena.

For example, the forces known in classical electrodynamics are inadequate for explaining the remarkable stability of atoms and molecules. Classical statistical mechanics enables one to establish a general connection between the total number of degrees of freedom of an assembly of vibrating systems and the specific heat. If one assumes that all the spectroscopic frequencies of an atom correspond to different degrees of freedom, one obtains a specific heat for any kind of matter incomparably greater than the observed value. This leads to a new clash between classical mechanics and the results of experiments. A similar clash is found in connection with the energy of oscillation of the electromagnetic field in a vacuum. In sum, attempts to construct a successful model of an atom on the basis of Newtonian mechanics have failed.

As another illustration of the failure of the classical mechanics we may consider the behavior of light (Ref. 25, p. 2). We have, on the one hand, the phenomena of interference and diffraction, which can be explained only on the basis of the wave theory; on the other, phenomena such as photo-electric emission and scattering by free electrons which show that light is composed of small particles. These particles, photons, have a definite energy and momentum, depending upon the frequency and velocity of the light, and appear to have just as real an existence as electrons, or any other particles known in physics. A fraction of a photon is never observed. Modern experiments have shown that this anomalous behavior is not peculiar to light, but is quite general. All material particles have wave properties, which can be exhibited under suitable conditions. We have here a striking and general example of the breakdown of classical mechanics--not merely an inaccuracy in its laws of motion, but an inadequacy of its concepts to supply a description of atomic events (Ref. 25, p. 3).

The need to depart from classical ideas in order to account for the ultimate structure of matter is obvious. In a classical explanation of the constitution of matter, one assumes a large number of small constituent parts and postulates laws for the behavior of these parts; from these postulates the laws of matter in bulk are deduced. But this cannot complete the explanation, since the structure and stability of the constituent parts are still unexplained. * To go into this question, it becomes necessary to postulate that each constituent part is itself made up of smaller parts, and there is no end to this subdividing.

So long as "big" and "small" are relative concepts, it is no help to explain the big in terms of the small and vice versa. It is therefore necessary to modify classical ideas in such a way as to give an absolute meaning to size. To do this, one must assume that there is a limit to the fineness of our powers of observation and the smallness of the accompanying disturbance--a limit which is inherent in the nature of things and can never be passed by improved technique or increased skill on the part of the observer (Ref. 25, p. 3). If the object under observation is such that the limiting disturbance is negligible, then the object is big in the absolute sense and we may apply classical mechanics to it. If, on the other hand, the limiting disturbance is not negligible, then the object is small in the absolute sense and one requires a new theory to deal with it. If a system is small, one cannot observe it without producing a serious disturbance and hence cannot expect to find any causal connections in the results of his observations. There is thus an essential indeterminacy in the quantum theory, of a kind that has no analogue in the classical theory. The quantum theory does not enable one to calculate the general result of an observation, but offers only the probability of obtaining a particular result when the observation is made.

Thus quantum mechanics starts out quite differently from classical mechanics and is more correct and more fundamental for statistical purposes. It does not deal with coordinates of the particles; it sets up a statistical assembly, and tells how that assembly changes with time without the intermediate steps of solving for the motion of individual systems by Newton's laws of motion.

In order to put quantum mechanics onto a quantitative basis, a new set of laws is required for the starting point of the new theoretical scheme; of these the principle of superposition is fundamental. This principle, the result of analysis and interpretation of typical microscopic phenomena such as polarization, corpuscular interference, radiation, etc., asserts that any state may be regarded as the result of a superposition of two or more states in an infinite number of ways (inconceivable in a classical view). The superposition principle implies that the states must be connected with mathematical quantities which when added together give further quantities of the same kind; one may therefore describe the state of a system by a vector quantity in a space of (generally) infinite dimensions, a quantity conveniently denoted by ψ . In general, any set of states may be dependent or independent, depending on whether the ψ 's are linearly dependent or independent.

In experiment, one determines the numerical value of a dynamic variable (called an observable); this is represented in the theory by a linear operator. The axioms and rules of manipulation governing these two mathematical quantities are then developed into a theoretical scheme. Particular operators are associated with particular modes of observation, and the laws of nature are expressed as relations among these operators.

The dynamic variables may be expressed in terms of a set of canonical coordinates and momenta; these quantities in theory obey the following laws in quantum mechanics:

*Exactly the same situation exists in recent problems in fluid dynamics.

$$[p_{i}, p_{j}] = (p_{i}p_{j} - p_{j}p_{i}) = 0, \text{ for all } i, j;$$
 (23)

$$[q_i, q_i] = (q_i q_i - q_j q_i) = 0$$
, for all i, j; (24)

$$[q_{i}, p_{j}] = \delta_{ij}; (q_{i}p_{j} - p_{j}q_{i}) = ih [q_{i}, p_{j}],$$
 (25)

i.e.,

$$(q_i p_j - p_j q_i) = ih \delta_{ij}, \qquad (25a)$$

where h is a new universal constant having the dimensions of action. From these fundamental points, the differential equations describing the behavior of systems obeying the laws of quantum mechanics may be derived. The assumption of superposition relationships between the states leads to a mathematical theory in which the equations that define a state are linear in the unknowns. In consequence of this, various attempts have been made to establish analogies with systems in classical mechanics which are governed by linear equations and for which a superposition principle holds. Such analogies have led to the name " wave mechanics" given sometimes to quantum mechanics. But one must remember that the superposition in quantum mechanics is essentially different from any occurring in the classical theory, as is shown by the fact that the quantum superposition principle requires indeterminacy in the results of observations in order to be capable of a sensible physical interpretation. Analogies are thus liable to be misleading (Ref. 25, p. 14).

1.3 Classical Statistical Mechanics

The principles of statistical mechanics permit us to make reasonable predictions as to the future conditions of a system, which may be expected to hold on the average, starting from an incomplete knowledge of its initial state. Historically, the science of statistical mechanics was specially devised for the treatment of complicated systems, composed of such an enormous number of individual molecules that it is too difficult to try to calculate the precise behavior of the system as a function of time by the methods of ordinary mechanics. Thus the general nature of the statistical mechanics procedure for the treatment of complicated systems consists in studying the behavior of a collection or ensemble of systems of structure similar to that of the system in question, distributed over a range of different precise states (Ref. 169, p. 2).

In order to investigate the behavior of such ensembles of systems it is convenient for any system of f degrees of freedom to construct a Euclidean space of 2f dimensions with 2f rectangular axes, one for each of the coordinates q_1, \ldots, q_f , and one for each of the momenta p_1, \ldots, p_f . Following Gibbs, we call such a space a phase space (Ref. 169, p. 43). The instantaneous state of any system in the ensemble can then be specified by the position of a representative point in the phase space, and the condition of the ensemble as a whole can be described by a set of such representative points, one for each system in the ensemble. The behavior of the ensemble with the time is described by the trajectories of points in the phase space.

The fundamental property of such a phase space can be expressed by means of Liouville's theorem referring to the density of distribution p of the representative points in the space. The Liouville's theorem states: dp/dt = 0, when one considers the rate of change of density in the neighborhood of any selected moving phase point rather than in the neighborhood of a fixed point in the phase space. This is called the conservation of density in phase.

The procedure and methods are statistical in character; the results which they provide are true on the average for the systems in an appropriately chosen ensemble rather than necessarily precisely true in any individual case.

The concept of averages introduces the necessity of providing a relationship between the time average (usually observable experimentally) and the ensemble average calculated by the methods of statistical mechanics for all the members of the corresponding representative ensemble. The postulate leading to the equality of these two averages was called by Boltzmann the ergodic hypothesis.

Recent work of a particularly applicable nature in this field is a study (Ref. 78) of the statistical mechanics of irreversible processes in linear assemblies and the application of results (Ref. 124) to three-dimensional crystals.

1.4 Quantum Statistical Mechanics

In classical mechanics we regard the state of a system at any time as specified by the values of its coordinates and momenta, and can regard the future behavior of the system as uniquely determined by its initial state (Ref. 169, p. 325). If the knowledge of the initial state is inexact, it is useful to apply the methods of the classical statistical mechanics.

Quite similar situations are also encountered in quantum mechanics. In general, the system in quantum mechanics is specified by a probability amplitude. Such probability amplitudes change with time in the case of an isolated system in the definite manner dictated by the Schrödinger equation, so that in principle it is also possible in quantum mechanics to make precise predictions as to the changes in the state of a system as time proceeds. But just as in classical mechanics one may encounter situations in which it is not practicable to treat the precise state of a system as time proceeds. Hence one may resort to the study of an ensemble of systems of the same kind as the one of interest but distributed over a range of possible states. The average behavior of the systems in such an ensemble will indicate the average behavior of a single system of interest. The Liouville theorem has here its analogue, giving the dependence on time of the density matrix of an ensemble of quantum mechanical systems.

1.5 Matrix and Wave Mechanics

The expression "quantum theory" embraces all the theories in which Planck's constant h plays a role. Quantum theory thus includes the Bohr-Sommerfield theory, sometimes called classical quantum theory, as well as quantum mechanics in its various forms: wave mechanics, matrix representation. (matrix mechanics), and operator representation.

The quantum mechanics of Heisenberg (matrix method) was inaugurated by W. Heisenberg in 1925 (Ref. 121, p. 63). The direct relations between observables are not in general expressible by ordinary algebra, and Heisenberg's development led to the utilization of matrix algebra.

Wave mechanics was originally suggested by de Broglie. Later it was developed by Schrödinger, who outlined its fundamentals in 1926. The Schrödinger method starts with the observation that the classical laws of point mechanics can be put into a form analogous to the laws of geometrical optics; i.e., classical point mechanics represents only a first approximation of more general laws. To retain the parallelism with optics, one must consider that these laws are analogous to the laws of wave optics.

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1.6 The Theory of Relativity

Until recently, time was regarded as something essentially distinct from space and from the behavior of material bodies. All motion involves displacement relative to something or other; but there may be various ideas in regard to the entity relative to which the displacement occurs. This kind of relativity has been called "Newtonian relativity."

Assume two different frames of reference, Cartesian coordinate systems (x, y, z), (x', y', z'), each in uniform translatory motion relative to the other. Then the equations of transformation for Newtonian relativity are:

$$x' = x - ut, y' = y, z' = z, t' = t.$$
 (26)

Einstein's postulates of the special or restricted theory of relativity are the following: (i) The laws of physical phenomena are the same when stated in terms of either of two inertial frames of reference (and involve no reference to motion through an ether), i.e., all frames of reference are equivalent; (ii) in any frame of reference, the fundamental laws of nature remain the same. In particular, the velocity of light is a fundamental constant.

An inertial frame is usually called an "unaccelerated" one. Thus, in the special theory of relativity the two frames of reference are in uniform translation relative to each other. In the mathematical formulation of this concept the Lorentz transformation finds a large application. Thus, for the motion of the frame (x', y', z') in the x-direction with the velocity v, the following formulas are valid:

$$\mathbf{x}' = (\mathbf{x} - \mathbf{v}\mathbf{t})(1 - \mathbf{v}^2/c^2)^{-1/2}; \ \mathbf{y}' = \mathbf{y}; \ \mathbf{z}' = \mathbf{z};$$
 (27)

$$t' = (t - xvc^{-2})(1 - v^{2}/c^{2})^{-1/2}.$$
 (27a)

Preservation of the law of conservation of momentum gives the law of variation of mass:

$$m' = m(1 - v^2/c^2)^{-1/2}$$
; c = velocity of light. (28)

Relativity puts time on a basis equivalent to the space coordinates and invariants are found only for four dimensional space. Calculation of the momentum gives for its four components:

$$(p_x, p_y, p_z, iEc^{-1}); E = mc^2.$$
 (29)

Similarly, for the radiation wave number vector the four components are found to be:

$$(\lambda_{x}^{-1}, \lambda_{y}^{-1}, \lambda_{z}^{-1}, i\nu c^{-1}),$$
 (30)

where: λ = wave length; ν = radiation frequency. The general theory of relativity takes up the problem of harmonizing space, time and the laws of gravitation. Einstein concludes that, in the neighborhood of any given point, there should be no difference of any kind between the gravitational field due to attracting matter and the apparent field due to acceleration of a frame of reference. This proposition adopted as a postulate is called the principle of equivalence.

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1.7 Quantum Theory of Fields*

In classical physics a field is described by one or several space-time functions $\psi_{\sigma}(\mathbf{x}, t)$ which satisfy certain partial differential equations, the "field equations" (Ref. 191). One may also start with a variational principle chosen in such a way that its Euler differential equations are the same field equations. Let L be a function of the $\psi_{\sigma}(\mathbf{x}, t)$ and of their first time and space derivatives:

$$\mathbf{L} = \mathbf{L} \left(\psi_1, \ \Delta \psi_1, \ \psi_1; \ \psi_2, \ \Delta \psi_2, \ \psi_2; \ \dots \right); \quad \psi_2 = \partial \psi_2 / \partial \mathbf{t}. \tag{31}$$

By integration over a volume V and a time interval from t' to t" one forms:

$$\int_{t'}^{t''} dt \int_{\mathbf{V}} \mathbf{L} (\psi_1, \ldots) d\mathbf{x} = \mathbf{I}.$$
(32)

Varying the function ψ_{σ} for a fixed region of integration subject to restriction that the variations $\delta \psi_{\sigma}$ vanish at the boundary of the domain of integration, i.e., at the surface of the volume V and for t = t' and t = t'', one obtains: +''

$$\delta I = \int_{t^*} dt \int_{V} \delta L dx.$$
 (33)

One requires that the classical field be determined by the condition that the integral I shall be stationary ($\delta I = 0$) for arbitrary variations $\delta \psi_{\sigma}$ which satisfy the above conditions and for an arbitrary choice of the integration region. From this it follows that for all times and for all positions:

$$5 \mathbf{L} = \mathbf{L}, \psi_{\sigma} = \sum_{\mathbf{k}} \frac{\partial}{\partial \mathbf{x}_{\mathbf{k}}} \partial \mathbf{L} / \left[\partial \left(\frac{\partial \psi_{\sigma}}{\partial \mathbf{x}_{\mathbf{k}}} \right) - \frac{\partial}{\partial \mathbf{t}} \mathbf{L}, \psi_{\sigma} = 0 \quad (\sigma = 1, 2...) .$$
(34)

These, the field equations, are partial differential equations of the second order at most for the field functions ψ_{α} . One calls

$$\mathbf{L}, \boldsymbol{\psi}_{\sigma} = \sum_{\mathbf{k}} \frac{\partial}{\partial \mathbf{x}_{\mathbf{k}}} \partial \mathbf{L} / \left[\partial \left(\frac{\partial \boldsymbol{\psi}_{\sigma}}{\partial \mathbf{x}_{\mathbf{k}}} \right) \right] \equiv \delta \mathbf{L} / \delta \boldsymbol{\psi}_{\sigma}, \qquad (35)$$

the "functional derivative" of $\int L dx$ with respect to ψ_{α} . With this notation, eq. (34) reduces to the form:

$$\partial /\partial t L, \dot{\psi}_{\sigma} = \delta L / \delta \psi_{\sigma},$$
 (36)

analogous to the ordinary equation of classical mechanics. This variational principle can be connected with Hamilton's least action principle of classical mechanics. By this procedure a field may be interpreted as a mechanical system of infinitely many degrees of freedom.

The above analogy may be further expounded by subdividing the space into finite cells $\delta x^{(s)}$ which we distinguish by the upper index s; the value of the field function ψ_{σ} in the cell (s) is denoted by $\psi_{\sigma}^{(s)}(t)$. In this way it is possible to represent the function L(31) in any cell (s) as a function of the generalized coordinates $q_i \equiv \psi_{\sigma}^{(s)}$. In order to make the transition to Hamilton's formalism in the

*The equations used in this section and parts of the discussion are taken from Quantum Theory of Fields by Gregor Wentzel (pp. 1-8), Copyright 1949 by Interscience Publishers, New York-London. Used by permission.

framework of the classical theory, one must introduce the momenta p_j , which are canonically conjugate to the coordinates $q_i = \psi_{\alpha}^{(s)}$; these are:

$$\mathbf{p}_{j} = \delta \mathbf{x}^{(s)} \cdot \partial \mathbf{L}^{(s)} / \partial \dot{\psi}_{\sigma}^{(s)}.$$
(37)

Hamilton's function is then obtained by

$$H = \sum_{j} p_{j} \dot{q}_{j} - L.$$
 (38)

This makes it possible to replace the field equations (34) by the "canonical field equations" corresponding to the canonical Hamilton equations of motion in classical particle mechanics:

$$\dot{q}_{j} = H, P_{j}; \dot{p}_{j} = -H, q_{j}.$$
 (39)

The transition from classical to quantum mechanics is effected by replacing the canonical variables q_j , p_j by Hermitian operators which satisfy the commutation rules:

$$[a, b] = ab - ba;$$
 (40)

$$[q_j, q_j] = [p_j, p_j] = 0; [p_j, q_j] = ih^{-1} \delta_{ij};$$
 (40a)

where h denotes Planck's constant divided by 2π and δ_{ij} is the Kronecker delta. The mechanical properties of the system are determined by its Hamiltonian, which is formally taken over from the classical theory but is interpreted as Hermitian operator. One may consider a quantized field as defined by its Hamiltonian $H = \int \overline{H} dx$ or by its Lagrangian $L = \int \overline{L} dx$ with:

$$\overline{\mathbf{H}} = \overline{\mathbf{H}} (\psi_1, \ \Delta \psi_1, \ \pi_1; \ \psi_2, \ \dots); \ \pi_\sigma = \partial \overline{\mathbf{L}} / \partial \dot{\psi}_\sigma; \tag{41}$$

$$\overline{\mathbf{L}} = \overline{\mathbf{L}} (\psi_1, \Delta \psi_1, \dot{\psi}_1; \psi_2, \ldots).$$
(41a)

The ψ_{σ} and π_{σ} in \overline{H} stand now for Hermitian operators, with commutation rules which result from those of $q_j = \psi_{\sigma}^{(s)}$, $p_j = \delta x^{(s)} \pi_{\sigma}^{(s)}$ by the transition to the continuum. This procedure is characteristic of the so-called "canonical field quantization" as it was first formulated for general fields by Heisenberg and Pauli. Writing $\psi_{\sigma}(x)$, $\pi_{\sigma}(x)$ instead of $\psi_{\sigma}^{(s)}$, $\pi_{\sigma}^{(s)}$, the following equations are postulated:

$$[\psi_{\sigma}(\mathbf{x}), \psi_{\sigma^{\dagger}}(\mathbf{x}')] = [\pi_{\sigma}(\mathbf{x}), \pi_{\sigma^{\dagger}}(\mathbf{x}')] = 0; \qquad (42)$$

$$[\boldsymbol{\pi}_{\sigma}(\mathbf{x}), \boldsymbol{\psi}_{\sigma}, (\mathbf{x}')] = \mathbf{i}^{-1} \mathbf{h} \boldsymbol{\delta}_{\sigma\sigma'} \boldsymbol{\delta}(\mathbf{x}, \mathbf{x}').$$
(42a)

Here $\delta(\mathbf{x}, \mathbf{x}^{t})$ stands for a function the value of which is $(\delta \mathbf{x}^{(\mathbf{s})})^{-1}$ or 0, according to whether the points **x** and **x'** lie in the same or different cells. Integrating for fixed **x'** with respect to **x**, one obtains $\int \delta(\mathbf{x}, \mathbf{x}') d\mathbf{x} = 1$. In the limit of the continuum (cell volume $\delta \mathbf{x}^{(\mathbf{s})} \rightarrow 0$), $\delta(\mathbf{x}, \mathbf{x}')$ goes over into the three-dimensional Dirac δ -function:

$$\delta(\mathbf{x}, \mathbf{x}') \longrightarrow \delta(\mathbf{x} - \mathbf{x}') = \begin{cases} 0 \text{ for } \mathbf{x} \neq \mathbf{x}', \\ \infty \text{ for } \mathbf{x} = \mathbf{x}', \end{cases}$$
(43)

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in such a way that

$$\int \delta(\mathbf{x} - \mathbf{x}') \, \mathrm{d}\mathbf{x} = 1 \,. \tag{43a}$$

This limiting process has meaning only if $\delta(x, x')$ appears in the integrand of a space integral. In quantum mechanics, the canonical equations of motions are valid as operator equations on account of the commutation rules of the q_i and p_i :

$$\dot{\mathbf{q}}_{j} = i \mathbf{h}^{-1} [\mathbf{H}, \mathbf{q}_{j}] = \mathbf{H}, \mathbf{p}_{j};$$
(44)

$$\dot{p}_{j} = ih^{-1} [H, p_{j}] = -H, q_{j}.$$
 (44a)

In general, the time derivative of any function ϕ of the q_j and p_j not depending explicitly on time may be expressed by:

$$\phi \equiv ih^{-1} [H, \phi]. \tag{45}$$

It must be kept in mind that the operator $\dot{\phi}$ is not simply the partial derivative of ϕ with respect to time but refers to expectation values:

$$\vec{\phi} = ih^{-1} \left[\overline{\mathbf{H}, \phi} \right] = d \, \overline{\phi} / dt \,. \tag{46}$$

The same result holds for the field theory:

$$\dot{\psi}_{\sigma}(\mathbf{x}) \equiv \mathrm{ih}^{-1} [\mathbf{H}, \psi_{\sigma}(\mathbf{x})]; \quad \dot{\pi}_{\sigma}(\mathbf{x}) = \mathrm{ih}^{-1} [\mathbf{H}, \pi_{\sigma}(\mathbf{x})].$$
(47)

The evaluation of these commutators with the help of the commutation rules (42, 42a), (43, 43a) leads to operator equations which are formally equivalent to the field equations (34) in the same way as the canonical equations of motion in particle mechanics ($q_j = H$, p_j ; $p_j = -H$, q_j) are equivalent to Lagrange's

equations. They refer to the operator equations which stem from the definitions (47) as "canonical field equations."

An attempt of a mathematical treatment of quantum field theory was done by Friedrichs (Ref. 29). At present the subject does not admit a systematic or rigorous presentation.

1.8 Groups, Statistical Mechanics, and Quantum Theory*

The theory of groups has a special significance with respect to statistical mechanics and quantum theory.

Wiener (Ref. 196) begins his description of the relation between groups and statistical mechanics by discussing the works of Gibbs and Lebesque. The key idea of Gibbs is this: in Newton's dynamics one is concerned with an individual system, with given initial velocities and momenta, undergoing changes according to a certain system of forces under the Newtonian laws. If one assumes a certain initial distribution of the known positions and momenta, he determines in a completely Newtonian way the distribution of the momenta and positions for any future time. Some of the statements about these distributions have the character of assertions that the future system will have certain characteristics with probability one or zero, and further that an event of probability one may be made up of an assemblage of instances of probability zero. The technique

^{*}This section is a condensation of Chapter II, <u>Cybernetics</u>, by N. Wiener, Copyright 1948 by Technological Press of Massachusetts Institute of Technology and John Wiley and Sons, Inc. Used by permission.

of the Gibbsian statistical mechanics uses the process of the resolution of a complex contingency into an infinite sequence of more special contingencies--a first, a second, a third, etc. --each of which has a known probability; and the expression of the probability of this larger contingency is the sum of the probabilities of the more special contingencies which form an infinite series. Thus one cannot sum probabilities in all conceivable cases to get a probability of the total event--for the sum of any number of zeros is zero--but we can sum them if there is a first, a second, a third member, and so on, forming a sequence of contir cies in which every term has a definite position given by a positive integer.

Lebesgue's work was based on the theory of trigonometric series. This goes back to the physics of waves and vibrations and to the question of the generality of the sets of motions of a linear system which can be synthesized out of the simple vibrations of the system. Thus a single function is expressed as the sum of a series. In these series, the coefficients are expressed as averages of the product of the function to be represented, multiplied by a given weighting function. The whole theory depends on the properties of the average of a series in terms of the average of an individual term. The average of a quantity, which is one over an interval from zero to A, and zero from A to 1, is A, and may be regarded as the probability that the random point should lie in the interval from 0 to A, if it is known to lie between 0 and 1. In other words, the theory needed for the average of a series is very close to the theory needed for an adequate discussion of probabilities compounded from an infinite sequence of cases. Thus Lebesque, in solving his own problem, had also solved that of Gibbs.

Assume a set of 2N coordinates, N of which are generalized coordinates and N the generalized momenta. They determine a 2N-dimensional volume. If we take any region of this space and let the points flow with the course of time, which changes every set of 2N coordinates into a new set depending on the elapsed time, the continual change of the boundary of the region does not change its 2N-dimensional volume. In general, for sets not so simply defined as these regions, the notion of volume generates a system of measure of Lebesque's type. In this system of measure, and in the conservative dynamical systems which are transformed in such a way as to keep this measure constant, the energy also remains constant. Sometimes the momentum and the moment of momentum of the system as a whole remain constant as well; these can be eliminated easily.

Let us assume a measure on a region in a phase space for which energy, possibly total momentum, and total moment of momentum are determined, and let the total measure of this restricted region be constant, or, as one can make it by a change in scale, one. As this measure has been obtained from a measure invariant in time, it is itself invariant. This is called phase measure, and averages taken with respect to it are known as phase averages.

But any quantity varying in time may have a time average. In Gibbs' statistical mechanics, both time averages and space averages occur. Thus, the appearance of ergodic theory and of the idea in Gibbs' attempt to show that these two types of average were, in some sense, the same, is obvious. Besides the notions of average and of measure, which are most urgently needed to understand Gibbs' theory, in order, in turn, to appreciate the real significance of ergodic theory one needs a more precise analysis of the notion of invariant and of transformation group. In general, in physics, one should be able to present a property of the system discussed which remains the same under the flux of particular circumstances. In the simplest case, the system is subject to a property which is invariant to a set of transformations. Thus one is led to the notions of transformations, transformation group, and invariants. A transformation A of a system is some alteration in which each element goes into another. The product or resultant of transformation AB is, in general, not equal to the product BA. If AB and BA are the same, A and B

are permutable. The identity transformation $A^{-1} A = I$ is a transformation which transforms every element into itself. In this case A^{-1} is called the inverse of A. Of course, A is the inverse of A^{-1} . I is its own inverse, and the inverse of AB is $B^{-1}A^{-1}$.

There exist certain sets of transformations in which every transformation belonging to the set has an inverse, likewise belonging to the set, and where the resultant of any two transformations belonging to the set itself belongs to the set. These sets are known as transformation groups. If any two transformations of the group are permutable, the group is Abelian. If any quantity attached to all the elements transformed by a transformation group is unchanged when each element is changed by the same transformation of the group, it is called an invariant of the group.

The bibliography includes references on the relation between the theory of group and quantum mechanics. The most outstanding in that respect are the works of Weyl (Refs. 192, 193). Also of value are the supplementary works on the physical aspect, such as those of Sommerfeld (Refs. 150, 151), Ruark and Urey (Ref. 132), Gerlach (Ref. 34), etc. The book of von Neumann is less known, but valuable (Ref. 118). The remarks below are based largely on Weyl's books.

The importance of the standpoint afforded by the theory of groups for the discovery of the general laws of quantum theory is apparent. The concepts arising in the theory of groups find their application in physics. Thus, for example, the theory of groups finds an immediate application to the theory of a single electron in a spherically symmetric electrostatic field. A rotation of physical space, i.e., an orthogonal transformation from the Cartesian coordinates (x, y, z) into (x', y', z') induces a unitary transformation $U(s): \psi \rightarrow \psi'$ defined by:

$$\psi'(\mathbf{x}',\mathbf{y}',\mathbf{z}') = \psi(\mathbf{x},\mathbf{y},\mathbf{z}), \qquad (48)$$

in the system space R of the electron, the vectors of which are the wave functions $\psi(\mathbf{x}, \mathbf{y}, \mathbf{z})$ describing the state of the electron. The correspondence $\mathbf{s} \longrightarrow \mathbf{U}(\mathbf{s})$ is a definite representation C, of infinitely many dimensions, of the rotation group δ_3 . This representation C can be reduced into the irreducible constituents D_i, and it is found that each D_i with integral ℓ occurs an infinite number of times.

On going over from one electron to two, the vectors of system space are the functions $\psi(\mathbf{x}_1, \mathbf{y}_1, \mathbf{z}_1; \mathbf{x}_2, \mathbf{y}_2, \mathbf{z}_2)$ of the Cartesian coordinates of both electrons. The unitary transformation U: $\psi \longrightarrow \psi'$ induced in system space by the rotation s is now defined by the equation:

$$\psi'(\mathbf{x'}_1, \mathbf{y'}_1, \mathbf{z'}_1; \mathbf{x'}_2, \mathbf{y'}_2, \mathbf{z'}_2) = \psi(\mathbf{x}_1, \mathbf{y}_1, \mathbf{z}_1; \mathbf{x}_2, \mathbf{y}_2, \mathbf{z}_2),$$
(49)

where x'_{1}, y'_{1}, z'_{1} and x'_{2}, y'_{2}, z'_{2} are obtained from x_{1}, y_{1}, z_{1} and x_{2}, y_{2}, z_{2} by the same orthogonal transformation s. In this situation the state space \mathbb{R}^{2} of the system consisting of two electrons is $\mathbb{R} \times \mathbb{R}$ and the representation \mathbb{C}^{2} induced in it is $\mathbb{C} \times \mathbb{C}$. This representation is determined by the kinematic constitution of the system alone, and is in no way influenced by the dynamic relationships. The rule for x-multiplication for the induced representation on composition of partial systems presupposes only kinematical, not dynamical, independence of the partial systems.

Similarly, one can find a relation between quantum kinematics and the Abelian group of rotation. The kinematic structure of a physical system is expressed by an irreducible Abelian group of unitary ray rotations in system space. The real elements of the algebra of this group are the physical quantities of

the system; the representation of the abstract group by rotations of system space associates with each such quantity a definite Hermitian form which "represents" it.

There seems to exist a plainly discernible parallelism between the more recent developments of mathematics and physics. Occidental mathematics has in past centuries broken away from the Greek view and followed a course which seems to have originated in India, and which has been transmitted. with additions, to us by the Arabs; in it the concept of number appears as logically prior to the concepts of geometry. The result has been that mathematics has applied this systematically developed number concept to all branches, irrespective of whether it is most appropriate for the particular applications in question. But the present trend in mathematics is clearly in the direction of a return to the Greek standpoint; one now looks upon each branch of mathematics as determining its own characteristic domain of quantities. The algebraist of the present day considers the continuum of real or complex numbers as merely one "field" among many; this newer mathematics, including the modern theory of groups and abstract algebra, is clearly motivated by a spirit different from that of "classical mathematics," which found its highest expression in the theory of functions of a complex variable. The development of the classical mechanics applied to a continuum had its parallelism in the development of classical mathematics and vice versa. The continuum of real numbers has retained its ancient prerogative in physics for the expression of physical measurements, but it can justly be maintained that the essence of the Heisenberg-Schrödinger-Dirac quantum mechanics is to be found in the fact that there is associated with each physical system a set of quantities, constituting a non-commutative algebra in the technical mathematical sense, the elements of which are the physical quantities themselves.

1.9 Dissipative Systems

There exist various approaches to generalize the principles of classical mechanics to systems with a dissipation. Rosen and Herivel, each discussed below, represent two such attempts.

1.9.1 Rosen (129)

Rosen formulates a variational principle for diffusional processes such as heat and matter diffusion, modifying Onsager's principle of minimum dissipation. Milliken in 1929 attempted to obtain a variational principle for describing the flow of a viscous incompressible fluid and came to the conclusion that for three-dimensional flow, unless the vector product of the vorticity and velocity is zero, such a principle could not be found. Rosen states that Milliken overlooked the possibility of a restricted variational principle similar to Onsager's in which forces are held fixed. Following his path of reasoning, Rosen derives a variational principle for the flow of viscous incompressible fluids which again has some analogy to Onsager's principle.

1.9.2 Herivel (50)

Herivel proposes a general variational principle for dissipative systems; he shows that it can be applied, in unchanged form, to a general dynamic system with dissipation, to the motion of perfect and viscous fluids, and to the flow of electricity in linear conductors. The papers of Herivel and Rosen seem to indicate the possibility of the formulation of a general variational principle for dissipation processes applicable without change of form to widely differing systems. Similarly, Hamilton's principle applies without change to all dynamical problems in which no dissipation occurs.

2. SOME FUNDAMENTAL MODELS AND CONCEPTS OF FLUID DYNAMICS

2.1 Continuum

The general procedure in theoretical mechanics can be divided into the following five steps (Ref. 155, p. 6):

- (1) A physical system is an object of investigation; one wishes to predict its behavior under various circumstances.
- (2) An ideal, mathematical model of the physical system is constructed mentally.
- (3) Mathematical reasoning is applied to the mathematical model; this includes a solution of the mathematical system in question.
- (4) The mathematical results are interpreted physically in the terms of the physical problem.
- (5) These results are compared with the results of observation.

The best known mathematical model applied to the investigation of phenomena in fluid dynamics is the model of continuum. It is, in fact, the basis of a great deal of Newtonian mechanics. Based on the notion of a particle, this mathematical model of matter is actually discontinuous: a collection of a vast number of particles. But since this model involves a very large number of things a statistical method may be used; instead of following individual particles, we may direct our attention to their average behavior. In fact, the discontinuous body, consisting of a great number of separate particles, is replaced by a continuous distribution of matter.

It seems obvious that a continuum model may present fairly enough the phenomena in solid bodies and incompressible media, i. e., liquids. But in compressible media the compressibility phenomena cannot be referred to the variations in the mutual locations of atoms inside a molecule (inter-atomic distances) or to the variations of distances between electrons and nuclei inside an atom. The reason is that the variations of the density and of the volume of a fluid due to such changes are of a negligible order. Consequently, the significant variations of density in compressible media can be referred only to the variations in intermolecular distances. This implies that the continuum model may give a reasonable approximation only for dense gases, that it may be questionable in the domains of rarefied gases, where the full statistical approach, corresponding to the full notion of "average," should be used.

The mechanics of continuum is fundamentally the Newtonian mechanics. A Newtonian continuum is defined as a finite or infinite closed region of Euclidean three-dimensional space, at each point of which, with the possible exception of isolated sets of points of dimension less than three, there exist the primitive characteristic functions for density, stress tensor, internal energy per unit mass, specific entropy, and heat flow vector, and whose topological transformation in time into a finite number of other closed regions is governed by the principles of conservation of mass, momentum, and energy. Basically, one has the following independent and dependent variables in the most general three-dimensional system in the Newtonian continuum: four independent scalar variables: x, y, z, t; 19 dependent scalar variables; kinematic variables: three velocity components u, v, w, and density ρ ; thermodynamic variables: temperature T, thermodynamic pressure p, specific entropy S, and three components of the heat flux vector; dynamic variables: nine components of a fluid stress dyadic.

There are 10 scalar equations connecting these variables: conservation of mass, momentum (three equations of motion and three equations expressing the equality of the fluid stress dyadic to its conjugate), conservation of energy, and two equations of state: $f(p, \rho, T) = 0$ and $T = T(S, \rho)$. To obtain a determinate problem, nine more equations must be added. To resolve the indeterminacy of the general theory,

it is customary to restrict attention to some particular ideal body, subject to the general laws already stated, which is specified by some particular postulated property intended to represent the behavior of a class of actual bodies. The defining property is now usually taken to be a functional relation among the stress dyadic and other variables, a functional relation between the heat flux and temperature, or both. Some particular cases may be distinguished:

- (i) The perfectly elastic body is defined by the condition that the stress depends only upon the strain from some preferred initial position and is independent of the rate of change of strain.
- (ii) The perfect fluid is defined by the condition that the stress dyadic is always a pure pressure, and shearing stress cannot occur.
- (iii) The viscous fluid is defined by the condition that the fluid stress dyadic depends only upon the deformation, without reference to any preferred initial configuration. The fluid is said to be isotropic if the constants in the linear stress-deformation relation are invariant under all possible rotations of Cartesian axes, or if the dissipation function is invariant in form under transformations of the Eulerian coordinates. For more details the reader is referred to special works on the subject (Refs. 170, 171, 172).

One may distinguish between kinds of fluid (171, 172):

- (i) The Stokesian fluid defined by a formulation equivalent to Stokes' principle: the stress power is a function of the rate of deformation only.
- (ii) The Maxwellian fluid, which is a generalization of the Stokesian fluid: the stress tensor and heat flux vector are functions of viscosity, thermal conductivity, pressure, temperature, rate of deformation tensor, vorticity, etc.; they are analytic functions of all the vectors and tensors listed.

Truesdell proposes a new definition of a fluid which may extend the validity of the proposed and derived equations to the regime of rarefied gases (Refs. 170, 171, 172). This is a rather general definition of a fluid as a special type of continuum susceptible to the principal phenomena observed in rarefied gases. His method proposes the development of the stress tensor in a power series in the vector and scalar variables listed in the Maxwellian fluid. The fundamental assumption is that of the tensorial and dimensional invariance. The proposed method is in one sense more general and more exhaustive, yet in another sense more definite, than those used previously. But a full knowledge of the order of magnitude of terms, and hence of the effects they represent, requires a knowledge not available at present, of the experimental values of the dimensionless higher order coefficients. This is a serious disadvantage of this proposition.

The classical theory of isotropic viscous fluids rests upon the Newton-Cauchy-Poisson law:

$$t_{j^{\circ}}^{i} = -p\delta_{j}^{i} + \lambda d_{k^{\circ}}^{k}\delta_{j^{\circ}}^{i} + 2\mu d_{j^{\circ}}^{i}, \qquad (50)$$

where:

 $t_{j^{\uparrow}}^{i}$ = the stress tensor; p = the pressure; λ, μ = the coefficients of viscosity; $d_{j^{\uparrow}}^{i}$ = the rate of deformation tensor; $\delta_{j^{\uparrow}}^{i}$ = Kronecker delta.

In a rectilinear shearing flow, according to eq. (50) the shearing stress t_y^x , and hence also the resistance, is proportional to the rate of shearing d_y^x . Since in many physical liquids this relation does not appear to be substantiated by experiments, considerable engineering literature on "non-Newtonian" fluids, in which $t_{y_{\gamma}}^x$ is represented as a polynomial or power series in $d_{y_{\gamma}}^x$, has accumulated. But these one-dimensional treatments can neither reveal nor reflect the characteristic phenomena of non-linear continuum mechanics.

2. 2 Kinetic (Molecular) Theory of Gases

The kinetic theory of gases is based upon a certain model of a gas which satisfies the following assumptions (Ref. 104):

- A gas consists of molecules which in a stable state and in a given type of gas are all alike. The mass of the molecule is denoted by m.
- (2) The molecules are in motion, and as they are material bodies Newton's laws of motion may presumably be applied.
- (3) The molecules behave as elastic spheres of diameter σ . In a perfect gas the number of molecules in the space considered is small enough that the mean distance between the molecules is large compared to their diameter, and thus for these considerations the space they occupy may be disregarded.
- (4) In perfect gases no appreciable forces of attraction or repulsion are exerted by the molecules on each other or on the substance of the containing vessel.

The assumptions of the stable state and similarity of the molecules are introduced to simplify the initial conditions. That the molecules are endowed with motion follows from the fact that they are assumed to have kinetic energies of agitation and are reflected from the walls, producing pressure. That they obey Newton's law is a consequence of the assumption that they are material bodies in motion, and Newton's laws are assumed applicable to all material bodies. The assumption of perfect elasticity is necessary in order to account for the reversibility of the absorption and emission of heat: if it is assumed that they are not elastic, kinetic energy gained on heating would go into the deformation of the atoms when inelastic impacts took place and unless this energy could be given back on cooling, heat would be lost in heating and cooling; if this elasticity does not hold, energy goes to atomic deformation, which may be radiated away as electromagnetic radiation. The assumption of point molecules corresponds to reality only as a rough approximation. In general, the inter-molecular forces of attraction are much greater than the gravitational forces which undoubtedly act between the molecules. For perfect gases all these forces are neglected for simplicity.

From this brief presentation it seems obvious that the mathematical tool applied to the kinetic theory may be taken from the field of classical mechanics of conservative systems. In the kinetic theory of gases viscosity is regarded as due to a transport phenomenon. A streamline instantaneously moving faster than its neighbors will lose more momentum than it gains as the molecules pass in a random manner from one streamline to another, and so it will be retarded in its motion. The coefficient of viscosity is a measure of the net momentum transferred under a specified gradient of mean velocity, and hence is proportional to the mean velocity of the molecules. In general, the nonuniformity in the thermodynamic and/or mechanical properties of a macroscopic system gives rise to phenomena which depend upon the mutual interactions of its microscopic structures. When the latter are identified as actual exchange of the composite microscopically defined particles between one region and another,

the resulting behavior of the system is classed among the transport phenomena.

Present kinetic theories of transport phenomena usually assume that any nonuniformity in the system is only a small deviation from equilibrium, and that any phenomena resulting from these nonuniformities are due to the perturbation terms in the modified expression for the molecular distribution function of momentum and position. This perturbation method was developed by Chapman and Enskog, with higher approximations due to Burnett. The expressions for the transport coefficients are in terms of sets of integrals depending upon the force laws assumed for molecular collisions, since the latter are considered in detail for the development of the "nonuniform" theory. Obviously, there are various transport phenomena.

The kinetic theory of matter furnishes a much more complete prediction of the behavior of gases than is possible with a continuum theory. Maxwell (Refs. 112, 113, 114), Boltzmann, Chapman (Refs. 19, 20, 21), Enskog (Refs. 28, 29), Rocard (128), Burnett (16), Cowling (21), and several others have developed expressions for the stress tensor in a fluid from statistical considerations. The results are not in perfect agreement, and there are indeed reasons to doubt the exact validity of all the analyses of this sort.

Ordinary diffusion is the transfer of mass from one region to another because of a gradient in the concentration; diffusion may also result from a temperature gradient (thermal diffusion or the Soret effect); viscosity is the transport of momentum through the gas because of a gradient in the velocity; and thermal conductivity is the transport of thermal energy resulting from the existence of a thermal gradient in the gas; the transfer of energy may also result from a concentration gradient (diffusion thermo or Dufour effect).

There are three main advantages of a kinetic theory derivation. First, numerical values for the coefficients in the stress tensor expansion may be computed. Second, theoretically the kinetic theory should allow one to predict the boundary conditions in more complicated cases like slip flow, etc. Although past computations (Ref. 141) have not received general acceptance, it seems that something can be done in that respect. The experiments of Knudsen (Refs. 79-81), Kundt and Warburg, and others, have established that, in general, the "non-slip" condition is valid only if the mean free path of the gas is completely negligible relative to the characteristic macroscopic dimension. Hence, for a rarefied gas, the "non-slip" condition must be replaced by some relation which specifies the slip velocity of the gas relative to the solid wall. The phenomenological assumption of Baset specifies that the slip velocity be proportional to the shearing stress at the wall. Similarly, the experiments of von Smoluchowski (Ref. 149) have shown that in rarefied gas there exists a "temperature jump" between the wall temperature and the temperature of the gas layer immediately adjacent to the wall. The third advantage is that it is possible to calculate the heat flux.

The fundamental assumption of the kinetic theory, that all macroscopic, observable properties of a substance can be deduced, in principle, from a knowledge of the forces of interaction and the internal structure of its molecules, has been demonstrated for the equilibrium state largely by the methods of statistical mechanics; the results are roughly equivalent to macroscopic thermodynamics. The study of nonequilibrium states is, of course, much more difficult mathematically (Refs. 38, 40, 41).

For a satisfactory description of a nonequilibrium state on any level, one must have equations which determine the variation in time of the variables of state once their initial values are given. The most detailed description is to specify the instantaneous values of the positions and velocities of all molecules. The equations governing the behavior of the system can be taken to be the Hamilton canoni-

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cal equations in the phase space (p, q). This description, of course, offers much more information than is ever available or even desired, but its disadvantage is that it is discrete rather than continuous. The latter difficulty is most easily remedied by the expedient of Gibbs. Instead of considering a single physical system (Refs. 38, 40, 41), one considers an assemblage of conceptual replicas of the given system or a continuum of such systems and introduces the probability $W(p, q, t) \equiv W(P, t)$ that the system is in the state P at the time t. The function W satisfies the Liouville equation which serves to determine the probability distribution W(P, t) at the time t when its initial value W(P, 0) is given. Gibbs' description is likewise much too detailed for most purposes since it gives the simultaneous probability distribution of all molecules. Another possibility is to consider the probability distribution of a single molecule, molecule (1), independent of the state of all the other molecules:

$$\mathbf{W}_{1}(\mathbf{P}_{1},t) = \int \mathbf{W}(\mathbf{P},t) \frac{d\mathbf{P}}{d\mathbf{P}_{1}}.$$
 (51)

(The notation dP/dP_1 indicates integration over the phase space of all molecules except [1]). The function

$$\mathbf{F} = \mathbf{n} \ \mathbf{W}_{1}, \tag{52}$$

where n = number of molecules, is defined over the phase space of a single molecule and is the distribution function. The expression $F(P_1) dP_1$ represents the number of molecules with coordinates within dP_1 of P_1 . If W is a smooth point function, so is F, and $F(P_1) dP_1$ represents the probable number of molecules in dP_1 even if dP_1 is small compared to the size of a molecule. One usually considers only molecules with no internal degrees of freedom, i.e., physically monatomic molecules.

Let us discuss briefly the assumptions that are needed to obtain a determined equation for F or W_1 . In order to assign a unique W to every W_1 , one usually assumes molecular chaos and binary collision (Refs. 38-41). One statement of molecular chaos is that the simultaneous probability distribution of r + s molecules, W_{r+s} , is the product of the individual probabilities $W_r W_s$, if no molecule of group r exerts a force on any of group s; i.e., in the sense of probability, the two groups are independent. The binary collision assumption states that the gas is so rarefied that collisions involving three or more molecules simultaneously can be ignored. Using the two assumptions, W is reduced to a product of W_1 's and W_2 's; it remains to determine W_2 for a pair of colliding molecules in terms of W_1 . Applying the molecular chaos assumption after the two molecules separate, W_2 for two colliding molecules is seen to be the product of two W_1 's having as arguments the ultimate positions and velocities that the molecules attain after completing the collision. With the addition of a few other minor assumptions, the Boltzmann equation for F results.

The following assumptions are used in the derivation of the Boltzmann equation: (1) point molecules; (2) complete collisions; (3) slowly varying distribution function; and (4) molecular chaos.

The second assumption is a stronger form of the binary collision assumption. The third assumption states that the molecular distribution function does not vary appreciably over a distance covered by the average molecule in a certain period dt. This restricts this function to be essentially constant over a distance comparable to the size of a molecule, but imposes no restriction on the variation in that function over distances comparable to the mean free path. In particular, flows around objects of molecular size cannot be handled by the Boltzmann equation, but object dimensions of the order of a mean free path cause no difficulty. The fourth or molecular chaos assumption cannot be given a simple physical interpretation; it has been proved only for the equilibrium state.

The problem of solving the Boltzmann equation has been attacked in several ways. Hilbert (Refs. 53, 54) constructed a method of finding all solutions F of the Boltzmann equation which are of the form:

$$\mathbf{F} = f_0 \, \lambda^{-1} + f_1 + f_2 \, \lambda + f_3 \, \lambda^2 + \dots, \tag{53}$$

where f_i (i = 0, 1, ...) are also solutions, and λ is an arbitrary parameter to be identified with the mean free path. Since as $\lambda \rightarrow 0$, the assumptions upon which the Maxwell-Boltzmann equation is derived lose their validity, and as $\lambda \rightarrow \infty$ any polynomial approximation to (53) becomes less accurate, the results obtained by this method can have at most a narrow range of validity and an asymptotic character (Refs. 171, 172). Enskog's accepted scheme (Refs. 28, 29) begins with a λ series, but while Hilbert's method determines the successive approximations at each stage, Enskog introduces a considerable arbitrariness, to be eliminated later by a formal procedure whose mathematical and physical meaning is not quite clear. The most general stresses yet derived from the kinetic theory by Enskog's method are those of Burnett (Ref. 16). A new method of integration of the Boltzmann equation proposed by Grad (Refs. 38, 40, 41) does not employ the notions of stress and heat flux, but instead yields gross equations of motion in terms of moments of the distribution function up to any specified order.

In general, a criterion for the range of validity of the approximate methods of solution of the Boltzmann equation is provided by the comparison of some characteristic length L with the mean free path L_c . When L becomes comparable with L_c , it is necessary to go to higher approximations to obtain adequate results. As discussed by Herzfeld (Ref. 52), Tsien and Schamberg (Ref. 180), Primakoff (Ref. 125), and others, important dynamic contributions appear only in approximations higher than the second, but none of these authors has been able to derive more than the third approximation, due to formidable difficulties.

Bhatnagar, Gross and Krook (Ref. 7) propose an iteration method for solving the Boltzmann equation which deals with the entire range of pressures in a unified manner and which satisfies general microscopic boundary conditions. Their treatment of the term involving the collision processes in gases leads to a simple mathematical formation of Boltzmann equation. Grad (Refs. 40, 41), considering the integral of angular momentum, concludes that the effects due to angular momentum are extremely small.

The problem of transport phenomena in polyatomic gases was attacked by Wang-Chang and Uhlenbeck (Ref. 187). Jaffe proposed finding a series solution of the Maxwell-Boltzmann equation in the form

$$F = f_0 + f_1 \lambda^{-1} + f_2 \lambda^{-2} + \dots$$

appropriate to very rarefied gases; the first approximation is "free molecule flow" rather than Eulerian hydrodynamics. Application of the hydrodynamic equations in the forms proposed by Burnett and Grad to the theory of the boundary layer was performed by v. Krzywoblocki (Refs. 86-89). A regime on the border between the slip flow and free molecule flow was treated by Epstein (Ref. 30), v. Krzywoblocki (Ref. 90), and others.

2.3 Continuum Versus Kinetic Theory

Comparing his proposition with Burnett's stress equations, Truesdell (Ref. 172, p. 143) concludes that an immediate comparison is not possible, not only because of the awkward form in which Burnett's equations are expressed, but also because they contain the superfluous dependent variable (density) which must be eliminated by the equation of state, following which there appear additional relations whose physical meaning is not apparent. In discussing results obtained by Enskog's method of integration of the Maxwell-Boltzmann equation, Truesdell (Ref. 172, p.145) points out that the successive approximations are uniquely defined only in terms of a certain formal procedure which perhaps may not yield all terms involving some magnitude at the mth stage. Thus some of the terms which appear in Burnett's equations may possibly be cancelled by terms from presently undetermined higher approximations. This anomaly is not inherent in the kinetic theory treatment, for Grad's results seem to be free of it. Truesdell (Ref. 172, p. 146) maintains that the whole subject of the derivation of hydrodynamical equations from the kinetic theory deserves to be re-evaluated, clarified, and presented from a more general point of view. The comparison of the results of the two approaches (continuum and kinetic theory) to the problem of determining the stress and heat flux in rarefied gas seems to indicate that the present form of the kinetic theory becomes less adequate for the ordinary prediction of gross phenomena the higher the degree of approximation required (Ref. 172, p.148).

One may summarize the advantages of the kinetic theory as follows:

- (a) In its broader features, the molecular model more closely resembles the accepted picture of physical matter. This advantage is seriously reduced, however, by the extreme idealizations which must be incorporated in the model if the calculations are actually to be carried out.
- (b) The numerical values of the coefficients are predicted, while in a continuum theory these must be experimentally determined. This argument is the strongest of all in favor of the kinetic theory.
- (c) In principle, it should be possible to calculate boundary conditions as well as equations of motion from the kinetic theory; to obtain boundary conditions in a continuum theory, one must in effect postulate them. A satisfactory kinetic theory treatment has yet to be given, however.
- (d) In a general kinetic theory the model may be adjusted so as to yield different results for very rare gases, very dense gases, liquids, etc.

Advantage of continuum theory are as follows:

- (a) It is not restricted to perfect gases, to compressible fluids, to homogeneous substances, etc.
- (b) Its results are free from the special relations among the coefficients, which kinetic theory predicts but does not explain or justify. On the other hand, it gives no hint of the numerical values assumed by these coefficients.
- (c) The terms of any given degree (following Truesdell's proposition) are relatively simple when compared with the elaborate calculations of the kinetic theory.
- (d) Continuum theory, being independent of deterministic mechanics of the ultimate particle, serves as a general guide with which any molecular model must be consistent.

In his discussion on the controversy regarding the bulk viscosity of fluids, Truesdell (Ref. 177) points out that recent physicists regard the Stokes relation as obviously false. Truesdell's paper is abstracted below.

The controversy concerning bulk viscosity $(\mu' + \frac{2}{3}\mu)$ separates into the following parts: (1) What is the effect of the value of $(\mu' + \frac{2}{3}\mu)$ upon solutions of the classical equations of fluid dynamics? (2) In physical fluids which obey these equations, how is $(\mu' + \frac{2}{3}\mu)$ to be measured? (3) Which physical fluids fail to obey the classical equations? (4) What mathematical theory is appropriate for these fluids?

Beginning with the first question, Truesdell maintains that there exist only three groups of solutions which seem to be useful: plane shock-layer solutions, infinitesimal wave solutions, and second order circulatory solutions. Gilbarg and Paolucci (Ref. 36) have solved the plane shock layer exactly and completely. Their results show: (1) that shock thicknesses computed earlier are much smaller than those given by the rigorous theory employing the physically appropriate dependence of viscosity upon temperature, and (2) that large enough bulk viscosity yields arbitrarily thick shocks. The position, relative to the exact theory, of solutions of the linearized equations for infinitesimal waves remains to be established mathematically. The exact solutions for free plane waves, forced or free spherical waves, and shear waves are not yet known. The solutions for acoustic streaming are more controversial.

The second question asks: "Which physical fluids obey the equations?" It is still widely believed that few, if any, physical fluids experiencing shock-layer or ultrasonic phenomena behave like the mathematical viscous fluid. Truesdell maintains that more physical fluids will show agreement with the mathematical model.

Concerning the value of the bulk viscosity, the question arises whether the hydrodynamical theory can account for "relaxation effects." Truesdell answers, "No, it cannot." Briefly, a systematic perturbation scheme to take into account the absorption and dispersion phenomena at higher frequencies reveals the difficulties usual for second order effects.

This brings the reader to the third question. Many ordinary fluids, all the common polyatomic gases being included, do not behave like the classical viscous fluids when subjected to an ultrasonic disturbance.

Now for the fourth question, which concerns the theory appropriate for these fluids. While there is a good deal of literature attempting to fit the data to viscoelasticity (the usual term among ultrasonic workers is "complex and frequency dependent viscosity"), the various proposals either fail to agree with experiment or contain so many empirical constants that almost anything can result. Recent proposals regarding such a physical fluid as a mixture of two or more components, each of which is a continuous medium diffusing through the rest, offer some possibilities. In the final step, the bulk viscosity appears in such a scheme as a crude equivalent which one may, but need not, introduce. For physical fluids which behave neither as pure fluids with linear viscosity nor as mixtures of such fluids, various theories of nonlinear viscosity have been proposed.

It is natural to suppose that the kinetic theory can give us much more dependable information. Such must indeed be the case ultimately, but it is not the case today. Beginning with the theory of moderately rarefied monatomic gases, one finds five essentially different types of methods proposed for solving the Maxwell-Boltzmann equation: the Hilbert-Enskog-Chapman (perturbation) series, the Jaffé-Keller (perturbation) series. Grad's method of moments, Mott-Smith's method of interpolation, and the Bhatnagar-Gross-Krook iteration method for a particular case. From the first three, none has been shown to converge or to be meaningful in any sense. Jeffreys (Ref. 62) has made some penetrating remarks which question whether for non-equilibrium states the Maxwell-Boltzmann equation itself is the correct mathematical statement of the physical ideas which constitute the kinetic view of the gaseous state. But the recent result of Morgenstern (Ref. 115) indicates that the doubts regarding the existence and uniqueness of a solution of the Maxwell-Boltzmann equation may soon be allayed.

When we come to polyatomic gases, the situation is worse. Every attempt to calculate bulk viscosity from the kinetic theory has proved incomplete or faulty (Ref. 175). Moreover, there exists no systematic theory analogous to those just mentioned for monatomic gases. The controversial state of the kinetic theory of liquids need hardly be emphasized. Thus for the immediate future one is not likely to gain any certain information from the kinetic approach to the problem of viscosity. But Truesdell (Ref. 177, p. 64) expresses hope that the substantial progress made recently in various parts of continuum mechanics will encourage pursuit of the basic problems concerning viscosity with the care and the criticism required for exact treatment of the appropriate nonlinear field equations.

In sum, it may be hoped that the indifferent mathematics applied in the past to the kinetic theory will be abandoned in favor of real mathematics which may permit better results based upon the kinetic theory, which theory must ultimately give a better picture than continuum. The controversy between continuum and kinetic theory seems to be interpreted wrongly. There is no question that the physical model of the kinetic hypothesis appears correct. A mathematical representation of this model, the Maxwell-Boltzmann equation, may not be quite correct in non-equilibrium conditions, but this does not indicate that the physical model of the kinetic hypothesis is wrong. Some techniques of the solution of the Maxwell-Boltzmann equation, like that of Chapman-Enskog-Burnett, may be incorrect. But again, this does not imply that the physical model of the kinetic hypothesis is wrong. Another question is that there are strong indications that fluid dynamics must take into account "sub-miscroscopic" phenomena, like those of the nature of atomic and molecular structure in order to explain macroscopic kinematic and thermodynamic phenomena.

And still another problem is the application of hydrodynamic equations to motions of the earth's atmosphere. What equations can describe such phenomena is not yet thoroughly understood. Until now the Navier-Stokes or even Euler's equation are generally used, often in a linearized form, i.e., $du/dt = \sim \frac{\partial u}{\partial t}$, with the omission of the uu_x, etc. The necessity, in fact, of using these nonlinear forms in describing the motions of the atmosphere at altitudes greater than 100 kilometers has been demonstrated by Pekeris (105).

2.4 Systems of Charged Particles and Scattering of Electromagnetic Radiation by Turbulence

The theory of oscillations in ionized gases is still tentative (Refs. 7, 8) although a number of features can be understood, at least qualitatively. An essential difference from the theory for neutral gases is that approximately undamped waves can be propagated not only at high but also at low pressures. The mechanism responsible for the cooperative behavior of the medium is different in the extreme cases of low density and high density (Refs. 12, 13). At low densities the collisions are of only secondary importance, and the forces acting to change the state of motion of a particle are electromagnetic in character. Energy and momentum are transferred from one group of particles to another through the intermediary of the electromagnetic field in a way now familiar from the study of microwave devices. It

is important to note, however, that the transfer of energy by the high frequency components of a pulse is a very slow process in low pressure plasmas (Refs. 7,8).

Some attempts have been made to treat the oscillations of ionized gases quantitatively by the methods of kinetic theory. The long range of the Coulomb force implies that the concept of definite binary collisions is inadequate except for very close encounters. Instead, it appears that every charged particle is continually interacting with all the particles of the assembly.

An important theoretical step, making possible the approximate treatment of many properties of ionized gases, was taken by Vlasov (Refs. 182, 183). Langmuir (Ref. 99) had already pointed out that the Debye length is characteristic of the dynamic behavior as well as of the static properties of an ionized gas. Vlasov assumed that apart from close collisions a particle moves in an average electric field arising from the other particles and proposed to describe the system by a one-particle distribution function.

Others (Refs. 11, 23, 33, 94, and 95) have treated various processes in ionized gases by using the binary collision approach even for distant collisions. Such distant collisions involve small momentum transfers, and thus expansion of the distribution functions in the collision integral term in powers of the momentum transfers leads to terms very similar to those given by the Fokker-Planck equation. Although this procedure is only approximate, in the present primitive state of the theory it is worthwhile exploring the consequences of this approach. The Fokker-Planck approach has already been used in the study of plasma oscillations by Logunov.

There exist several studies of the oscillations of ionized gases using transport equations. For example, the Thomsons (Ref. 163, ii, 353) and subsequently Bailey (Ref. 4) base their discussions on Maxwell's equations of transfer, and the Thomsons' approach is further brought out in an alternative treatment by Linder (Ref. 102).

The recent approach of Bhatnagar, Gross, and Krook (Ref. 8), although an approximate one, offers some possibilities, since the equations for neutral and ionized gases are extremely complicated in practice because of the intractable nature of the Boltzmann binary collision term. While Linder, Bailey, and the Thomsons discuss some simple kinetic models which permit exact mathematical treatment including the solution of the definite boundary value problem, Bhatnagar, Gross, and Krook refer to both electron-neutral or ion-neutral collisions and electron-electron or ion-ion collisions, which are important in high pressure ionized gas. The modified collision terms are constructed so that each collision conserves particle number, momentum, and energy; other characteristics, such as persistence of velocities and angular dependence, may be included. Their article illustrates the technique for a simple model which involves assuming a collision time independent of velocity.

In the field of electro-magneto-fluid dynamics, Villars and Weisskopf (Ref. 182) apply to the electromagnetic problem in compressible medium the results of the statistical theory of locally isotropic homogenous turbulence developed for incompressible media. In particular, they apply the hypotheses of Weizsäcker and Heisenberg. According to this theory, the pressure fluctuations produce density fluctuations in refractive index and hence a scattered field. Silverman and Balser (Ref. 148) apply the theory of Villars and Weisskopf to derive the amplitude distribution of the scattered radiation. Good agreement with experimental results is obtained.

Severnyi (Ref. 147) derives a mathematical analysis of the motion of nodes and streams in protuberances, based on the fundamental equations of magneto-hydrodynamics for small scale motions in the neighborhood of the hydrostatic equilibrium of plasma. The passage of a plane aerodynamic wave

through a plane ionosphere in a magnetic field is discussed by Lucas (Ref. 109). The phenomenological theory of turbulence in magneto-hydrodynamics was developed by Chandrasekhar (Ref. 17) on the basis of the equations of motion derived by Batchelor (Ref. 5). It was generalized to compressible fluid flow regime by v. Krzywoblocki (Refs. 83-85). Some particular problems in that regime are discussed by Gjellestad (Ref. 37). The solution of Boltzmann's equation for a Lorentzian gas and the application to weakly ionized gases is treated by Bayet, Delcroix, and Denisse (6). The hydrodynamic equation of an electron stream, similar to the Navier-Stokes equation of motion with one additional term is derived by Howard (56). Application of this equation to the boundary layer of an electron stream was done by v. Krzywoblocki (Ref. 91).

2.5 Free Molecule Flow and Newtonian Gasdynamics

Above a certain degree of rarefaction of the body of the gas, neither the mechanics of continuum nor the kinetic (molecular) theory of gases can describe the phenomena. Here the collision between the molecules of the gas may usually be neglected, partially or completely, as compared to the collisions of molecules with the object. The hypothesis of Newton on the drag of a body moving in a gas is revived and readjusted; the drag is caused by collision of a solid body with particular discrete molecules of the gas. In this regime Epstein (Ref. 30) has obtained the drag on a sphere at very low Mach numbers, Zahm (Ref. 198) the drag on a plate, and Tsien (Ref. 179) on an element of surface at all Mach numbers. Epstein's work was generalized and extended by v. Krzywoblocki (90).

The bibliography lists several other papers on the subject in question. They distinguish two regimes: (1) free molecule flow, where after the reflection the molecules possess both normal and tangential velocity components, i.e., the molecules are fully elastic; (2) Newtonian gas dynamics where following the collision only the tangential velocity component is preserved, i.e., the molecules are inelastic. The latter type of flow is extremely unlikely and probably physically impossible.

The momentum transmitted to the object each second depends partly on the way the molecules are reflected at the surface. Experiments show that at least three different types of reflection can occur depending on the state and nature of the surface, the kind of gas, the density of the impinging stream, and the respective temperatures of the gas and surface (46). These are: specular reflection, diffuse reflection, and condensation and re-emission.

In specular reflection, the components of the molecular velocity tangent to the surface remain unchanged, but the component normal to the surface reverses its sign. The most conclusive experimental results have been obtained by Stern and collaborators (46), who showed that specular reflection, under the condition that the surface forces are not too strong, can occur in two cases: (1) when the surface irregularities are of the same or smaller order of magnitude than the de Broglie wave length of the incident particle, which condition can be satisfied by having very smooth surfaces or by allowing the molecules to strike the surface at very small glancing angles; (2) when the molecules are scattered from a crystal whose grating space is of the same order of magnitude as the de Broglie wave length of the incident particles.

In the diffuse case, the molecules are reflected at random from the surface, all traces of their past history having been lost; they obey a cosine law similar to that of a surface emitting radiant energy.

In the case of condensation and re-emission, the molecules condense on the surface for a certain period of time T, after which they are re-emitted in a random way. In true condensation and re-emission,

the number of molecules emitted by the surface each second is not necessarilly equal to the number that hits the surface each second.

Sänger (Ref. 139) assumes in calculating the flux of momentum and energy that the gas molecules collide with single atoms in the solid; apart from this assumption the familiar kinetic theory is applied The contribution of elastic collisions is taken into account. A regime on the border between slip flow and free molecule flow was treated by Epstein (Ref. 30), v. Krzywoblocki (Ref. 90), and others.

2.6 Relativistic Approach

There exist various approaches to macroscopic theories of fluid dynamics from the standpoint c relativity. One can mention here the works of Lamla (Ref. 93), Eckart (Ref. 26), Jüttner (Ref. 65), Taub (Refs. 160, 161), Salzman (Ref. 134), and Salzman and Taub (Ref. 135).

In particular, Khalatnikov (Ref. 77) in anticipation of future application to nuclear physics has studied the adiabatic, nondissipative flow of liquids according to special relativity, obtaining the general solution of the resulting equations for flow in one dimension.

2.7 Statistical Mechanics of Fluids

An extensive application of statistical methods in the theory of turbulence inspires many to investigate the statistical mechanics of fluids. In the purely descriptive theory, the kinematics of a turbulent velocity field and the stationary random functions seems to be a well suited tool; but when one turns to the dynamics, he is stopped almost immediately if he restricts himself to the domain of mechanics of continuum. Kampé de Fériet (Ref. 63) concludes that the mixture of the methods of probability used in the statistical approach and of equations suggested by the fluid dynamics of continuum is perhaps unfortunate. A return to the foundations in constructing a statistical fluid mechanics is thus suggested.

The characteristic features of the statistical mechanics of a conservative dynamical system having a finite number of degrees of freedom and satisfying the Hamilton-Jacobi equations are as follows:

- (1) definition of the phase-space Ω ; every state of the system is characterized by a point $\omega \epsilon \Omega$;
- (2) proof of a uniqueness theorem; starting at the initial time t = 0 from a given initial state ω ; all the subsequent or prior states $T_{\pm}\omega$, where t varies from $-\infty$ to $+\infty$, are perfectly well determined and described, in Ω , a curve, the trajectory $\Gamma(\omega)$;
- (3) definition of a measure μ in Ω invariant under the transformations $T_{+}\omega$ (Liouville's theorem);
- (4) proof of the ergodic theorem: the time-average computed along a trajectory $\Gamma(\omega)$ exists for almost all ω ; time-average and statistical average are equal if the transformation $T_t \omega$ of Ω into itself is metrically transitive.

Since in the most general approach a fluid flow system has an infinite number of degrees of freedom, one has to take a function space instead of a phase space, a new difficulty but not an impossibility; Kampé de Fériet has shown that for some continuous medium having a function space it is easy to build a complete statistical mechanics (Refs. 72, 73).

From the Lagrangian point of view a fluid state at a given time t is defined by the positions and the velocities of all the particles. Let us call $a(a_1, a_2, a_3)$, a ϵX , the position of a particle at the initial time t = 0; the coordinates of the same particle at the time t are three continuous functions of four variables $\{a_1, t\}$ (i = 1, 2, 3), i.e.:

$$x_{j} = x_{j}(a, t)$$
 $j = 1, 2, 3,$ (54)

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the correspondence between x and "a" being one-to-one. The components of the velocity of the particle are given by:

$$\mathbf{x}_{j} = \frac{\partial}{\partial t} \mathbf{x}_{j} (\mathbf{a}, t).$$
 (55)

One has to take as the phase space Ω a function space in which a point ω is defined by a set of six functions of three variables $\{\partial_i\}$ (i = 1, 2, 3):

$$\omega = \{\alpha_i(a), \beta_i(a)\}$$
 $j = 1, 2, 3,$ (56)

the functions $\alpha_j(a)$, $\beta_j(a)$ being continuous to any order "n" that we want to use later in the equations of fluid dynamics. A state of the fluid is represented in the function space Ω by the point ω such that:

$$\begin{aligned} \mathbf{x}_{\mathbf{j}} &= \alpha_{\mathbf{j}}(\mathbf{a}) \\ \mathbf{u}_{\mathbf{j}} &= \beta_{\mathbf{j}}(\mathbf{a}), \end{aligned}$$
 (57)

and a motion of the fluid is represented in Ω by the set of points ω (trajectory Γ) such that:

$$\alpha_{j}(a) = x_{j}(a; t)$$

 $\beta_{j}(a) = u_{j}(a; t).$
(58)

To proceed further we must have a uniqueness theorem: starting from a given initial state $\omega \in \Omega$ at t = 0, we must be assured that all the subsequent states of the fluid are fully determined. But at present the results are indefinite for both a perfect and a viscous fluid. Although Leray (Ref. 101) has proved that with regular initial conditions in an incompressible viscous fluid filling the whole space X there is one and only one regular motion in a finite interval for the case of finite total energy of the fluid, normally the interest is in velocity fields for which total kinetic energy is infinite, and thus his results are of little use. The fact remains that no uniqueness theorem has been advanced which is broad enough to be used as a foundation for statistical fluid dynamics.

Kampé de Fériet discusses briefly the question of an invariant measure (Ref. 71, p. 158). In classical statistical mechanics the existence of an invariant measure in Ω (Liouville's theorem) is connected with the fact that the system is a conservative one; if there are dissipative forces acting on the system, the energy will tend toward zero as the time increases: all trajectories in Ω will have the particular point ω corresponding to equilibrium as the limiting point; this fact is obviously not comparable with the invariance of measure along a trajectory. The same contradiction will appear for a viscous fluid when the total kinetic energy is finite at the initial time; the final state of the fluid will always be the equilibrium; thus the definition of a measure invariant along energy trajectory is impossible.

If the total kinetic energy is infinite there is hope that an escape from the logical contradiction is possible in some cases. Kampé de Fériet (Ref. 71, p. 159) concludes that an invariant measure would exist only in the case of conservative systems--that is, only for perfect fluids.

New possibilities in this field are opened by Morrey (Ref. 116), who suggests several methods for deriving the laws of the mass motion of a "continuous medium" from the study of the motions of finite systems of particles (point-masses). Since such systems are not continuous media, some way must be found to "pass from the discrete to the continuous." Morrey employs three methods: (1) a study of the motions of the particle systems themselves by means of the Fourier-Stieltjes transforms of the corres-

ponding (finite) distribution of mass, momentum, and energy; (2) the introduction of a continuous family of systems of particles by introducing a probability distribution in "phase-space" (an idea originally conceived by Gibbs); (3) the reduction of a problem of finding time averages to that of finding space averages using the ergodic theorem.

2.8 Quantum Hydrodynamics

Below is a brief chronological review of some papers on quantum hydrodynamics. Similar reviews are in the dissertation by Whittenbury (Ref. 194) and in the paper by v. Krzywoblocki and Whittenbury (Ref. 82).

2, 8, 1. Madelung (110)

Using the second form of Schrödinger's equation:

$$\Delta \psi - 8\pi^2 \, \mathrm{mh}^{-2} \, \mathrm{U} \psi - 14\pi \, \mathrm{mh}^{-1} \, \psi_{,+} = 0, \qquad (59)$$

and the proposition $\psi = \alpha \exp(i\beta)$, Madelung obtains two equations:

$$\Delta \alpha - \alpha \,(\text{grad }\beta)^2 - 8\pi^2 \,\text{mh}^{-2} \,\text{U} + 4\pi \,\text{mh}^{-1} \,\alpha\beta_{1,\nu} = 0 \tag{60}$$

$$\alpha \Delta \beta + 2 (\operatorname{grad} \alpha \operatorname{grad} \beta) - 4\pi h^{-1} \alpha_{,+} = 0.$$
 (61)

The second equation with $\phi = \beta h(2\pi)^{-1}$ gives

div
$$(\alpha^2 \text{ grad } \phi) + (\alpha^2)_{+} = 0,$$
 (62)

which can be interpreted as a continuity equation with $\rho = \alpha^2$ and $\vec{u} = \text{grad } \phi$. Equation (60) gives with curl $\vec{u} = 0$:

$$d\bar{u}/dt = -m^{-1} \text{ grad } U + \text{ grad } [\alpha^{-1} \Delta \alpha h^2 (8\pi^2 m^2)^{-1}],$$
 (63)

which can be interpreted as Euler's equation of motion with the first term on the right side of eq. (63) equal to mass force $t\rho^{-1}$ and the second one to the pressure term - $\int \rho^{-1} dp$.

2.8.2 London (105-108)

London in 1938 advanced the hypothesis that the transition of liquid helium I into liquid helium II might be caused by the condensation mechanism of the degenerating Bose-Einstein gas. He suggested that the superfluid flow might be connected with the condensed phase which consists of molecules of macroscopic de Broglie wave length. His 1945 paper discusses low temperature transfer.

2.8.3 Tisza (165-168)

The idea of applying results of the ideal gas theory to the liquid state appears at first sight somewhat daring. Yet for liquid helium the gas picture is probably not quite so unrealistic as it would be for any other liquid. It was Tisza who first recognized the possibility of evading the pitfalls of a rigorous molecular kinetic theory employing the qualitative properties of a degenerating Bose-Einstein gas to develop a consistent macroscopic theory. This two-fluid theory is based on the following assumptions:

(1) Liquid helium consists of two mutually interpenetrating fluids, the "superfluid" of density ρ_s and the "normal" fluid of density ρ_n . Each is supposed to have its own velocity field v_{si} and v_{ni} , respectively. At any point in the space the mass velocity ρ is written in the form $\rho = \rho_s + \rho_n$ and the mass current density $J_1 = \rho_s v_{si} + \rho_n v_{ni}$. (2) The entropy $s_s = 0$. (3) The viscosity coefficient of the superfluid is zero. (4) The normal fluid is supposed to be the carrier of the whole thermal excitation of the liquid; the entropy of liquid helium II is entirely attributed to the normal liquid.

2.8.4 Yvon (197)

Yvon shows that the relativistic mechanics of Dirac gives the same transformation as the procedure of Madelung, who uses the Schrödinger mechanics in a more mechanical than a quantum sense.

2.8.5 Landau (94-96)

Landau rejects the gas statistics approach, arguing that a liquid is generally much more like a solid than a gas, and he attempts to put his two-fluid theory on an entirely new basis. His point of departure is an extension of the quantum theory of fields, and accordingly he tries to represent the liquid as a quasi-continuum whose excitations are quantized, as in the Debye theory of the solid body or in quantum electrodynamics. He assumes that the excited states of liquid can be represented by two kinds of elementary excitations, the "phonons" and the "rotons." The phonons are the excitations of the longitudinal sound waves, and represent the potential motions of the liquid, characterized by curl $\vec{V} = 0$. The rotons are described as the elementary excitations of a vortex spectrum (curl $\vec{V} \neq 0$). The roton spectrum is assumed to be separated by an energy gap from the lowest phonon state, the ground state of the potential motions being the lowest state of the system. Both rotons and photons are supposed to have an effective mass and a momentum which are attributed to the "normal fluid." The remaining mass corresponds to the superfluid, which is assumed to be able to move as a whole with its own velocity and without dissipation. Once the possibility of the two velocity field is granted, the development of the macroscopic hydrothermodynamics has to proceed along the same line as in Tisza's theory.

2.8.6 Dingle (24)

The paper reviews the theories which have been proposed to explain the peculiar properties of liquid helium. Dingle discusses the Bose-Einstein condensation of an ideal gas, order-disorder transition theories, Landau's quantum hydrodynamics, Green's theory of quantum liquids, etc.

2.8.7 Takabayasi (156)

By re-expression of the generalized Schrödinger equation in its coordinate representation in terms of amplitude and phase of the state vector, a quantum mechanical change of a system can be made to correspond to an ensemble of classical motions of the system to which is added some internal potential. Bohm's renewed form (9) of the statistical interpretation of quantum mechanics is criticized in several points. The hydrodynamical picture formally equivalent to the statistical picture in one-body problems is considered, and from such analogy a formal generalization of the Schrödinger equation is suggested.

2, 8, 8 Kronig and Thellung (82)

The classical hydrodynamics of non-viscous fluids for the case of irrotational motion in the absence of external forces is represented in terms of general field theory. The velocity potential and the density

appear as canonically conjugate variables in a rigorous sense. A quantization is carried out along the usual lines, justifying a number of results previously presented by Landau and his collaborators.

In the second paper Thellung (Ref. 162) extends his previous work to include vortex motions. With the aid of a transformation by Clebsch it is possible in this general case to bring the hydrodynamical equations into a canonical form. The total Hamiltonian is then found to consist of three parts involving: (1) the phonon field; (2) the roton field, and (3) an interaction between the two. In this way Landau's interpretation of the properties of helium Π can be given a more secure foundation.

2.8.9 Ziman (199)

The Clebsch formula for fluid velocity allows the classical hydrodynamical equations, including vorticity, to be derived from a variational principle and put into canonical form. The standard quantization procedure of the theory of fields then gives a set of field operators satisfying the commutation relations obtained by Landau in 1941. The Hamiltonian contains terms corresponding to the excitation of the "roton" states of Landau's theory.

2.8.10 Itô (57)

A canonical formalism in hydrodynamics is developed with the aid of Clebsch's transformation. If one considers the adiabatic process where the entropy is preserved, the vortex motion is found to be closely connected with the entropy. Euler's hydrodynamical equation emerges factorized into four fundamental equations which are discussed from the thermodynamical point of view. Although Itô has succeeded in constructing a Lagrangian formalism in hydrodynamics, the idea of "roton" is not clarified in this paper. The commutation relations do not assume the validity of the standpoint of quantum hydrodynamics if Itô's results are the same as London's or Landau's.

2.8.11 Takabayasi (157)

The formulation of quantum mechanics in terms of the picture of trajectory ensemble or of the hydrodynamical picture, developed in Takabayasi's previous paper (Ref. 156), is further supplemented Individual trajectories for some typical non-stationary state are explicitly obtained, illustrating that they generally show complicated fluctuations due to the action of quantum potential. Next, emphasis is placed on the fact that the Schrödinger field admits a mechanical model. Finally, the picture of trajectory ensemble is generalized to represent wave equations with sources.

2.8.12 Tyabji (181)

A number of authors (Itô, Kronig and Thellung, Ziman) have recently quantized the motion of an inviscid fluid. The starting point has been Bateman's variational principle, which uses the Clebsch variables. The density turns out to be the canonical conjugate to the velocity potential, and the transition to the quantum theory is then made in the usual way. If the fluid is making small vibrations, "phonons," which are scalars, appear as a result of the quantization.

In this paper the Lagrange variables of classical hydrodynamics are used because of their similarity to the variables of particle dynamics. The principal difference from the work in the Clebsch variables is that vector rather than scalar "phonons" appear. If these "phonons" are resolved in the direction of the wave-number vector \vec{k} , and transverse to it, the transverse part may be identified with "rotons."

2.8.13 Kaempffer (68)

Attempts by Takabayasi and Kaempffer at an entirely different method of field quantization are examined in the light of Ziman's successful approach to the quantum hydrodynamical problem. It is pointed out that the energetic impossibility of a roton spectrum in an ideal continuum fluid makes it necessary to introduce a fundamental length, which acts as high frequency cut-off. Takabayasi's generalized hydrodynamic formulation of the nonrelativistic Schrödinger equation is treated as an example.

2.8.14 Kaempffer (69)

There exist at present two entirely different approaches toward quantization of classical field theories. In the conventional approach the field under consideration is described in terms of a wave function ψ and its complex conjugate ψ^* , and these are subjected to commutation of the type:

$$[\psi(\mathbf{x}); \ \psi^{*}(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}'), \tag{64}$$

where a quantization leading to Bose statistics is used. The eigenvalues of the operator $\int \psi^* \psi dx$ turn out to be integers and are therefore interpreted as the number of particles present in a given state of the field.

In the approach of quantum hydrodynamics, the same field is described in terms of suitably chosen density ρ and velocity potential ϕ , and these are subjected to commutation relations of the type:

$$[\boldsymbol{\phi}(\mathbf{x}); \boldsymbol{\rho}(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}'). \tag{65}$$

This gives rise to a description in terms of an excitation gas of Bose particles, which is made responsible for all observable effects of the field, while the ψ -field is demoted to the somewhat inferior role of the underlying fluid, in which observable effects appear as excitations of the motion.

As there is no <u>a priori</u> reason for preferring one or the other of these approaches toward quantization of a given classical field theory, there is still doubt about the justification for the quantum hydrodynamical approach. The reason is the belief that the conventional quantization method gives an essentially correct many-particle quantum theory, and that a justification for the procedure of quantum hydrodynamics has to consist of a proof that the commutation relations (Eq. 65) follow from the commutation relations (Eq. 64), or that quantum hydrodynamics can at best yield only an approximate description of a many-particle system. Kaempffer in this paper examines the conditions under which the procedure of quantum hydrodynamics is a consequence of the conventional quantization procedure, and vice versa.

2.8.15 Morita (115)

Morita derives the equations of hydrodynamics from the equations of hydrodynamics given by Irving and Kirkwood by means of the statistical mechanics. The newly derived equations contain explicitly the quantities concerning both phonons and macroscopic fluid flow.

2.8.16 Schönberg (143, 144)

Schönberg discusses a new hydrodynamical model for the Schrödinger equation which differs from that of Madelung by the existence of turbulence. It follows directly from the ordinary interpretation of quantum mechanics, by the introduction of operators for the charge and current densities and the components of the stress tensor in the one particle formalism. The model is developed for any values of the

spin. The Madelung fluid corresponds to the mean motion of the special turbulent medium. The quantum potential appears as a combination of pressure with terms arising from the turbulence. It is shown that the quantization of the motion of the Madelung fluid introduces the right kind of turbulence. The trajectories of the deBroglie-Bohm theory appear as trajectories of the mean motion of the turbulent medium. Schönberg shows clearly that the Madelung fluid corresponds to the expectation values of the quantities of the quantized fluid in the one of quantum states. The quantization of the fluid regenerates the turbulence eliminated by taking the expectation values in the one particle formalism. The regeneration of the turbulence can be related to the vacuum fluctuations of the quantized Madelung fluid.

2.8.17 Schönberg (145)

Schönberg discusses the general motions of the continuous medium (Madelung fluid), whose irrotational motions are described by the Schrödinger equation. It is shown that many of the the basic theorems of the vortex motions of the inviscid barotropic fluids are also valid for the Madelung fluid.

2.8.18 Alcock and Kuper (1)

The quantum mechanical Hamiltonian obtained by Ziman and by Thellung for an ideal liquid is diagonalized in the vicinity of small compressibility. On taking account of the interaction between "phonon" and "roton" variables, the roton rest energy is found to be proportional to the inverse of the sound velocity and to the ninth power of the wave number cut-off. The effective mass μ_{inc} of the incompressible roton is given by

 $\mu_{\rm inc} = 9\rho_0 \pi^2 k_0^{-3}$

where

 ρ_{0} = the mean value of the density,

 k_{o} = the cut-off in wave-number space.

It seems reasonable to picture the roton as a moving sphere of liquid, with a radius of the order $\pi(2k_0)^{-1}$ to πk_0^{-1} . On this basis the effective mass should be of the order $\rho_0 \pi^4(6k_0^3)^{-1}$ to $4\rho_0 \pi^4(3k_0^3)^{-1}$, which is not in disagreement with the exact value of the equation. The possibility of classical vortices of this type was originally demonstrated by Hill in 1894 (see also Lamb, 1932) and has recently been pointed out by Pekeris (1953). Vorticity must arise, for instance, at the edges of the moving sphere, so that such excitations would be forbidden in an irrotational fluid. For illustrative purposes, πk_0^{-1} is equal approximately to six or seven atomic distances.

2.8.19 Discussion

It is difficult to divide the field of quantum hydrodynamics into distinct groups. Nevertheless, it is certainly desirable to fill out the gap between various approaches and to construct a unique theory of quantum hydrodynamics. I have tried here to divide the existing approaches into three distinct groups.

<u>Group I.</u> In this group are included attempts to derive the equations of classical hydrodynamics and to describe phenomena of a hydrodynamical nature starting from the fundamental equations of wave mechanics. As might be expected, the starting point is often the Schrödinger equation, but here and there are attempts to obtain the same goal by starting from relativistic mechanics. These approaches seem to be more formal, and the mathematical formulation of the problem is primary, serving to

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describe the physical concepts that are behind the continuum theory. In this group, as Kaempffer points out, one may distinguish two groups: (a) descriptions of the field in terms of a wave function; (b) descriptions of the phenomena of a hydrodynamical nature in terms of density and velocity potential. The following may be included in this group. Madelung has shown the relation between Schrödinger's and Euler's equations. Yvon has shown the relation between Madelung's mechanical approach and Dirac's relativistic mechanics. Takabayasi, in two papers, presents the hydrodynamical picture formally equivalent to the statistical picture and suggests a formal generalization of Schrödinger's equation. Bohm presents a deterministic interpretation of quantum mechanics. Schönberg shows that Madelung's approach can be generalized to include the turbulence, which can be related to the vacuum fluctuations of the Madelung fluid. Mori and Ono derive the quantum mechanical Boltzmann equation determining the molecular phase space distribution for non-uniform gases. Ross and Kirkwood present an alternative method of averaging.

<u>Group II.</u> In this group one may include the works which approach the solution of the problem of describing phenomena of a hydrodynamical nature starting from the method of quantum field theory, i.e., introducing canonical formalism and quantization. It seems that workers in this group propose methods of a rather intuitive nature, in which physical description of phenomena in the medium in question is primary. This group is almost exclusively concerned with liquid helium I and II. London, using Bose-Einstein statistics for the gas advances the hypothesis concerning the transition from liquid helium I to II. Tisza develops the idea of the two-fluid theory further. Landau puts the two-fluid theory on an entirely new basis; he assumes two kinds of elementary excitations in the fluids, phonons and rotons. Dingle reviews the theories of liquid helium. Thellung, using the Clebsch transformation, gives Landau's hypothesis a more secure foundation. Ziman shows that the hydrodynamical equations valid in the domain of Landau's hypothesis can be derived from a variational principle. Itô, using the Lagrange formalism, obtains a result similar to Ziman's.

Group III. In this group one may include papers which attempt to find the relation between the two approaches of Group I and Group II. In this group we can include the works of Kaempffer, who shows that the approaches of the two previous groups can be related to each other. In the conventional approach the field under consideration is described in terms of the wave function and its complex conjugate, which are subject to the commutation rules. In the second approach of quantum hydrodynamics the same field is described in terms of the density and the velocity potential. Kaempffer expresses the opinion that there is still considerable doubt about the justification of the second approach,

3. SOME ELEMENTS OF ATOMIC STRUCTURE

3.1 The Quantum Hypothesis

The quantum theory of radiation was derived by Planck (1900) on a classical basis from fundamental thermodynamic considerations of black body radiation. Einstein successfully applied the theory to the explanation of the photoelectric effect, which we will now describe. When light falls on a metal surface electrons are liberated. The energy of the individual electrons is not dependent on the intensity of the light. No electrons at all will be emitted if the frequency of the incident light is less than a threshold frequency ν_0 . At frequencies above ν_0 the emitted electrons possess energies in the range $0 < E < E_{\rm max}$, where

$$\mathbf{E}_{\max} = \mathbf{h}\boldsymbol{\nu} - \boldsymbol{\phi} \quad .$$

Here h is Planck's constant, and ϕ , the work function, is a constant for the particular metal and equal to $h\nu_0$. Einstein's hypothesis (1905) was that the energy of the incident light wave is associated with small particles (photons) of energy $h\nu$.

This idea of quantization was extended to the energy levels of the atom by Bohr (1912). According to his theory, electrons circle the nucleus in stationary orbits under Coulomb attraction. The orbital velocity of an electron may be derived by equating the centrifugal and Coulomb attractive forces, and we may then write the momentum as

$$P = mv = (mZe^{2}/r)^{1/2}$$
(66)

where m and e are the electronic mass and charge, Z is the atomic number, and r the orbit radius. We now make a heuristic argument which will be completely justified below. If we raise an electron from its ground state to some excited state, we must do this by adding energy in the form of a photon of energy $h\nu$. The excited electron now possesses this energy, and we may visualize it as being stored in the form of a standing wave associated with the electronic orbit. In order that the wave be stable we require that its wavelength be an integral sub-multiple of the orbit circumference:

$$r = \frac{n\lambda}{2\pi}$$
(67)

where n is an integer larger than zero.

A full understanding of the relation between eqs. (66) and (67) was not attained until de Broglie (1924) made the bold generalization which bears his name. From the theory of special relativity, we know that the momentum p_{ϕ} of a photon is

$$\mathbf{p}_{\rm c} = \mathbf{E}/\mathbf{c} \tag{68a}$$

where c is the velocity of light (and of course of the photon). Using the Planck equation, $E = h\nu$, we obtain from (68a)

$$\mathbf{p}_{\mathbf{d}} = \mathbf{h}\nu/\mathbf{c} = \mathbf{h}/\lambda \quad . \tag{68b}$$

We now assert that (68b) is true for the waves associated with any particle, whatever its velocity. That this is indeed a valid assumption was shown experimentally by Davisson and Germer (1927), who succeeded in diffracting the waves associated with a beam of low-energy electrons.

We can now combine eqs. (66), (67), and (68b), and obtain the expression

$$p = 2\pi m Z e^{2} n^{-1} h^{-1} {.} {(69)}$$

Remembering that $E = T + V = \frac{p^2}{2m} - \frac{p^2}{m} = -\frac{p^2}{2m}$ (where T is the kinetic and V the potential energy of the orbital electron) we obtain the Bohr quantum levels

$$E_{n} = -2\pi^{2}me^{4}Z^{2}h^{-2}n^{-2} .$$
 (70)

We can see that \mathbf{E}_n is limited to discrete values depending on n, where n is the principal quantum number.

3.2 Radiation

If we now calculate the energy of the photon emitted by an electron falling from a level of larger n to a level of smaller n, we obtain

$$h\nu = E_{n_1} - E_{n_2} = 2\pi^2 m e^4 Z^2 h^{-2} (n_2^{-2} - n_1^{-2})$$
 (71a)

Balmer and others have established the empirical rule, based upon spectroscopic measurements on hydrogen,

$$h\nu = R_{exp}(n_2^{-2} - n_1^{-2})$$
(71b)

where R_{exp} is the Rydberg constant, which can be measured experimentally. The experimental value corresponds with remarkable accuracy to

$$R_{\text{theor.}} = 2\pi^2 \text{me}^4 \text{h}^{-2}$$
(71c)

where, for hydrogen, Z = 1.

The Bohr theory thus explains most satisfactorily the gross features of the atomic spectrum of hydrogen. The fine structure, as well as the details of the spectrum of more complex atoms, requires the development of a more sophisticated theory for its explanation.

3.3 Wave Mechanics

A more general interpretation of atomic structure was proposed by Schrödinger (1925). The starting point in the development of the so-called "new" quantum mechanics is the above-mentioned de Broglie hypothesis. In the Schrödinger formalism, one investigates the motion of a particle in terms of a function associated with the de Broglie waves, whose modulus squared is a measure of the probability of finding the particle at any given point as a function of time. We introduce the wave function

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$$\Psi = \psi \exp\left(-2\pi i\nu t\right), \quad \psi = \psi(\mathbf{x}) \tag{72}$$

For a point of mass m, the wave equation has the form

$$\Delta \psi + 8\pi^2 \,\mathrm{mh}^{-2}(E-V)\,\psi = 0 \tag{73}$$

where $\mathbf{E} = h\nu$ is the total energy of the mass point and V is the potential energy.

While heuristic justifications can be made for presenting (73) as the equation of motion of a quantum mechanical particle, we must in the final analysis accept it as an axiom which is nothing but the quantum mechanical equivalent of Newton's second law, F = ma. The analogy becomes more evident if one writes Newton's second law in the Hamiltonian formulation; we will not here digress to do this. It is often convenient to write the Schrödinger equation as

$$H\psi_{i} = E_{i}\psi_{i} \tag{73a}$$

where H is the Hamiltonian of the system and E_i is the set of energy eigenvalues. In general, eq. (73) possesses solutions only for certain values of the total energy E. These eigenvalues of E correspond, in the particular case of the Bohr model, to discrete orbits of an electron around the nucleus. When one wishes to deal with several non-interacting particles in the same potential, the equation has the form

$$\sum_{k} m_{k}^{-1} \Delta_{k} \psi + 8 \pi^{2} h^{-2} (E-V) \psi = 0$$
(74)

where the subscript k refers to the kth particle, and where

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{i}} \frac{\partial^2}{\partial \mathbf{x_{ik}^2}}$$

Consider the case of an electron with charge -e moving in a potential of the form $V = -Ze^2r^{-1}$; then the solution of the Schrödinger equation leads to the following eigenvalues of the energy E:

$$E_n = -2\pi^2 m e^4 Z^2 h^{-2} n^{-2}$$

which agrees with the solution derived implicitly from the Bohr quantum condition, eq. (70).

If the nucleus of the atom is not fixed, it and the electron revolve about a common center and we must substitute for the electronic mass m in eq. (70) the reduced mass

$$\mu = \mathbf{m}\mathbf{M}(\mathbf{m} + \mathbf{M})^{-1} \tag{75}$$

where M is the nuclear mass. With this modification to eq. (70), we have again the expression for the energy levels of the Bohr model of one hydrogen atom.

3.4 The Uncertainty Principle

The Heisenberg uncertainty principle is implicit in the above formalism. It states that the position of a particle and its momentum cannot simultaneously be measured to an arbitrary degree of accuracy. Let us denote by Δx_i the uncertainty in the measurement of the coordinate x_i of a particle. Similarly, let Δp_{x_i} denote the uncertainty in the conjugate momentum. The uncertainty principle states that

$$\Delta x_i \Delta p_{x_i} \stackrel{\geq}{=} h(2\pi)^{-1} = h \quad . \tag{76}$$

This notion can be generalized to any pair of canonically conjugate quantities; in particular,

$$\Delta E \Delta t \stackrel{\geq}{=} \frac{h}{h} \quad . \tag{77}$$

Bohr has proposed an idealized experiment which provides a clear (although not completely rigorous) derivation of the uncertainty principle. Consider a particle in the field of view of a microscope whose objective lens subtends an angle 2θ at the position of the particle. The Rayleigh criterion gives the resolving power of a microscope as

$$\Delta \pi_i = \lambda / (2 \sin \theta) \tag{78}$$

where λ is the wavelength of the radiant energy used to illuminate the particle. Now in order to see the particle, we must illuminate it with at least one photon, which will be deflected by the particle into the microscope and there collected by a suitable detector at the focus. In the process of being deflected, the photon transfers a certain quantity of momentum to the particle. Since we know the initial momentum of the photon, we could calculate the momentum transferred to the particle if only we could measure the final momentum of the photon. However, all we know of the post-collision history of the photon is that it is deflected into the microscope somewhere within the cone of apex angle 2θ . This introduces an uncertainty in our knowledge of the photon momentum (and hence of the particle momentum) of

$$\Delta p_{x_1} = 2p \sin \theta = 2h \lambda^{-1} \sin \theta .$$
 (79)

From (78) and (79) we immediately obtain

$$\Delta \mathbf{x}_i \Delta \mathbf{p}_{\mathbf{x}_i} = \mathbf{h} \quad . \tag{80}$$

The fact that (78) and (80) differ by a factor of 2π is a consequence of the choice of a resolution criterion, and is of little consequence.

3.5 Angular Momentum

In section 3.1 above we have shown that the states of the hydrogen atom are discrete and describable in terms of a set of eigenvalues called quantum numbers. The quantum number is the analogue of a constant of the motion in the classical scheme. An important example is angular momentum. Just as angular momentum is a constant of the motion for the classical sun-planet system, it can be expressed in terms of a quantum number for the hydrogen atom.

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Let us represent the angular momentum of the hydrogen atom as a vector of appropriate magnitude. It can be shown that the square of the orbital angular momentum is limited to the values

$$|\ell|^2 = \ell(\ell+1) \frac{h^2}{h^2}$$
, (81)

where $0 < \ell \le n$, and n is the principal quantum number mentioned in eq. (70). This corresponds to a generalized Bohr model in which elliptical as well as circular electron orbits are permitted. The azimuthal quantum number, ℓ , measures the eccentricity of the orbit. The orbit is circular for $\ell=n$. The restriction of the angular momentum to units of h is a typical consequence of the quantum mechanical approach and can be derived straightforwardly from the Schrödinger equation. An older semi-classical treatment based on the Bohr model was given by Sommerfeld and yields the same result except that $\ell(\ell+1)$ is replaced by ℓ^2 . It is clear that in the classical limit, where $\ell \rightarrow \infty$, $\ell(\ell+1) \rightarrow \ell^2$.

Clearly, we cannot specify the direction of the angular momentum vector except in relation to some direction in space. For the case of the free atom in free space, however, such specification is meaningless, since we take it as axiomatic that free space is isotropic. But if we place the atom in the presence of a magnetic field, its electron, being charged and in motion, will interact with the magnetic field, which thus serves to pick out as unique some special direction in space.

We can visualize the $\vec{\ell}$ vector as precessing about the direction of the magnetic field (arbitrarily chosen in the \vec{z} direction), describing a cone. The component of $\vec{\ell}$ along the field will be constant. Using the formalism described in Section 3.3, one inserts into the Schrödinger equation (73a) the interaction energy of the electron with the field,

$$H = \frac{1}{2m} (\vec{p} - \frac{e}{c} \vec{A})^2$$
(82)

where \overrightarrow{A} is the vector potential of the magnetic field and the other symbols are defined above. The solution yields a set of eigenvalues for \overrightarrow{l}_{z} . One finds

$$|\vec{\ell}_{\sigma}| = m_{\ell} h \tag{83}$$

where $-\ell \leq m_{\ell} \leq \ell$. When $m_{\ell} = \ell$, the atom is aligned with its angular momentum vector parallel to the magnetic field; $m_{\ell} = -\ell$ corresponds to antiparallel alignment, and the intermediate values to intermediate alignments.

3.6 The Zeeman Effect

Consider again a hydrogen atom in a magnetic field. In the light of the above discussion, the energy of the atom can be described in terms of three quantum numbers, n, ℓ , and m_{ℓ} . It can be shown that except for a relativistic correction, all values of ℓ (for a given n) lead to the same energy--that is, they are degenerate. Now, when the atom emits a photon, n changes and (in conformity with certain selection rules) m_{ℓ} also changes. The latter change involves considerably less energy than the former, but results in a splitting of each of the spectral lines described in equation (71a) into a characteristic number of components. This number depends upon the selection rules, and also upon the number of values which m_{ℓ} can take under the restrictions $|m_{\ell i}| \leq \ell_i \leq n_i$, $|m_{\ell f}| \leq \ell_f \leq n_f$. Here the subscripts

i and f refer to the initial and final states respectively. A detailed description of this splitting, known as the Zeeman effect, is beyond the scope of this discussion.

3.7 Electron Spin

If the electron were the inert particle originally described in the Bohr theory, the basis of the description of atomic states and atomic spectra would now be essentially complete. However, the electron (in common with many other elementary particles) possesses an angular momentum of its own, which is frequently visualized as a spin about its own axis. This angular momentum, called \vec{s} , is constant in value, and, like the angular momenta treated above, is expressed in units of h, viz:

$$\overrightarrow{s} \stackrel{2}{=} s(s+1) h^2$$
(84)

where the quantum number s = 1/2 always. Hence,

$$\overrightarrow{|\mathbf{s}|}^2 = 3/4 \, \mathbf{h} \quad . \tag{84a}$$

Just as the vector $\overrightarrow{\ell}$ precesses in the presence of a magnetic field, so does \overrightarrow{s} . The quantum number analogous to m_{ℓ} is $m_{\underline{s}}$, and, as might be expected,

$$m_g = \pm \frac{1}{2}$$
 and $\overrightarrow{s}_z = m_g h = \pm \frac{1}{2} h$. (85)

We can define the total angular momentum of the hydrogen atom, \vec{j} , as the vectorial sum

$$\overrightarrow{j} = \overrightarrow{l} + \overrightarrow{s}$$
 . (86)

The corresponding quantum number j describes the range of allowed values of $|\vec{j}|^2$:

$$\vec{j} = j(j+1) h^2$$
 (87)

in complete analogy to (81) and (84) above. Further, we have in a magnetic field

$$\vec{j}_{z} = m_{j} h .$$
(88)

We have now discussed the quantum numbers n, ℓ, m_{ℓ} , s, m_s , j, and m_j . It is clear from eq. (86) that of $\vec{j}, \vec{\ell}$, and \vec{s} , only two are necessary for a complete description of the system, since the third is derivable from the other two. A complete description of the state of the hydrogen atom can be made in terms of four quantum numbers. Such a choice is called a representation. Two very useful ones are $\{n, \ell, s, j\}$ and $\{n, \ell, m_{\ell}, m_s\}$.

The significance of such a representation is as follows. We remember that classically a system can be described completely for all time if we can specify at a given moment the position and momentum of each constituent particle with complete exactitude. In view of the uncertainty principle, this is a goal which cannot be attained in quantum mechanics, and we are obliged to abandon such a representation of the system. The quantum number representations discussed above are the quantum mechanical analogues of the classical representation of a system in terms of constants of the motion.

3.8 Nuclear Spin

We have discussed above a number of angular momenta associated with atomic electrons which are of importance in describing atomic spectra. Each is quantized in units h, and they add vectorially. The nucleus, too, possesses an angular momentum because of its small radius, (10⁻⁵ atomic radius). The nucleus contains only a very small part of the total angular momentum of the atom. Nonetheless, the splitting of spectral lines due to the vectorial addition of the nuclear spin is detectable by means of high-resolution spectrographs and is one of the causes of the hyperfine structure. The nuclear spin may also be observed by means of nuclear magnetic resonance. The radiation emitted by a transition in the nuclear spin is in the radio frequency region of the spectrum.

The nuclear angular momentum is called \overrightarrow{I} , and its magnitude is

F

$$\overrightarrow{|\mathbf{I}|}^2 = \mathbf{I}(\mathbf{I}+\mathbf{1}) \, \mathbf{h}^2 \quad . \tag{89}$$

There is an associated magnetic quantum number

$$|\vec{M}_{I}|^{2} = M_{I}(M_{I}+1)h^{2}$$
 (90)

Adding the nuclear angular momentum \vec{I} to the electronic angular momentum \vec{j} gives a total atomic angular momentum $\overrightarrow{\mathbf{F}}$, restricted to the values

$$|\vec{F}|^2 = F(F+1)h^2$$
 (91)
= (j+I), (j+I-1), ..., (j-I) .

3.9 Many-Electron Atoms

The above discussion has been restricted to the hydrogen atom. While the principles enunciated apply to more complicated atoms, the treatment becomes considerably more involved. In particular, care must be taken as to the rules which apply in adding the angular momenta of the various electrons. In practice, the exact calculation can become exceedingly difficult, and approximations must be made.

The total angular momenta of all the electrons are represented by capital letters; we replace l by L, s by S, etc.

4. ELEMENTS OF MOLECULAR STRUCTURE

4.1 General Description of the Diatomic Molecule

If we combine two atoms into a molecule, the individual atoms will continue to display all the properties described above. There will be additional properties, however, which must be ascribed to the cooperative effect of the two atoms interacting with each other, and must hence be called molecular properties.

We have seen that isolated atoms produce various types of spectral emissions which can be ascribed to combinations of electronic and nuclear motions within the atom. In a molecule, we must add to these motions two more. First, the two atoms may rotate about their common center of mass much as do the electron and proton in the hydrogen atom. Secondly, the atoms may vibrate about some equilibrium distance of separation. We will treat these phenomena separately.

4.2 The Rigid Rotator

For the time being, we eliminate the vibrational mode from consideration by regarding the molecule as a rigid dumbbell-like structure. We first make the usual calculation of reduced mass (see eq. 76) and also observe that there can be no potential energy of rotation in a rigid body. The Schrödinger equation then becomes

$$\Delta \psi + 2\mu \hbar^{-2} \mathbf{E} \, \psi = 0 \tag{92}$$

where E now contains only kinetic energy;

$$\mathbf{E} = 1/2 \, \mathrm{I}\omega^2 \quad . \tag{93}$$

Here ω is the angular frequency of the rotator and I its moment of inertia, equal to the classical value μr^2 , where μ is the reduced mass and r the interatomic distance. The solution of eq. (92) is simple, and leads to the energy eigenvalues

$$E = J(J+1) h^{2} (2\mu r^{2})^{-1}$$
(94)

where J, the rotational quantum number, is restricted to the values 0, 1, 2, 3, \ldots .

The transitions from one value of J to another are accompanied by the emission or absorption of a light quantum. For most molecules, μ and r are of such magnitude that the wavelengths associated with these quanta are in the infrared region.

4.3 The Harmonic Oscillator

We now take into consideration the fact that the molecule is not a rigid dumbbell. Clearly, there is some equilibrium interatomic separation. If the atoms are pushed closer together (but not too far) a mutual repulsion comes into play. If they are pulled apart (not too far) the atoms attract each other. We assume in first approximation that the restoring force is proportional to the difference between the interatomic distance and the equilibrium distance. The problem then becomes the familiar one of the quantum mechanical harmonic oscillator. The Schrödinger equation is

$$\Delta_{\psi} \psi + 2\mu h^{-2} \left[\mathbf{E} - 1/2 \mathbf{k} (\delta \mathbf{r})^2 \right] \psi = 0$$
(95)

where k is the force constant and δr the displacement from equilibrium position. The equation possesses solutions only for the energy eigenvalues

$$E(v) = h(k/\mu)^{1/2} (v + 1/2)$$
(96)

where the vibrational quantum number v can take the values 0, 1, 2,

4.4 The Anharmonic Oscillator

It is clear that the molecular restoring force cannot be of a strictly harmonic character. On the one hand, we know that if we pull the two atoms far enough apart, the attractive force ceases to increase and in fact decreases to zero at infinite separation. In the case of any pair of atoms which will not combine exothermally at absolute zero, e. g., SiC, there will even be a natural repulsion at some distance larger than the molecular diameter. On the other hand, if we compress the molecule sufficiently, electron core interactions and later nuclear interactions will become significant. The resulting anharmonicity will be observable in the molecular spectrum. For the lower vibrational states, which are encountered almost exclusively if one remains sufficiently below the dissociation temperature, the deviations from harmonicity are small, and can be handled by means of perturbation theory.

4.5 The Molecular Spectrum

Selection rules, the details of which we will not treat here, usually forbid a vibrational transition except when a rotational transition occurs simultaneously. Since the rotational energy levels are very close together, the vibrational spectrum is broadened into a group of very closely spaced lines which form a characteristic band, in a manner similar to that in which the main atomic levels are split into components in the Zeeman effect.

4.6 The Electronic Energy Levels

In a diatomic molecule, the valence electrons are shared by the two constituent atoms. Thus, these electrons lie in a Coulomb field which is produced by both atoms, and which, moreover, varies in time as the molecule oscillates. These and other interactions complicate the molecular spectrum as well as modify the individual atomic spectra, and must be taken into account in a complete description of molecular behavior.

4.7 More Complicated Molecules

As one considers larger and larger molecules the problem becomes more complicated very rapidly. More vibrational and rotational modes are added, the electronic configuration may become quite complicated, and the molecules tend to become anisotropic. A number of very powerful techniques of approximation and computation have been developed to treat such molecules and their spectra, and such experimental methods as nuclear magnetic resonance and electron paramagnetic resonance, together with isotope substitution techniques, are used to add to the information gathered by classical optical and infrared spectroscopy.

A special case of the very large molecule is the crystal. Here a number of very important simplifications can be made by virtue of the periodicity of the crystalline lattice and consequently of the potential field in which the electrons find themselves. The most striking effect upon the atomic structure is that an electron can no longer be said to belong to a certain particular atom. In quantum mechanical language, its wave function extends throughout the crystal. This results in the broadening of the lowerenergy spectral lines into broad bands, which in some cases actually overlap. The relative position of these bands will determine whether the solid is a dielectric, a semiconductor, or a conductor. A full ireatment of this and related effects lies in the domain of solid state physics.

5. POSSIBLE TRENDS IN FLUID DYNAMICS

5, 1 General Remarks

The development of fluid dynamics has been briefly outlined. Beginning from hydraulics, fluid dynamics of incompressible media, and the concept of continuum, the field of fluid dynamics subsequently introduced the concept of compressible continuous media and the principles of the kinetic hypothesis with transport phenomena. From the concept of a particle and the phenomena associated with it, fluid dynamics passed to the concept of a molecule with the corresponding phenomena. But the modern requirements superimposed upon the field of fluid dynamics are much stronger. As a field of science, fluid dynamics should be able to describe such phenomena as radiation, ionization, dissociation, etc., in moving laminar and turbulent gaseous media; one may mention as well a liquid-gaseous system with nuclear phenomena and transformation of mass into energy (the sun).

It is obvious that the existing concepts of a particle or a molecule as the fundamental element of fluid, are insufficient. The molecular and atomic structure of the medium in question must be taken into account. Fluid dynamics considered as a field of classical physics or applied mathematics must adjust itself to the modern development in mathematical physics.

5.2 Classical Models

Assume that the definition of the word "mechanics" includes the notion of statistical mechanics. Then the following charts (Matrices Ia, and Ib) contain an elementary description of the contents of some subfields of the field of mechanics. Similarly, one can discuss subfields of acoustics with related subfields such as hydro(aero)-acoustics, etc., and the subfield of electromagnetism with related subfields such as hydro(aero)-electro-magnetism, etc. One may also discuss the possibility of application of various modern theories to fluid dynamics and related subfields. Matrix 3 briefly outlines a few such possibilities. Matrix 2 divides fluid dynamics according to the magnitude of the Mach number and according to the main phenomena of the system in question.

5.3 Brief Discussion of Some Subfields

The field of fluid dynamics was originated and developed as a field of the dynamics of liquids. The first approach considered only laminar motion in the macroscopic sense, and considered not the phenomena due to internal friction but only due to the external forces. Later, the need to consider the effect of internal (frictional) stresses became obvious.

The first model used was that of continuum; there is no free space between the particles or molecules of the medium in question. The fluid represents a homogeneous non-porous medium subject to deformation and action of internal stresses. Since there is no free space between the molecules, the only way to change the volume is to change the volume of each molecule. The volume of a molecule of a polyatomic gas can be changed by changing the following molecular energies: E_T , E_{rotat} , E_{vibr} , E_{elect} . In a monatomic gas the above requirement implies a change of the volume of an atom. But the changes in volumes of atoms and molecules are insignificant; changes in volume of a gas are caused by the changes in intermolecular distance. Consequently the model of mechanics of continuum cannot represent phenomena in all kinds of gases, being

Main subfield: Fluid Dynamics.	Phenomena of motion of a medium (fluid) with no heat addition from outside, no electro-magnetic phenomena (radiation), no nuclear reaction; principally: distribution of the velocity, density, pressure and temperature.	
Related subfields:		
Thermo-fluid dynamics (thermo-aerodynamics)	Heat phenomena in moving media due to internal friction are taken into account; emphasis upon fluid dynamics phenomena	
Acoustico-fluid dynamics (-hydrodynamics)	Bordering subfield between acoustics and fluid dynamics; acoustic phenomena in moving media; emphasis upon fluid dynamics phenomena	
Electro-magneto-fluid dynamics (radiation-fluid dynamics)	Bordering subfield between electromagnetism and fluid dynamics; radiation phenomena in moving media; emphasis upon fluid dynamics phenomena.	
Nuclear-fluid dynamics	Bordering subfield between nuclear physics and fluid dynamics; nuclear reaction phenomena in moving media are considered; emphasis upon fluid dynamics phenomena.	

Matrix 1a. Elementary Description of the Subfields: Fluid Dynamics and Related Subfields.

at best only a first approximation. In case one uses the model of continuum and some average (mean) functions, the problem needs to be referred to statistical mechanics.

Thus the most justified model to account for the phenomena in moderately and strongly rarefied gases is a model of physics of gases: for example, that of the kinetic hypothesis of gases.

All the other regimes and fields in Matrices 2 and 3 are self-explanatory. The subfield nuclear-fluid dynamics can be illustrated as follows: the sun can be treated as a liquid state system subject to continuous nuclear reactions, which implies a continuous change of mass into energy. The fundamental equations of such a system are yet unknown.

From the matrices presented, it seems obvious that the field of fluid dynamics tends to proceed along the same lines as the modern field of mathematical physics, i.e., a description of macroscopic phenomena in the system in question by means of microscopic phenomena in molecules and atoms.

Main subfield: Thermodynamics	Phenomena in a medium at rest due to heat addition from outside, no electro-magnetic phenomena (radiation), no nuclear reaction; principally: distribution of heat and temperature.	
Related subfields:		
Hydro-(Aero)- Thermodynamics	Thermodynamic phenomena in moving media; emphasis upon thermodynamic phenomena.	
Acoustic-Thermodynamics	Bordering subfield between acoustics and thermodynamics; acoustical phenomena in thermodynamic systems; emphasis upon thermodynamic phenomena.	
Electro-Magneto- Thermodynamics	Bordering subfield between electro-magnetism and thermo- dynamics; radiation phenomena in thermodynamic systems; emphasis upon thermodynamic phenomena.	
Nuclear-Thermodynamics	Bordering subfield between nuclear physics and thermo- dynamics; nuclear reaction in thermodynamic systems; emphasis upon thermodynamic phenomena.	
Nuclear-Hydro-(Aero)- Thermodynamics	As above, in moving media; emphasis upon thermodynamic phenomena.	

Matrix 1b. Elementary Description of the Subfields: Thermodynamics and Related Subfields.

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Regime of Fluid Dynamics	Possible Mach No.	
·	and other characteristics	
Incompressible fluid: liquid-continuum	$\rho = \text{const.}$	
Compressible medium: gas	$\rho \neq \text{const.}$	
Subsonic: pseudo-continuum, or physics of gases	M < 1	
Transonic: pseudo-continuum, or physics of gases	M = 1	
Supersonic: pseudo-continuum, or physics of gases, slip flow	1 < M < 7	
Hypersonics, hyperballistics (rarefied gas); slip flow	\sim 7 < M \sim 15 ÷ 20	
Free molecule flow, Newtonian gas dynamics (rarefied gas)	\sim 15 ÷ 20 < M	
Meteoritical fluid dynamics (meteors)	$100 \stackrel{<}{=} M$	
Fluid dynamics of system subject to electro-magnetic phenomena	Ionosphere, radiation	
Cellestial fluid dynamics		
Fluid dynamics of systems subject to nuclear reaction	Hydrodynamics of the sun	
Meteorological fluid dynamics		

Matrix 2. Division of Fluid Dynamics

	Field	Fundamental Model	Possibility of Application
1.	Mechanics of continuum	Deformation of a particle, shearing stress tensor	Fluid dynamics of incom- pressible media, extended to compressible media
2,	Physics of gases- kinetic theory of gases-(statistical mechanics)	Collision of molecules, transport phenomena	Fluid dynamics of compressible media, thermo-fluid dynamics slip flow
3.	Free molecule flow	Reflection of fully elastic molecules from the surface of a body with normal and tangential velocity components	Hypersonic flow regime, hyperballistic
4.	Newtonian gas dynamics	Motion of fully inelastic molecules along the surface of a body with normal velocity component equal to zero	Hypersonic flow regime, hyperballistics
5.	Molecule dynamics- quantum theory	Motion of atoms inside a molecule: translation, rotation, vibration	Variation of c_p , c_v , γ with the temperature, dissociation, heat-capacity lag (relaxation time) thermo-fluid dynamics, hypersonic regime
6.	Quantum theory- quantum mechanics- theory of structure (model) of an atom	Motion of electrons around nucleus (proton), radiation, electro-magnetic phenomena	Radiation, ionization, hyper- sonic regime, electro-mag- neto-fluid dynamics, meteor- itical fluid dynamics, celles- tial fluid dynamics
7.	Electron theory	Electrical charges of electron and proton	As in 6
8.	Theory of rela- tivity, special (systems moving with uniform velocity) and general (acceler- ated systems)	There is no absolute motion and no absolute set of coordinate axes; velocity of light in free space is a universal and invariant constant of nature; acceleration due to gravity is indistinguishable from any other acceleration; equivalence of mass and energy	Cellestial fluid dynamics; phenomena between cellestial bodies; application to the atomic structure (Dirac rela- tivistic approach to atomic structure).
9.	Nuclear reaction	Equivalence of mass and energy: $H^2 + H^2 \longrightarrow H^3 + n + 3.3^{-4} ev$	Nuclear fluid dynamics (the sun)

Matrix 3. Possible Physical Models as Applied to Fluid Dynamics and Related Subfields

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5. 4 Radiation and Dissociation Phenomena in Moving Media

To illustrate let us discuss briefly the possible model of a dense fluid dynamic moving system with radiation and dissociation phenomena. Since each phenomena in a fluid are obviously described by the methods of quantum mechanics, the following combination can be considered:

- (i) A system (one or more) of Schrödinger equations combined by means of the proper "links" with the system of macroscopic fluid dynamics equations based upon continuum which equations are expressed in terms of kinematic properties u_i , ρ , thermodynamic properties p, T, and the proper coefficients μ_i (i = 1, 2), λ ; the "links" may contain T, or other magnitudes, expressing the relation between the microscopic phenomena due to radiation and dissociation and the macroscopic properties such as heat content. The resultant system may be subject to boundary conditions superimposed upon the kinematic, thermodynamic, electro-magnetic, and radiation magnitudes. For example, the ionosphere is subject to high energy electro-magnetic radiation impinging upon this gaseous domain from the sun. This model is a simple one and although acceptable from the mathematical point of view, it may be challenged from the physical standpoint in its marriage of continuum and atomic structure.
- (ii) As above, applied to the kinetic theory. This model seems to be highly desirable from the physical standpoint due to realistic features of the kinetic hypothesis. But if transport phenomena are considered, this model may present enormous mathematical difficulties: the molecules are not perfectly elastic spheres, etc. The already extremely difficult equation similar to the Maxwell-Boltzmann equation will be accompanied by a simultaneous system of Schrödinger equations.
- (iii) As above, applied to the free molecule flow.

As a final remark, one can mention that the application of nuclear phenomena to combustion processes is also under investigation (Ref. 2, p. 68, Ref. 15).

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