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THE MACROSCOPIC  
LEVEL OF  
QUANTUM MECHANICS

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## Synopsis

A synthetic account is given of a general treatment of large quantal systems, allowing of a clear-cut characterization of the macroscopic level of description of such systems. The time-evolution of the density operator is given by a Liouville equation, which is written down in a superspace formed by the direct product of the Hilbert space with itself. It is shown how to construct a projector  $\tilde{I}$  in this superspace such that the subspace it defines contains the asymptotic time-evolution of the density operator for time intervals very large compared with those typical for atomic processes: this asymptotic subdynamics shows the characteristic features of macroscopic behaviour.

A quantitative criterium is formulated in superspace for the existence of a well-defined and unique macroscopic level in the sense just outlined of a separate subdynamics governing the asymptotic behaviour of the system. This "condition of dissipativity" can be directly tested on the Hamiltonian of any given system.

In general, the subdynamics can only be formulated in superspace: it is not possible to return from the  $\tilde{I}$  subspace to a Hilbert space description of the system in terms of state-vectors. Thus, the scope of the latter description is clearly limited, and a precise formulation is obtained of the complementarity between the dynamical account of the system on the atomic scale and its description at the level of macroscopic observation.

The epistemological problems of quantum mechanics receive from the present point of view an especially transparent treatment. In particular, the consistency of the use of classical concepts for the account of quantal phenomena is obvious, since the macroscopic description operates directly with probabilities, all quantal interference effects being eliminated from the  $\tilde{I}$  subspace; thus, the rule of "reduction" of the state-vector following a measurement performed upon an atomic system appears as an immediate consequence of the macroscopic character of the measuring process.

## 1. Introduction

In a detailed discussion of the epistemological problems of atomic physics, where explicit reference to the conditions of macroscopic observation is essential,<sup>1,2)</sup> a decisive part is played by the analysis of the asymptotic approach to equilibrium of material bodies consisting of a very large number of interacting atomic constituents (and possibly also of a field of electromagnetic radiation). In the first place, such an analysis serves in its own right to establish the consistency of the atomistic description of macroscopic phenomena, by clarifying the relation of complementarity between the irreversible character of the macroscopic behaviour of the large system and the time-reversal invariance of its dynamical description at the atomic level.<sup>3)</sup> In the second place, applied to the process of observation of an individual atomic phenomenon by means of a macroscopic apparatus interacting with the atomic object, it throws light on the conceptual foundations of quantum mechanics.<sup>4,5)</sup>

Recent progress in the quantum theory of large systems allows us, as we intend to show in this paper, to treat these problems with more precision and more completely than was hitherto possible. The method we use was initiated by one of us<sup>6)</sup> and developed in numerous publications by the Brussels group during the last decade. This method may be applied to arbitrary systems but becomes especially interesting and fruitful in the limit of large systems, whose energy spectrum is (at least in part) continuous. It is then possible to follow directly the time-evolution of observables depending on a finite number of degrees of freedom through the time evolution of the density operator, and in particular to study the asymptotic behaviour of the system for times of macroscopic order of magnitude. It turns out that this behaviour can be given a remarkably simple formal expression under very general assumptions about the correlations between the constitutive elements of the system: in physical terms these correlations should be of limited range and their effects should only persist for times of atomic order of magnitude. The asymptotic density operator will then exhibit the expected



approach to equilibrium, provided that a further condition – playing here somewhat the same part as the condition of mixing in the theory of classical systems – is fulfilled by the interactions. In contrast with the ergodicity and mixing conditions for classical systems\*) this condition of “dissipativity” can be explicitly tested for typical systems of actual physical interest. Of course, our method can also be applied to classical systems, for which it again leads, in the limit of large systems, to a condition of dissipativity.

This condition plays a fundamental role in our theory, inasmuch as its fulfilment guarantees the existence of a well defined macroscopic level of description of a large system, besides its dynamical description on the atomic level. This new mode of description contains the usual phenomenological account of the behaviour of the system in terms of thermodynamics, chemical kinetics and other macroscopic theories. Thus, the condition of dissipativity, when fulfilled, establishes the possibility of introducing in a well defined way two complementary levels of description of atomic systems.

To illustrate the significance of this remarkable result, let us consider the evolution of the temperature of a gas. We may proceed in two ways: either we use the statistical definition of temperature and solve the dynamical problem (which is possible, at least in principle, by means of an appropriate computer), or we use the Fourier equation of heat conduction. These two quite different procedures, so far as we know, give results in agreement with each other. This shows that the complete dynamical description contains elements which in fact are irrelevant for the evolution of such an observable as the temperature. Now, our method, in the form elaborated in recent papers of the Brussels group,<sup>9–18)</sup> allows us to define with precision the part of the dynamical description that is relevant and to discard in an unambiguous fashion the remainder.

As shown by PRIGOGINE, GEORGE and HENIN,<sup>14)</sup> the evolution of a mechanical system may be split into formally independent “subdynamics”, characterized by certain projection operators, as explained in subsection 2.7 below. One of these subdynamics, belonging to the projector  $\tilde{I}$  defined in subsection 2.7, contains all the information about equilibrium and linear transport properties, and the macroscopic level of description of a large quantal system is accordingly defined as that entirely expressed in terms of the variables corresponding to this  $\tilde{I}$ -subdynamics. The consideration of the macroscopic level of a system thus entails an enormous reduction of its mode of description, since all the variables associated to the other subdynamics are excluded

\*) For a discussion of these conditions and their extension to finite quantal systems, see in particular refs.<sup>7,8)</sup>.



from it. In relation to the macroscopic description so defined, the condition of dissipativity plays a fundamental part. For non-dissipative systems, such as quantal systems with a discrete, non-degenerate energy spectrum, there is no dynamical evolution in the  $\tilde{H}$ -space, and a macroscopic level of description cannot be defined. The consideration of large dissipative systems is therefore essential. There also exist large quantal systems, with continuous spectrum, which are not dissipative (an extreme example would be a superfluid system at zero temperature): for such systems there is no macroscopic description, in the above sense, of their dynamical evolution.

In the next section, we present a synthetic account of the formal framework of our theory, leading to the concept of subdynamics and the definition of the macroscopic level of quantum mechanics. Section 3 is devoted to a discussion of the physical content of the theory, with special emphasis on the epistemological problems of the atomic theory of material bodies. In section 4 the theory is applied to the analysis of the observation of an individual atomic process and its bearing on the epistemological aspects of quantum mechanics. This still leaves out of consideration a number of important problems upon which our approach throws new light, such as those related to transformation theory, the introduction of collective modes or quasiparticles, or the definition of unstable particles.\*) We hope nevertheless that the aspects discussed here are sufficient to show that the theory of large quantal systems is an essential part of quantum mechanics, both by its physical applications and its contributions to the questions of principle concerning the foundations of atomic theory. Indeed, it makes possible an incorporation in quantum theory of deep-lying, general properties of matter, which could not be achieved by means of the usual Hilbert space formalism of quantum mechanics.

\*) A monograph by I. PRIGOGINE, C. GEORGE and F. HENIN, dealing with these problems, is in preparation.

## 2. Dynamics and asymptotic behaviour of very large systems

### 2.1. The Liouville equation in superspace

The study of the time evolution of a quantal system can be performed in either of two ways. One may represent the state of the system by a vector  $|\psi(t)\rangle$  in a Hilbert space and describe the change of the system in time as a rotation of this state vector, the rate of which is governed by the Hamiltonian  $H$  according to the Schrödinger equation. Alternatively, one may define the density operator

$$\varrho(t) = |\psi(t)\rangle\langle\psi(t)|$$

whose time derivative  $\dot{\varrho}(t)$  is then given by the Liouville equation

$$i\dot{\varrho}(t) = \frac{1}{\hbar} [H, \varrho(t)],$$

where the right-hand side denotes  $\hbar^{-1}$  times the commutator of  $H$  and  $\varrho(t)$ . With the help of the density operator, one can compute the expectation value at any time of any quantity represented by a Hilbert space operator  $A$  as the trace of the operator  $\varrho(t)A$ . This mode of representation of the dynamics of the system exhibits most directly the correspondence, in the limit  $\hbar \rightarrow 0$ , with the classical formulation of the kinetic approach to statistical thermodynamics, and is accordingly generally adopted for the quantal treatment of the same problem.

Since the quantal density operator embodies both density distributions in given states of the system and correlations between pairs of states, it is natural to regard it as describing the evolution of the system in the product space  $\mathcal{H} \times \mathcal{H}$ , which we shall call “superspace” (using the prefix “super-”, when necessary, to distinguish vectors and operators in it from those in Hilbert space). Operators in Hilbert space are thus “supervectors”, and the scalar product of two supervectors  $A, B$  is defined as the trace of the product  $A^+B$ , where  $A^+$  denotes the Hilbert space operator adjoint to the operator  $A$ . The expectation value of the operator  $A$  in the state represented by the (self-adjoint) density operator  $\varrho$  is then the scalar product  $\text{tr}(\varrho A)$  of the two supervectors  $\varrho, A$ . We may now introduce linear superoperators  $O$  acting

upon supervectors; the *adjoint*  $O^\dagger$  of the superoperator  $O$  is defined<sup>\*)</sup> by the condition

$$\text{tr}[A^+(OB)] = \text{tr}[(O^\dagger A)^+B].$$

The *transposition* of a superoperator, i.e. its operating "to the left", denoted as  $AO$ , is defined by requiring that  $\text{tr}[(A^+O)B] = \text{tr}[A^+(OB)]$ ; therefore,  $AO = (O^\dagger A^+)^+$ , or

$$(OA)^+ = A^+O^\dagger.$$

Since, moreover, one has for the product of two superoperators  $O, Q$ ,

$$(OQ)^\dagger = Q^\dagger O^\dagger,$$

the adjoint of any expression involving products of superoperators and supervectors is obtained by the uniform rule of taking the adjoint of every superoperator and supervector and inverting the order of factors in every product.

A frequently occurring type of superoperator, which we shall call *factorizable*, is defined by a pair of supervectors  $M, N$  as follows:

$$OA \equiv MAN;$$

we shall denote such a factorizable superoperator as  $O \equiv M \times N$ ; its adjoint is  $O^\dagger = M^+ \times N^+$ , its transpose is given by  $A(M \times N) \equiv (N \times M)A$ . The product of two factorizable superoperators  $M \times N, P \times Q$  is again factorizable:  $(M \times N)(P \times Q) = MP \times QN$ . A unitary transformation  $U$  in Hilbert space,  $U^+U = UU^+ = 1$ , gives rise to a linear transformation in superspace, which is represented by the factorizable superoperator  $\mathcal{U} = U \times U^+$  and is accordingly also unitary in superspace, in the sense that  $\mathcal{U}^\dagger \mathcal{U} = \mathcal{U} \mathcal{U}^\dagger = 1 \times 1 = 1$ . The invariance of the scalar product of supervectors for unitary transformations is immediately proved:

$$\text{tr}[(\mathcal{U}A)^+ \mathcal{U}B] = \text{tr}[(\mathcal{U}^\dagger \mathcal{U}A)^+ B] = \text{tr}[A^+ B].$$

The Liouville equation may now be written in the form

$$i\dot{\varrho}(t) = L\varrho(t) \tag{1}$$

with the help of a Liouville superoperator, which is a sum of factorizable superoperators:

$$L \equiv \frac{1}{\hbar} \{H \times 1 - 1 \times H\}.$$

<sup>\*)</sup> The matrix representation of the superoperators defined in this subsection is given in the Appendix.



The solution of eq. (1) corresponding to an initial state  $\varrho(0)$  is formally expressed as

$$\varrho(t) = e^{-iLt} \varrho(0);$$

the time-evolution superoperator  $T(t) \equiv \exp(-iLt)$  is readily shown to be factorizable:\*)

$$T(t) = e^{-iLt} = e^{-iHt/\hbar} \times e^{iHt/\hbar}. \quad (2)$$

The Liouville superoperator is self-adjoint, and the time-evolution superoperator unitary.

Projection operators in superspace will play a fundamental part in the following argument, and we shall be led to generalize their usual definition. Let us briefly explain what this generalization amounts to. Besides idempotency, the most essential property of a projection superoperator  $P$  must be to make the projection of any density supervector  $\varrho$  self-adjoint:  $(P\varrho)^+ = P\varrho$ , in order to ensure the physical interpretation of the projection as density supervector in the projected subspace, and above all the reality of the expectation value

$$\langle A \rangle_P = \text{tr}[(P\varrho)^+ A]$$

of the quantity represented by the self-adjoint supervector  $A$ . A superoperator  $O$  satisfying the condition  $(OA)^+ = OA$  for any self-adjoint supervector  $A$  will be said to be *adjoint-symmetrical*, or to have *adjoint symmetry*. (This terminology is suggested by the special form  $M \times M^+$  which a factorizable superoperator must have in order to satisfy the above condition.) If the superoperator  $O$  is adjoint-symmetrical, its adjoint  $O^\dagger$  has the same property; this may be seen by considering the scalar product  $\text{tr}[B(OA)]$ , where  $A$  and  $B$  are two arbitrary self-adjoint supervectors and  $OA = AO^\dagger$ : this product may in fact be written  $\text{tr} AO^\dagger B$  as well as  $\text{tr}[A(O^\dagger B)^+]$ . Now, in virtue of

\*) The proof is given here as an example of the calculus of factorizable superoperators. Putting  $L_1 = -iLt/\hbar$ ,  $H_1 = -iHt/\hbar$ , we have

$$\begin{aligned} \frac{1}{n!} L_1^n &= \frac{1}{n!} \left\{ H_1 \times 1 + 1 \times H_1^+ \right\}^n = \sum_{p=0}^n \frac{1}{n!} \binom{n}{p} (H_1 \times 1)^p (1 \times H_1^+)^{n-p} \\ &= \sum_{p=0}^n \frac{1}{p!(n-p)!} (H_1^p \times 1) (1 \times [H_1^+]^{n-p}) = \sum_{p=0}^n \frac{1}{p!} H_1^p \times \frac{1}{(n-p)!} [H_1^+]^{n-p}, \end{aligned}$$

and since

$$\sum_{n=0}^{\infty} \sum_{p=0}^n \dots = \sum_{p=0}^{\infty} \sum_{n=p}^{\infty} \dots,$$

it follows that

$$e^{L_1} = e^{H_1} \times e^{H_1^+}.$$

the idempotency of  $P$  and  $P^\dagger$ , the expectation value  $\langle A \rangle_P$  may also be written  $\text{tr}[(P_\rho)(P^\dagger A)]$ : this shows that if we want to interpret it as that of the projected supervector  $PA$ , we must impose upon the projector the further requirement of being self-adjoint. This is the case for the usual projectors constructed from (self-adjoint) projection operators in Hilbert space  $P_m, P_{m'}$ :

$$P = \frac{1}{2} [P_m \times P_{m'} + P_{m'} \times P_m] \equiv \overline{P_m \times P_{m'}},$$

the symmetrization being necessary in order to satisfy the adjoint-symmetry requirement. However, this further specification of the expectation value will prove too restrictive for our purposes, and the physical meaning of the above definition of  $\langle A \rangle_P$  is perfectly clear and precise without it, provided that the adjoint-symmetry condition is fulfilled. Hence, we shall give up the requirement of self-adjointness for projectors in superspace, and consider as such the wider class of idempotent superoperators satisfying the condition of adjoint symmetry.

Although the superspace representation is equivalent to the usual one might therefore appear as no more than a convenient formalism, it will turn out that it actually opens possibilities of description of fundamental physical properties, not adequately dealt with in the Hilbert space representation, because they essentially require the use of non-factorizable superoperators, in particular projection superoperators in the generalized sense just defined.

## 2.2. Energy spectrum and time-behaviour of large systems

The structure of the energy spectrum leads to a clearcut distinction between two types of large systems: systems of finite degree of freedom and finite extension, whose energy spectrum is discrete, and systems of infinite degree of freedom and infinite extension, but finite density of constitutive elements: the latter have essentially a continuous energy spectrum, possibly combined with a set of discrete states. The spectral decomposition of the Hamiltonian may be written as a Stieltjes integral

$$H = h \int v_k dP(k),$$

where the symbol  $k$  represents a set of appropriate quantum numbers, and  $hv_k$  the energy eigenvalue corresponding to definite values  $\{k\}$  of this set. According to eq. (2), the corresponding decomposition of the time-evolution superoperator is

$$T(t) = \iint dP(k) \times dP(k') e^{-2\pi i (v_k - v_{k'})t}. \quad (3)$$

Any discrete sequence of states, with eigenvalues  $h\nu_n$ , will accordingly give a contribution to  $T(t)$  almost periodic in time. This shows that finite quantal systems, with discrete spectrum, cannot be expected to exhibit any irreversibility in their asymptotic behaviour. Infinite systems, on the other hand, allow of a direct approach to their dynamical time-evolution.

Indeed, it follows from eq. (3) that the contribution to  $\varrho(t) = T(t)\varrho(0)$ , with  $\varrho(0) = |\psi_0\rangle\langle\psi_0|$ , of a continuous part of the energy spectrum, has matrix elements of the form

$$\langle k|\varrho(t)|k'\rangle = \langle k|\psi_0\rangle\langle\psi_0|k'\rangle e^{-2\pi i(\nu_k - \nu_{k'})t}.$$

Now, an amplitude like  $\langle k|\psi_0\rangle$ , when continued analytically in the plane of the complex variable  $\nu_k$ , is in general<sup>\*)</sup> a multivalued function of this variable, with branch-points on the real axis at various thresholds of excitation, and its domain of uniformity of physical interest for  $t > 0$  (owing to the time-reversal invariance of the evolution, it suffices to consider positive times) consists of adjacent parts of Riemann sheets below the real axis limited by cuts issuing from the thresholds. The integrations occurring in the calculation of an average  $\text{tr } \varrho(t)A$  may be transformed so as to involve integrations over the energy variables  $\nu_k$  and  $\nu_{k'}$ . The contour of integration in the plane of each variable may then be closed by a parallel to the real axis at infinite distance in the lower half-plane, with indentations along the cuts. The "resonance" poles of the integrand inside this contour,

$$2\pi\nu_r = 2\pi\varepsilon_r - \frac{1}{2}i\gamma_r \quad (\gamma_r > 0),$$

will yield exponentially decaying terms to the integral, to which is added a "background" whose time variation is more complicated. The resonance contributions to  $\text{tr } \varrho(t)A$  have accordingly a time dependence of the form  $\exp[-2\pi i(\nu_r - \nu_r^*)t]$ , corresponding to processes of frequencies  $\varepsilon_r - \varepsilon_r'$ , decreasing exponentially with decay times  $[\frac{1}{2}(\gamma_r + \gamma_r')]^{-1}$ . These life-times vary over a very wide range, extending from the time-scale characteristic of individual atomic processes to that of macroscopic relaxation times. In the simplest case, in which only these two extreme time-scales appear, one may expect that it would be possible, at least approximately, to separate the direct effects of short-lived atomic processes from the slower evolution of the system on the macroscopic time-scale.

Before pursuing this line of argument, we must mention another essential difference between finite and infinite systems, which, as we shall see, is of relevance for their asymptotic behaviour: it concerns the invariants of the

\*) Cf. on this point, e.g., refs.<sup>6)</sup> and <sup>19)</sup>.



system, i.e. those Hilbert space operators  $\Phi$  which commute with the Hamiltonian, and accordingly satisfy the equation  $L\Phi = 0$ . Whereas the invariants of finite systems are regular operators within the Hilbert space of state vectors of finite norm, those of infinite systems are of two distinct types: besides "regular" ones, there is an infinity of invariant operators which do not have the regularity property just mentioned.\*) We shall discuss this point in detail in subsection 2.8.

### 2.3. Independent modes of motion and correlations

In order to proceed further, we must introduce a more explicit characterization of the constitutive elements of the system and the interactions between them, which would allow us to account for the continual change of the system in the course of time as the result of transition processes brought about by such interactions. As usual, this is done by reference to an idealized "model system", susceptible of independent, non-interacting, modes of motion, defining a complete orthogonal basis of representation in Hilbert space. The interactions producing correlations between these modes are then defined as those which transform the model into the real system. The choice of the model system is dictated by physical considerations: for a dilute gas, the natural model will be a perfect gas, for a crystal, a perfect lattice susceptible of collective harmonic oscillations. The essential requirement is that the basic modes should have some operational meaning, in the sense that we can imagine situations conveniently represented by them. In any case, all physical results of the theory, expressed as expectation values of suitable operators, are of course independent of the choice of the model system, since a change of basis is effected by a unitary transformation.

The total Hamiltonian  $H$  is thus decomposed into the Hamiltonian  $H^{(0)}$  of the model system and a residual interaction Hamiltonian  $H^{(1)}$ . The spectrum of the model Hamiltonian

$$H^{(0)} = h \int v_m^{(0)} dP(m),$$

will generally be a continuum, in which a set of discrete states may be embedded; the "Friedrichs model"<sup>21)</sup> is of this type, with only one discrete state. The collective index  $m$  stands, as the case may be, for a set of quantum

\*) The distinction between regular and singular invariants also applies to classical systems; the first mention of it occurs in a paper by P. RÉSBOSIS and I. PRIGOGINE,<sup>20)</sup> devoted to classical dilute gases. Cf. also ref.<sup>6)</sup>.

numbers of single-particle states (properly symmetrized or antisymmetrized) or for a set of occupation numbers. In superspace, a complete orthogonal basis consists of the Hilbert space projection operators<sup>\*)</sup>  $P_m = |m\rangle\langle m|$ ; the corresponding orthogonal projectors in superspace are the factorizable superoperators  $\overline{P_m \times P_{m'}}$  formed by all the pairs of supervectors  $P_m, P_{m'}$ .

With a view to distinguishing the effects of the correlations from the behaviour of the model system, we now introduce a subdivision of the total basis in superspace into two orthogonal and complementary subsets, defined by two superprojectors  $P_o, P_c$  with  $P_o + P_c = 1$ . Thus, for the Friedrichs model, where we wish to study how the correlations  $H^{(1)}$  couple the discrete state of the Hamiltonian  $H^{(0)}$  with its continuum, we may take for the subspace  $P_o$  that defined by the discrete state, and consequently  $P_c$  by the continuum.<sup>16, 17)</sup> More generally, we shall include in  $P_o$  all the projectors  $\overline{P_m \times P_m}$  formed of pairs of identical states; if the external conditions allow for a bulk flow of the system, we shall add to these the projectors  $\overline{P_m \times P_{m'}}$  for all the pairs  $P_m, P_{m'}$  representing the same internal physical state of the system; the subspace  $P_c$  consists of all the remaining projectors  $\overline{P_m \times P_{m'}}$ , corresponding to those pairs of states between which transition processes take place owing to the short-range, atomic correlations. Still other decompositions may prove useful for specific problems;<sup>18)</sup> for our general argument, the precise mode of decomposition chosen is irrelevant, provided that it confines the short-range correlation effects to one of the two subsets.

The adopted decomposition effects a separation of the density supervector into two components:<sup>\*\*)</sup>

$$\varrho(t) = \varrho_o(t) + \varrho_c(t), \quad \varrho_o(t) = P_o \varrho(t), \quad \varrho_c(t) = P_c \varrho(t).$$

The density  $\varrho_o(t)$  represents an average distribution referred to the states of the model system, whereas the supervector  $\varrho_c(t)$  accounts for the effects of the fluctuating correlations among these states. Between  $\varrho_o$  and  $\varrho_c$  we derive from eq. (1) a set of coupled Liouville equations:

\*) For a continuous spectrum, we define  $P_m = \int_{\epsilon(m)} dP(m)$ , where  $dP_m = |m\rangle\langle m|$ , and  $\epsilon(m)$  is an infinitesimal neighbourhood of  $m$ . We further interpret a summation over  $m$  as  $\int dm \dots$  and the Hilbert space scalar product  $\langle m | m' \rangle$  as the distribution  $\delta(m - m')$ . Then, the idempotency, orthogonality and completeness relations  $P_m P_{m'} = P_m \delta_{mm'}$  and  $\sum_m P_m = 1$  hold for both the continuous and the discrete part of the spectrum.

\*\*) From now on, we adopt the elegant formalism developed by M. BAUS,<sup>10)</sup> of which we present a version improved in some important respects, and extended to take account of later progress.<sup>12-17)</sup> Some mathematical aspects are discussed by J. RAE.<sup>11)</sup> Another general exposition has lately been given by BALESCU and WALLENBORN.<sup>18)</sup>

$$i\dot{Q}_o = L_{oo}Q_o + L_{oc}Q_c, \quad (4)$$

$$i\dot{Q}_c = L_{cc}Q_c + L_{co}Q_o, \quad (5)$$

where

$$L_{oo} = P_oLP_o, \quad L_{cc} = P_cLP_c, \quad L_{oc} = P_oLP_c, \quad L_{co} = P_cLP_o.$$

We shall especially use the equivalent integrated form of eq. (5),

$$Q_c(t) = e^{-iL_{cc}t} \left\{ Q_c(0) - i \int_0^t d\tau e^{iL_{cc}\tau} L_{co}Q_o(\tau) \right\}, \quad (6)$$

exhibiting the occurrence of the time-evolution superoperator

$$T_c(t) \equiv e^{-iL_{cc}t} = e^{-iP_cL t} P_c = P_c e^{-iLP_c t}, \quad (7)$$

which is going to play an essential part in our analysis.

The superoperator  $T_c(t)$  describes a time-evolution proceeding entirely by transitions between states of the correlation subspace; we have called such sequences of processes confined to the correlation subspace the “irreducible dynamics” of the system: its explicit consideration is one of the main points of our approach.<sup>6, 10)</sup> Indeed, in contrast with the total time-evolution superoperator  $T(t)$ , we may expect that the superoperator  $T_c(t)$  may have a simple asymptotic behaviour:\*) in view of its exclusive dependence on correlation effects, its time-variation may be dominated by decaying pole terms of atomic life-times. More precisely, we shall consider the possibility that the application of the superoperator  $T_c(t)$  to any regular super-vector which is not an invariant in the correlation subspace gives a result which, in the asymptotic limit of positive values of the time of macroscopic order of magnitude, becomes of negligible importance. This condition may be formally expressed as

$$\lim_{t \rightarrow +\infty} T_c(t)A = 0 \quad (\text{if } LP_cA \neq 0); \quad (8)$$

in terms of the Laplace transform

$$\mathcal{F}_c(z) = \int_0^{\infty} T_c(t) e^{-zt} dt = -iP_c \frac{1}{LP_c - iz} = -i \frac{1}{P_cL - iz} P_c, \quad (9)$$

an equivalent expression for it is

\*) We must exclude from consideration in this respect the time-evolution superoperator  $\exp(-iL_{oo}t)$ ; e.g., for homogeneous systems, where  $P_o = \sum_m P_m \times P_m$ , one has  $L_{oo} = 0$ .



$$\lim_{z \rightarrow +0} z \mathcal{F}_c(z) A = 0 \quad (\text{if } LP_c A \neq 0), \quad (10)$$

implying that  $\mathcal{F}_c(z)A$  is a regular function of  $z$  in the neighbourhood of  $z = +0$ . If  $P_c A$  is an invariant, one has instead  $z \mathcal{F}_c(z)A = P_c A$ .

This analyticity condition may be used in principle for a classification of dynamical systems. It has indeed been shown that it is satisfied in the thermodynamic limit for large systems with short-range interactions, when a perturbation expansion can be carried out with respect to a ‘‘small’’ physical parameter, such as the coupling constant or the density. Moreover, it is seen to be exactly fulfilled (independently of any perturbative approach) for soluble systems such as the Friedrichs model.<sup>17)</sup> It is not the aim of the present paper to investigate this question any further. We shall simply assume that we are dealing with systems that satisfy the condition (8) or (10): it is for this class of systems that we shall arrive at a unique definition of a macroscopic level of description, complementary to the dynamical one. The assumption (8) will indeed prove convenient for the derivation of simple asymptotic forms for the density supervectors  $\varrho_o$  and  $\varrho_c$ . It must be stressed that the introduction of this assumption destroys the invariance of the description for time-reversal: for in retrodiction the operator  $T_c(-t)$  describes the buildup of the resonance states of the system – an aspect of the evolution on the atomic scale which is all but negligible. An interesting type of system from the physical point of view is that in which the interactions between the constitutive elements are such as to determine two characteristic time-scales of very different orders of magnitude: on the one hand, any coherent processes involving states collected in the subspace  $P_o$  have relaxation times belonging to the macroscopic time-scale; on the other, the individual processes due to the finite-range interactions between the basic modes of the model system, which occur between states of the subspace  $P_c$ , have decay times of atomic dimension. Systems for which no such separation of time-scales can be made may be discussed by more general methods.

#### 2.4. Asymptotic density supervectors and evolution equations

By means of the assumption (8), we will now set up solutions of the Liouville equations (4), (5) valid for large positive values of  $t$ ; these solutions, which we shall denote as  $\tilde{\varrho}_o(t)$ ,  $\tilde{\varrho}_c(t)$ , will then be associated with the actual density supervectors  $\varrho_o(t)$ ,  $\varrho_c(t)$  by an appropriate condition: this will allow us to interpret  $\tilde{\varrho}_o(t)$ ,  $\tilde{\varrho}_c(t)$  as the respective asymptotic forms of  $\varrho_o(t)$ ,  $\varrho_c(t)$ . Taking eq. (6) first, we neglect the first term on the right-hand side

(which means, physically, that we assume the effect of any initial correlations to be dissipated), and in the second term, re-written as

$$-i \int_0^t d\tau e^{-iL_{cc}\tau} L_{co} \varrho_o(t-\tau),$$

we replace  $\varrho_o(t-\tau)$  by the asymptotic solution  $\tilde{\varrho}_o(t-\tau)$ , since the integrand is only important for small values of  $\tau$ ; we thus obtain

$$\tilde{\varrho}_c(t) = -i \int_0^t d\tau e^{-iL_{cc}\tau} L_{co} \tilde{\varrho}_o(t-\tau). \quad (11)$$

Next, let us consider eq. (4); for large values of  $t$ , it becomes, on account of eq. (11), an integro-differential equation for  $\tilde{\varrho}_o$ :

$$i\dot{\tilde{\varrho}}_o = L_{oo}\tilde{\varrho}_o - iL_{oc} \int_0^t d\tau e^{-iL_{cc}\tau} L_{co} \tilde{\varrho}_o(t-\tau).$$

Let us introduce<sup>\*)</sup> an asymptotic time-displacement superoperator  $\theta$  in the  $P_o$  subspace by the definition

$$i d\tilde{\varrho}_o = \theta \tilde{\varrho}_o dt,$$

or, alternatively,

$$\tilde{\varrho}_o(t) = e^{-i\theta t} \tilde{\varrho}_o(0) \quad (\text{for } t > 0). \quad (12)$$

Inserting this expression in eq. (11) yields the asymptotic relation

$$\left\{ \theta - L_{oo} + iL_{oc} \int_0^t d\tau e^{-iL_{cc}\tau} L_{co} e^{i\theta\tau} \right\} \tilde{\varrho}_o(t) = 0,$$

which can be further modified, according to our assumption (8), by extending the integration over  $\tau$  to infinity. We thus obtain a functional equation for the superoperator  $\theta$ :

$$\theta = L_{oo} - iL_{oc} \int_0^\infty d\tau e^{-iL_{cc}\tau} L_{co} e^{i\theta\tau},$$

which may be solved by iteration,<sup>9, 18)</sup> starting from the *ansatz*  $\theta = 0$  (which would correspond to a stationary asymptotic distribution). By defining a time-independent superoperator

\*) The superoperator  $\theta$  was first considered by P. RÉSIPOIS and further studied by C. GEORGE.<sup>9)</sup>

$$iC \equiv \int_0^{\infty} d\tau T_c(\tau)L_{co} e^{i\theta\tau}, \quad (13)$$

we may re-write the equation for  $\theta$  as

$$\theta = L_{oo} + L_{oc}C, \quad (14)$$

and treat the equations (13), (14) as a set of coupled equations for the determination of  $\theta$  and  $C$ . The role of the latter appears when, returning to eq. (11), we repeat on the right-hand side the preceding transformations; this gives the very simple result

$$\tilde{\varrho}_c(t) = C\tilde{\varrho}_o(t). \quad (15)$$

According to its definition (13),  $C$  describes the effect of an infinite sequence of processes starting from a state in the subspace  $P_o$  and leading to a state of the correlation subspace  $P_c$  either directly or through intermediate states: in other words,  $C$  describes the ‘‘building up’’ of the correlation component  $\tilde{\varrho}_c$ , as expressed by eq. (15). We therefore call  $C$  the ‘‘creation superoperator’’ of correlations. It should be noted that one may derive from the definition (13) of  $C$ , by partial integration, the identity

$$C\theta = L_{co} + L_{cc}C, \quad (16)$$

use being made once more of the assumption (8). Combining this with eq. (14), one obtains a non-linear equation for the determination of  $C$ :

$$CL_{oo} + CL_{oc}C = L_{co} + L_{cc}C.$$

So far, we have defined the asymptotic supervectors  $\tilde{\varrho}_o(t)$ ,  $\tilde{\varrho}_c(t)$  by eqs. (12), (15), as solutions of the ‘‘kinetic equations’’

$$i\dot{\tilde{\varrho}}_o = \theta\tilde{\varrho}_o, \quad i\dot{\tilde{\varrho}}_c = C\theta\tilde{\varrho}_o.$$

If, in these equations, we substitute for  $\theta$  and  $C\theta$  their respective expressions (14) and (16), and take account again of eq. (15), we see that they become identical in form with the Liouville equations (4), (5): in other words, *the asymptotic density supervectors are exact solutions of the Liouville equations*. It remains to be seen how they are related to the solutions  $\varrho_o(t)$ ,  $\varrho_c(t)$  which describe the behaviour of the system on the atomic scale.

## 2.5. Heisenberg representation and time-reversal

As a preparation to the elucidation of this point, it will be necessary to repeat the preceding considerations from the point of view of Heisenberg's



representation. In the latter, any (time dependent) operator  $A(t)$  satisfies the Liouville equation

$$i\dot{A}(t) = -LA(t),$$

where the Liouville superoperator is, of course, time-independent. Let us now define the time-inversion of any supervector or superoperator as the transformation which consists in both changing the direction of time and taking the adjoint:

$$\bar{A}(t) = A^+(-t), \quad \bar{O}(t) = O^\dagger(-t).$$

Since the Liouville superoperator, which is self-adjoint, changes sign on transposition, the time-inverse supervector  $\bar{A}(t)$  obeys the same Liouville equation

$$i\dot{\bar{A}}(t) = L\bar{A}(t)$$

as the density supervector. The projectors  $P_o, P_c$  being invariant for time-reversal, we may define components

$$\bar{A}_o(t) = P_o\bar{A}(t), \quad \bar{A}_c(t) = P_c\bar{A}(t)$$

and corresponding asymptotic components  $\tilde{A}_o(t), \tilde{A}_c(t)$ , with a time-evolution governed by the superoperators  $\theta$  and  $C$ :

$$\tilde{A}_o(t) = e^{-i\theta t} \tilde{A}_o(0), \quad \tilde{A}_c(t) = C\tilde{A}_o(t).$$

In this context, these superoperators appear as the time-inverses of new superoperators

$$\eta = \bar{\theta}, \quad D = \bar{C},$$

determined by functional equations derived from eqs. (14), (16) and (13) by time-inversion:

$$\eta = L_{oo} + DL_{co}, \tag{17}$$

$$\eta D = L_{oc} + DL_{cc}; \tag{18}$$

$$iD = \int_0^\infty d\tau e^{i\eta\tau} L_{oc} T_c(\tau), \tag{19}$$

In contrast to  $C$ , the superoperator  $D$ , according to its definition (19), leads from a state of the correlation subspace  $P_c$  to a state of the subspace  $P_o$ : it describes the processes leading to a “destruction” of correlations, and is called, accordingly, the “destruction superoperator”.

It is important to notice that in applying the time-inversion transformation to the right-hand side of eq. (13) in order to obtain eq. (19), one has to leave the integration variable  $\tau$  unchanged, but change the interval of integration over  $\tau$  to  $(0, -\infty)$ . This clearly shows that the change of the direction of time can affect seemingly time-independent superoperators like  $C$  and  $D$  which are defined through an asymptotic time-limiting procedure. A comparison of the expressions (13) and (19) for  $C$  and  $D$ , together with eqs. (14) and (17), shows that the time-inversion transformation, for such superoperators, consists in taking the adjoint and inverting the sign of  $L$ . The time-inversion may obviously be performed in the same way for operators depending explicitly on the time variable, since this time dependence may always be expressed as a functional dependence on  $iLt$ ; one may therefore consider the transformation just defined as equivalent to time-inversion.

According to this definition, it is clear that time-reversal invariance of a superoperator depending on  $L$  does not in general imply its self-adjointness: this is only the case if its functional dependence on  $L$  is not affected by a change of sign of  $L$  – in particular (trivially), if the superoperator does not depend on  $L$ . Thus, time-inversion appears as a natural generalization of adjointness for superspace operators, and time-reversal invariance as a natural generalization of self-adjointness. The adequacy of this generalization with respect to the requirements of physical interpretation is guaranteed by the simple, but very important fact that the superoperator  $iL$ , and consequently any superoperator which is a functional of  $iL$ , is adjoint-symmetrical. The equality  $(iLA)^+ = iLA$  for any self-adjoint supervector  $A$  follows indeed immediately from the self-adjointness of  $L$  and its transposition property  $LA = -AL$ . The superoperators  $C$ ,  $i\theta$  as well as  $D$ ,  $i\eta$ , as appears from eqs. (13), (14), (17), (19) which define them, offer examples of superoperators which are functionals of  $iL$ , and accordingly adjoint-symmetrical. It will soon turn out that the time-dependence (in the extended sense just introduced) of all density supervectors of physical interest (such as  $\varrho(t)$  and  $\tilde{\varrho}(t)$ ) can be expressed in the general form  $\varrho_o(t) \equiv O[iL] \varrho$ , where  $\varrho$  is the initial density supervector and  $O[iL]$  an appropriate superoperator which is always a functional of  $iL$ : these time-dependent density supervectors are therefore self-adjoint, as well as their time-inverses, and the expectation value of any self-adjoint supervector  $A$ , which can accordingly be written

$\text{tr } \varrho_o(t)A$ , or equivalently\*)  $\text{tr } \overline{\varrho_o(-t)} A$ , is always real — a property essential for its physical interpretation.

The functional equations for  $\theta$  and  $\eta$ , given by the combination of eqs. (14), (13) and (17), (19), respectively, can be put into a more compact form:

$$\theta = L_{oo} - i \int_0^{\infty} d\tau \Psi(\tau) e^{i\theta\tau}, \quad \eta = L_{oo} - i \int_0^{\infty} d\tau e^{i\eta\tau} \Psi(\tau), \quad (20)$$

with the help of the superoperator

$$\Psi(t) = L_{oc} T_c(t) L_{co}. \quad (21)$$

The superoperator  $\Psi(t)$  represents a transition from the subspace  $P_o$  to the same subspace exclusively through states of the correlation subspace; it is therefore called the “irreducible collision operator”. The formulae (20) show how the asymptotic superoperators  $\theta$  and  $\eta$  essentially arise from sequences of interaction processes belonging to the “irreducible” dynamics of the system. The interaction superoperator  $\Psi(t)$ , or its Laplace transform

$$\Psi_{\mathcal{L}}(z) = L_{oc} \mathcal{F}_c(z) L_{co} = z L_{oc} \frac{1}{P_c L - iz} P_o, \quad (22)$$

has an important function, as we shall soon see, in the formulation of a general characterization of the asymptotic behaviour of infinite systems.

An explicit relation between  $\theta$  and  $\eta$  is readily derived from eqs. (14), (16) and (17), (18):

$$N_o \theta = \eta N_o, \quad \text{with } N_o = 1 + DC; \quad (23)$$

according to eqs. (13), (19) and (21), one may write

$$N_o = 1 - \int_0^{\infty} d\tau \int_0^{\infty} d\tau' e^{i\eta\tau} \Psi(\tau + \tau') e^{i\theta\tau'}. \quad (24)$$

\*) Such time-dependent expectation values are conserved under a group of time-dependent transformations  $U[iL]$ , defined in such a way that the transforms  $A', \varrho'(t)$  of  $A, \varrho(t)$  are, respectively,

$$A' = U[iL]A, \quad \varrho'(t) = U[-iL]\varrho(t),$$

and characterized by the condition

$$\overline{U[iL]} U[iL] = U[iL] \overline{U[iL]} = 1.$$

This condition indeed ensures that  $\text{tr} \overline{\varrho'(-t)} A' = \text{tr} \overline{\varrho(-t)} A$ . This is a generalization of the group of unitary transformations, in which adjointness is replaced by time-inversion. It has been considered under the name of “star-unitary” group in previous papers of the Brussels group; see especially the second paper of ref.<sup>15</sup>). In contrast to the unitary transformation superoperators, the star-unitary ones are not factorizable: they belong specifically to the superspace.



In general,  $N_o$  will have an inverse, and the relation (23) between  $\theta$  and  $\eta$  will then take the form

$$\eta = N_o\theta N_o^{-1}, \quad \theta = N_o^{-1}\eta N_o. \quad (25)$$

### 2.6. Relation between asymptotic and dynamical behaviour

Let us now return to the asymptotic density supervector  $\tilde{\varrho}_o(t)$  and its time-evolution (12). From the relation (23) we see that this evolution can be expressed by means of the superoperator  $\eta$  as follows:

$$N_o\tilde{\varrho}_o(t) = N_o e^{-i\theta t}\tilde{\varrho}_o(0) = e^{-i\eta t}N_o\tilde{\varrho}_o(0); \quad (26)$$

in other words, the time-evolution of  $N_o\tilde{\varrho}_o(t)$  is governed by the superoperator  $\eta$ . On the other hand, it follows from eqs. (17) and (18) that

$$\eta(P_o + D) = (P_o + D)L. \quad (27)$$

This remarkable commutation property implies that the time-evolution of the supervector  $(P_o + D)\varrho(t)$  is also given by the superoperator  $\eta$ :

$$i(P_o + D)\dot{\varrho} = (P_o + D)L\varrho = \eta(P_o + D)\varrho. \quad (28)$$

Hence, if we choose at any ‘‘initial’’ time

$$\tilde{\varrho}_o(0) = N_o^{-1}[\varrho_o(0) + D\varrho_c(0)], \quad (29)$$

this relation will subsist at any future time and thus ensure the interpretation of  $\tilde{\varrho}_o(t)$  and  $\tilde{\varrho}_c(t)$  as the asymptotic form of the dynamical density supervectors  $\varrho_o(t)$ ,  $\varrho_c(t)$ .

### 2.7. Projection onto orthogonal subspaces and ‘‘subdynamics’’

The relationship just established is part of a set of similar ones, which it is interesting to present systematically. According to eq. (15), the asymptotic density supervector  $\tilde{\varrho} = \tilde{\varrho}_o + \tilde{\varrho}_c$  is contained in a subspace defined by the idempotent superoperator  $P_a = P_o + C$ :

$$\tilde{\varrho}(t) = P_a\tilde{\varrho}(t).$$

Being also adjoint-symmetrical, the superoperator  $P_a$  is a (generalized) projector. Let us consider the subdivision of the superspace into the orthogonal subspaces determined by the projector  $P_a$  and its orthogonal complement:

$$P_a = P_o + C, \quad P_b = P_c - C, \quad (30)$$

as well as the similar subdivision by means of the time-inverse projectors

$$\bar{P}_a = P_o + D, \quad \bar{P}_b = P_c - D. \quad (31)$$

Besides the superoperator  $N_o$  defined by eq. (23), we introduce another one,  $N_c$ :

$$N_o = 1 + DC, \quad N_c = 1 + CD, \quad (32)$$

and we readily verify the relations

$$\bar{P}_a P_a = P_o N_o = N_o P_o, \quad P_b \bar{P}_b = P_c N_c = N_c P_c. \quad (33)$$

Further, we note that

$$P_a P_o = P_a, \quad P_o \bar{P}_a = \bar{P}_a; \quad P_c P_b = P_b, \quad \bar{P}_b P_c = \bar{P}_b. \quad (34)$$

We already know the mutually time-inverse superoperators

$$\theta = P_o L P_a, \quad \eta = \bar{P}_a L P_o; \quad (35)$$

they satisfy the relation (27) and its time-inverse, i.e.

$$P_a \theta = L P_a, \quad \eta \bar{P}_a = \bar{P}_a L, \quad (36)$$

from which eq. (23) follows at once. We may now introduce a further superoperator  $\zeta$  and its time-inverse  $\lambda$ :

$$\zeta = P_c L \bar{P}_b, \quad \lambda = P_b L P_c; \quad (37)$$

they satisfy the relations

$$\bar{P}_b \zeta = L \bar{P}_b, \quad \lambda P_b = P_b L. \quad (38)$$

Hence we have, together with eq. (23), an analogous relation involving  $\zeta$ ,  $\lambda$  and  $N_c$ :

$$N_o \theta = \eta N_o, \quad N_c \zeta = \lambda N_c. \quad (39)$$

With this notation the results of the preceding subsection, expressed by eqs. (12), (15 and (29), take the compact form

$$\tilde{\varrho}(t) = \tilde{\Sigma}(t - t_o) \varrho(t_o), \quad (40)$$

with

$$\tilde{\Sigma}(t) = P_a e^{-i\theta t} N_o^{-1} \bar{P}_a = P_a N_o^{-1} e^{-i\eta t} \bar{P}_a, \quad (41)$$

the last form for  $\tilde{\Sigma}(t)$  following from the first on account of eq. (23); the equivalence of these two forms shows that the superoperator  $\tilde{\Sigma}(t)$  is invariant

for time-reversal. Eq. (40) expresses the general correspondence between the asymptotic density supervector  $\tilde{\varrho}(t)$  at any time  $t$  and the dynamic supervector  $\varrho(t_0)$  at any former time  $t_0$ . By using eqs. (33) and (34) one readily verifies that the superoperator  $\tilde{\Sigma}(t)$  has the semi-group property

$$\tilde{\Sigma}(t_1) \tilde{\Sigma}(t_2) = \tilde{\Sigma}(t_1 + t_2) \quad (t_1, t_2 > 0). \quad (42)$$

Taking the limit  $t_0 \rightarrow t$  in eq. (40), we obtain from it a relation between the asymptotic and the dynamic density at the same time:

$$\tilde{\varrho}(t) = \tilde{I}\varrho(t), \quad (43)$$

where the superoperator

$$\tilde{I} \equiv P_a N_o^{-1} \bar{P}_a \quad (44)$$

is a projector in superspace, since it is adjoint-symmetrical and, according to eq. (42), idempotent. We have, moreover, in virtue of eq. (42),

$$\tilde{\Sigma}(t) = \tilde{\Sigma}(t) \tilde{I} = \tilde{I} \tilde{\Sigma}(t), \quad (45)$$

and therefore also, by combining eqs. (40) and (43),

$$\tilde{\varrho}(t) = \tilde{\Sigma}(t - t_0) \tilde{\varrho}(t_0). \quad (46)$$

Finally, eqs. (36), (39) and (44) allow us to write

$$P_a \theta N_o^{-1} \bar{P}_a = L \tilde{I} = \tilde{I} L = P_a N_o^{-1} \eta \bar{P}_a \quad (47)$$

and consequently

$$\tilde{\Sigma}(t) = e^{-iLt} \tilde{I} = \tilde{I} e^{-iLt}. \quad (48)$$

We thus arrive at the remarkable conclusion<sup>\*)</sup> that the asymptotic density supervector is a solution of the Liouville equation, characterized as the projection of the dynamical solution onto a subspace  $\tilde{I}$  of the Hilbert superspace, and that the asymptotic time-evolution is entirely contained in this "asymptotic subspace".

The orthogonal complement of the subspace  $\tilde{I}$  is susceptible of an equally simple characterization, by means of the superoperator

$$\hat{I} = \bar{P}_b N_c^{-1} P_b. \quad (49)$$

Indeed the latter is immediately recognized to be a projector orthogonal to

<sup>\*)</sup> This result was first derived by I. PRIGOGINE, C. GEORGE and F. HENIN.<sup>14, 15)</sup>



$\tilde{H}$ ; it is actually  $= 1 - \tilde{H}$ , since the idempotent operator  $1 - (\tilde{H} + \hat{H})$  has zero trace, according to eqs. (33), and is therefore  $= 0$ . The time-evolution of the supervector

$$\hat{\varrho}(t) \equiv \hat{H}\varrho(t) = \varrho(t) - \tilde{\varrho}(t) \tag{50}$$

is given, according to eqs. (38) (39), by the superoperator

$$\hat{\Sigma}(t) = \bar{P}_b e^{-i\zeta t} N_c^{-1} P_b = \bar{P}_b N_c^{-1} e^{-i\lambda t} P_b \tag{51}$$

which has the same semi-group property as  $\tilde{\Sigma}(t)$  and satisfies the similar relations

$$\hat{\Sigma}(t) = e^{-iLt} \hat{H} = \hat{H} e^{-iLt}. \tag{52}$$

In other words, the time-evolution of the supervector  $\hat{\varrho}(t)$ , which describes the fluctuations of the system on the atomic scale,<sup>\*)</sup> is entirely contained in the ‘‘fluctuation subspace’’  $\hat{H}$ , orthogonal to the asymptotic subspace  $\tilde{H}$ . Both components  $\tilde{\varrho}(t)$ ,  $\hat{\varrho}(t)$  of the dynamic density supervector  $\varrho(t)$  are, like the latter, solutions of the Liouville equation: they receive their respective characteristics – asymptotic irreversibility, atomic-scale fluctuations – exclusively from the projection onto the corresponding subspaces. One may say that the asymptotic evolution results from a ‘‘subdynamics’’ of the system,<sup>\*\*)</sup> unfolding itself on the macroscopic time scale in the subspace  $\tilde{H}$ .

### 2.8. Invariants of the system

Let us finally examine the relation of the subdynamics with the invariants of the system; as already mentioned in subsection 2.2, this relation is an important aspect of the theory of large systems. If we decompose the invariant  $\Phi$  into its components  $\Phi_o$ ,  $\Phi_c$ , the invariance conditions take the form

$$L_{oo}\Phi_o + L_{oc}\Phi_c = 0, \tag{53}$$

\*) Clearly, the density distribution  $\hat{\varrho}(t)$  includes only those fluctuations that cannot be detected under the given conditions of observation. For instance, the usual fluctuations around the thermodynamic equilibrium state can be derived from the corresponding asymptotic distribution density  $\tilde{\varrho}(\infty)$  and are therefore contained in the asymptotic subspace  $\tilde{H}$ .

\*\*\*) In the preceding argument, we have started from the construction of an asymptotic solution of the Liouville equation and shown that it corresponds to a ‘‘subdynamics’’. A different point of view may be adopted:<sup>22, 23)</sup> we may first study the conditions enabling us to separate the density supervector into two components evolving independently, and then discuss under which conditions one of the components represents an asymptotic solution of the Liouville equation. The conception of subdynamics may be extended to relativistic dynamical systems, for which R. BALESCU and L. BRENGI<sup>24)</sup> have shown that the projector  $\tilde{H}$  commutes with the ten generators of the Poincaré group.

$$L_{co}\Phi_o + L_{cc}\Phi_c = 0. \quad (54)$$

Multiplying eq. (54) on the left with  $-iT_c(t)$  and integrating over  $t$  yields

$$-i \int_0^t dt T_c(t) L_{co}\Phi_o + [T_c(t) - 1] \Phi_c = 0. \quad (55)$$

If  $\Phi_c$  is a regular supervector, not itself an invariant, our fundamental asymptotic assumption, expressed by eq. (8), ensures that  $\lim_{t \rightarrow \infty} T_c(t) \Phi_c = 0$  and that the supervector  $C(0) \Phi_o$ , with

$$C(0) \equiv -i \int_0^{\infty} dt T_c(t) L_{co}, \quad (56)$$

exists. Eq. (55) thus becomes, in the limit  $t \rightarrow \infty$ ,

$$\Phi_c = C(0)\Phi_o; \quad (57)$$

inserting this expression for  $\Phi_c$  into eq. (53), we get

$$[L_{oo} + L_{oc}C(0)] \Phi_o = 0. \quad (58)$$

As a comparison with eqs. (13), (14) shows, this means

$$\theta\Phi = 0 \quad (59)$$

(and therefore also, by time-reversal,  $\Phi_\eta = 0$ ). Making use of the notation (30) for  $P_b = P_c - C(0)$ , we may re-write eq. (57) as  $P_b\Phi = 0$ , and therefore, according to eq. (49),

$$\hat{H}\Phi = 0; \quad (60)$$

the invariant  $\Phi$  is contained in the asymptotic subspace  $\tilde{H}$ .

The above argument could be formulated with the help of the Laplace transform  $\mathcal{F}_c(z)$  of  $T_c(t)$  and the related superoperator  $\mathcal{C}(z) = -i\mathcal{F}_c(z)L_{co}$ : instead of eq. (55), one could start from

$$\mathcal{C}(z)\Phi_o + [z\mathcal{F}_c(z) - 1] \Phi_c = 0. \quad (61)$$

The assumed properties of  $\Phi_c$  imply, according to eq. (10),  $\lim_{z \rightarrow +0} z\mathcal{F}_c(z)\Phi_c = 0$  as well as the existence of  $\lim_{z \rightarrow +0} \mathcal{C}(z)\Phi_o = C(0)\Phi_o$ . Eq. (58) may then be written, in terms of the Laplace transform (22) of the interaction superoperator,

$$[L_{oo}-i\Psi_{\mathcal{G}}(+0)]\Phi = 0, \quad (62)$$

– an equation equivalent to eq. (59), but of a more convenient form for concrete applications of the theory. This limiting process is not permissible if  $\Phi_c$  does not have the two properties assumed in the preceding argument; but one may always combine eq. (61) directly with eq. (53) to obtain

$$[L_{oo}-i\Psi_{\mathcal{G}}(z)]\Phi + iz\mathcal{D}(z)\Phi_c = 0, \quad (63)$$

where

$$\mathcal{D}(z) = -iL_{oc}\mathcal{T}_c(z). \quad (64)$$

If  $\Phi_c$  is a regular invariant, one has (as pointed out in subsection 2.2 after eq. (10))  $\lim_{z \rightarrow +0} z\mathcal{T}_c(z)\Phi_c = \Phi_c$  and therefore  $\lim_{z \rightarrow +0} z\mathcal{D}(z)\Phi_c = 0$ : in this case, eq. (62) is still valid. If  $\Phi_c$  is a singular supervector, the limit of  $z\mathcal{D}(z)\Phi_c$  for  $z \rightarrow +0$  exists, but does not vanish, and eq. (62) does not hold. This discussion shows, therefore, that eq. (62) and the equivalent equation (59) are characteristic for the regular invariants. Moreover, it is readily seen that any supervector obeying these equations is an invariant if it belongs to the asymptotic subspace. Indeed, it follows from eq. (36) that the relation  $\theta F = 0$  implies  $LP_a F = 0$ , i.e. the invariance of the supervector  $P_a F$ , and consequently the invariance of  $F$  if  $F = P_a F$ ; but according to the definition (44) of  $\tilde{I}$  the equations  $F = \tilde{I}F$  and  $F = P_a F$  are equivalent. We thus arrive at the remarkable conclusion that the asymptotic subspace  $\tilde{I}$  contains all the regular invariants of the system and only those; the validity of eq. (62) is a criterium for deciding whether any supervector of the asymptotic subspace is a regular invariant.

A further simple result can be obtained if the projectors  $P_o, P_c$  can be adequately chosen in such a way that  $L_{oo} = 0$ , as is the case, in particular, for homogeneous systems. Then, those systems for which the superoperators  $\Psi_{\mathcal{G}}(+0)$  and, equivalently,  $\theta, \eta$ , vanish identically are such that all supervectors contained in their asymptotic subspace are invariant. The behaviour of systems of this class is strictly dynamical: in the asymptotic subspace, the density supervector, as well as, in the Heisenberg representation, all supervectors contained in this subspace, are stationary; all processes occur in the subspace  $\tilde{I}$ , in an entirely reversible way. The systems exhibiting the normal thermodynamic irreversibility are therefore characterized by the existence of a superoperator  $\theta$  or  $\eta$  which does not vanish identically: we call<sup>13, 14, 15</sup> such systems *dissipative*, and the condition just formulated “condition of dissipativity”. Especially in the form



$$\Psi_{\mathcal{L}}(+0) \neq 0, \quad (65)$$

this condition offers a convenient criterium to decide whether a given system has the normal asymptotic behaviour. Thus, the Friedrichs model, for which explicit calculations can be carried out completely and rigorously,<sup>17)</sup> offers in this context a very precise picture: if the coupling between the discrete state and the continuum preserves the former (leading for instance to a bound state), the superoperator  $\theta$  vanishes identically; if the coupling destroys the discrete state, the system is dissipative.

Among the regular invariants one distinguishes the important set of those which KHINTCHIN has called "controllable", because their values can be fixed by the external conditions of observation. Besides the Hamiltonian, this set consists of the operators defining the infinitesimal transformations of the groups with respect to which the system is invariant: space translations and rotations, for instance, with which the components of the total momentum and the total angular momentum are respectively associated. In the theory of classical finite systems, the controllable invariants determine the manifold in phase space on which the ergodicity condition can be formulated: the other invariants do not lead to any reduction of the dimensionality of this manifold. In the case of infinite systems, as we just have seen, only the regular invariants are retained at the macroscopic level of description, whereas the singular ones play no part in the definition of this level or of the asymptotic time-evolution taking place in it; in simple examples, such as that of a gas of weakly coupled particles or the more general Friedrichs model, one finds that the regular invariants are just the controllable set.<sup>17)</sup> This clear-cut discrimination of the set of invariants which enter into the description of the irreversible macroscopic behaviour of the system is paralleled in the account of phase transitions: here also it is in the limit of infinite systems that a sharp distinction becomes possible between the regular points of an isotherm and those singular points at which a phase transition occurs.

### 3. Epistemological problems of the atomic description of macroscopic phenomena

#### 3.1. The historical background

The epistemological problems raised by the attempt to base the description of the directly observed phenomena on the atomic constitution of matter have forced themselves on the attention of physicists since the pioneering work of MAXWELL and BOLTZMANN, but they could only be clearly formulated after the dynamical behaviour of the atomic constituents had found its definitive expression in quantum mechanics and the conceptual foundations of this theory had been elucidated. In the perspective of XIXth century physics it was natural enough to assume that the dynamics of the atoms was the same as that of large bodies, and accordingly to interpret the quantities characterizing the properties of these bodies as suitable averages over quantities pertaining to the constituent atoms. This averaging process seemed so far from being problematic that in the early papers of CLAUSIUS and BOLTZMANN it was not even mentioned explicitly.

However, the apparent contradiction between the irreversible evolution of macroscopic bodies and the time-reversal invariance of their description as atomic systems soon led MAXWELL and his follower BOLTZMANN to their still fundamental analysis of the role of statistical causality in atomic physics. Of course, sharing the universal belief in determinism as the ultimate causal pattern of natural laws, they regarded any recourse to statistics as a *pis-aller*, but they correctly insisted on the fact that such a recourse was dictated by the very conditions of macroscopic observation. This point was variously elaborated both by GIBBS and by the EHRENFESTS; the former forcibly pointed out that irreversibility at the macroscopic level results from the circumstances defining the corresponding mode of observation, while the latter introduced the notion of “coarse-grained” distribution as a mathematical expression for a mode of observation not reaching down to the dynamical determination of the atomic system. On the other hand, it was clear to MAXWELL and BOLTZMANN that the equilibrium distribution had to arise naturally from the dynamics, and they had the correct intuition (albeit incorrectly formulated) of ergodicity as the dynamical property primarily



responsible for fixing the form of the asymptotic distribution. GIBBS wanted to express the same physical conception by his “mixing” simile, which, however, turned out to be a stronger dynamical requirement than ergodicity.\*)

The development of quantum mechanics cannot affect the specific epistemological problems arising from the atomistic structure of matter, but it makes it easier to cope with them, by supplying us with adequate mathematical and logical tools for handling statistical averages of atomic quantities and probabilities of atomic processes. The statistical form of causality is now prevailing both in the account of individual atomic processes and of macroscopic phenomena; it is essential, however, to maintain a sharp distinction between these two forms of statistical causality, which are logically independent: the former has its origin in the existence of the quantum of action, the latter depends on the degree of freedom of the systems investigated, which may be characterized by some critical parameter, such as Avogadro’s number, defining the order of magnitude we call “macroscopic”. The formalism offers us uniform rules for dealing with both types of statistics and the relations of complementarity associated with each of them. In particular, as pointed out in the preceding section, the quantal density operator determines both the average distributions and the correlation coefficients of any system of interacting constituents, and accordingly yields a unified formal basis for the discussion of the two aspects of the asymptotic time-evolution – existence of the asymptotic distribution and “mixing” effect of the correlations.

The ergodic approach leaves unanswered the question as to which physical characteristics of a dynamical system are decisive for its exhibiting a thermodynamic behaviour on the macroscopic time-scale; for the conditions of ergodicity and mixing are mere mathematical formulations of properties characteristic of such behaviour, but not explicitly related to the physical structure of the system. One lacks here, for distinguishing systems which allow of a thermodynamical description from those that do not, a criterium linking this property more directly to the Hamiltonian.

### 3.2. Kinetic approach vs. ergodic theory

Even from the formal point of view, the extension of classical ergodic theory to quantal systems is far from straight-forward: the stumbling block is the difficulty of finding a representation of the conditions of macroscopic observation of comparable simplicity to the classical concept of coarse-graining. In classical theory, it is permissible to replace a coarse-grained

\*) See, e.g., ref. 7).



distribution, referred to some arbitrary subdivision of phase space into finite cells, by an idealized continuous distribution, and thus to make it independent of the mode of subdivision adopted. It is certainly possible, as the Italian school has shown,<sup>8)</sup> to introduce a “cell” subdivision of the Hilbert space of state vectors and to arrive at certain quantal generalizations of the ergodic and mixing properties of classical theory, but both the enunciation of these results and the algorithm leading to them – so long as one insists on mathematical rigour – are very cumbersome.

It must be observed, however, that the use of a coarse-grained cell subdivision is a consequence of the cyclic character of the time-evolution of the closed, finite systems dealt with in ergodic theory: in the classical case, this cyclic character is expressed by POINCARÉ’S theorem; in the quantal case, the discreteness of the energy spectrum leads to an almost periodic time dependence of the density operator. As a result, the idealized definitions of macroscopic quantities can only use averages taken over an infinite time, and it is then the object of the theory to express these as statistical averages, necessarily coarse-grained in view of their physical meaning. The time-evolution of infinite systems, on the other hand, is, as we have pointed out in subsection 2.2, radically different: the classical Poincaré cycle becomes of infinite duration, and the quantal energy spectrum, being continuous, allows of no almost-periodicity in time; but the correlations may lead to the occurrence of states idealized, as is usual in the theory of aperiodic processes, by (non-normalizable) state vectors with amplitudes decaying or building-up exponentially in time. This makes it possible, as we have seen, to study directly such one-sided effects of the correlations over long, but finite time intervals: the asymptotic form the density operator takes after a time of macroscopic order of magnitude can then be immediately interpreted as representing the conditions of macroscopic observation, without any need for the explicit consideration of coarse-graining. In this kinetic approach, the part of coarse-graining is played by the projection into the asymptotic subspace of our Hilbert superspace; besides its simplicity, this operation has the advantage of clearly exhibiting the fact that the macroscopic mode of description is uniquely fixed by the dynamics of the system.

### 3.3. Main features of the macroscopic aspect of the kinetic theory

The form given to the kinetic theory in section 2 has several noteworthy features. The most prominent is doubtless the clear-cut separation it effects, through the projection just mentioned, between the level of macroscopic

observation, contained in the asymptotic subspace  $\tilde{H}$ , and the fluctuating atomic behaviour of the system, which is fully accounted for by the density operator  $\varrho(t)$  describing the dynamical behaviour in the total superspace. If the system is initially in a pure state, its density operator at any time can be factorized as a dyadic product of state vectors: in the asymptotic subspace  $\tilde{H}$ , however, no such factorization is possible, no analogue to a state vector can be defined. Indeed, the function of the projector  $\tilde{H}$  is to sort out the part of the density operator that subsists after time intervals long enough to “wipe out” all initial phase relations between state vectors responsible for the fluctuations at the atomic level. In the asymptotic subspace, therefore, no “interference” of probability amplitudes occurs, but the asymptotic density operator  $\tilde{\varrho}(t)$  embodies the description of any correlation effect observable at the macroscopic level.

Indeed, the formalism is not restricted to the study of the approach to thermodynamic equilibrium, but is applicable as well to systems presenting kinematic properties of macroscopic order of magnitude. It is important for the completeness of the theory that it should contain a formal criterium allowing us to recognize the type of asymptotic behaviour we may expect for a given system. This criterium is supplied by the condition of dissipativity, which gives a simple characterization of the class of systems exhibiting an irreversible approach to equilibrium. It is important to note that the dissipativity condition is amenable to explicit evaluation at least in simple cases, such as the Friedrichs model, and relates the dissipative character of the system directly to the structure of its energy spectrum.

For dissipative systems, a particularly clear picture is obtained of the origin of the irreversibility observed in their macroscopic behaviour. The projector  $\tilde{H}$ , effecting the subdivision of the superspace into the subspaces which are the respective seats of the macroscopic and atomic evolution of the system, is invariant for time-reversal: this subdivision applies indeed to all systems, whether or not they are dissipative. The time evolution operator  $\tilde{\Sigma}(t)$  in the asymptotic subspace is also time-reversal invariant; its form (48), if we use the spectral decomposition  $\int \lambda dP(\lambda)$  of the superoperator  $L$ , just amounts to a Fourier integral representation  $\int \exp(-i\lambda t) dP(\lambda) \tilde{H}$  of the time-evolution. The expressions (41) for  $\tilde{\Sigma}(t)$  illustrate more explicitly how the asymptotic time-evolution starting from any given initial state proceeds by sequences of processes of “creation” and “destruction” of correlations between the elements of the system. The time direction in which one considers these processes is fixed by the choice of the conditions under which



we want to observe the behaviour of the system: on the information supplied by observation at a single instant, we normally base expectation of future behaviour; but the symmetry in time of the two equivalent forms (41) of  $\tilde{\Sigma}(t)$  shows what retrodiction we can also make, on the basis of the same information, about the evolution of the system, on the macroscopic time-scale, most likely to have led to its observed state: the sequences of creations and destructions of correlations appear inverted when, so to speak, we look back in time, and for dissipative systems we arrive at the well-known situation discussed by EHRENFEST in connexion with the *H*-theorem.\*)

The collision superoperator  $\Psi_{\mathcal{L}(+0)}$  does not only govern the condition of dissipativity; it also clarifies, as we have seen, the role of the dynamical invariants. In particular, it allows us, by eq. (62), to characterize the regular invariants (which, at least in typical cases, coincide with the controllable ones). This solves one of the main riddles of the kinetic theory: it was indeed never clear why the “collision operators” occurring in the usual formulations of the theory, such as the Boltzmann operator, were only in simple relation with the controllable invariants, independently of the possible existence of other invariants. At the same time, we see how decisive in this respect is the distinction between regular and singular invariants, – a distinction which can only be made for infinite systems.

Finally, it must be stressed that the macroscopic description we arrive at by projection into the  $\tilde{H}$  subspace is not the “classical” one: it still contains Planck’s constant wherever quantal effects occur on a macroscopic scale, as in the spectral distribution of electromagnetic radiation in thermal equilibrium, or in superconductivity and superfluidity. The laws of classical physics only appear as a limiting case of this macroscopic description in which all quantal effects are neglected, i.e. formally where  $\hbar$  is treated as infinitesimal.

Nevertheless, it would be a serious logical error to imagine that the procedure we have been following – starting from the quantal description of the system, obtaining by the projection  $\tilde{H}$  its macroscopic description, and letting in the latter  $\hbar$  tend to zero – would be a deduction of classical physics

\*) It must be observed, in this connexion, that while both  $\tilde{q}(t)$  and  $\varrho(t)$  appear as functions of the same time variable  $t$ , and in fact as solutions of the same Liouville equation, their time variations may be extremely different:  $\varrho(t)$  exhibits variations at the rate of atomic processes, whereas the variations of  $\tilde{q}(t)$  may look quite smooth in comparison. This circumstance may be made quite explicit, as shown by L. LANZ, L. A. LUGIATO and G. RAMELLA,<sup>25)</sup> at the unavoidable cost of formal complication: one must then renounce using the asymptotic time-displacement superoperator  $\theta$  acting at any time, but introduce a similar superoperator, whose action is only defined for an arbitrary finite sequence of separate instants.



from quantum mechanics. For we must not forget that the quantal description from which we start has to be made in terms of the very concepts of classical physics. All we have done, therefore, is to prove the logical consistency of the rules by which a connexion is established between the mathematical formalism and the classical description, upon which our account of macroscopic observation must ultimately rest. Obviously, there can be no question of any formal axiomatization of such a scheme: it must be based upon some set of classical concepts (e.g. space-time localization and momentum-energy) which remain unanalysed and are treated as “primitive”. These concepts (and these only) must be explained by processes of measurement, i.e. prescribed manipulations of specially designed apparatus, entirely describable in classical terms. Typically quantal concepts, on the other hand, like Planck’s constant or the electron spin, cannot be related directly to such purely classical measuring apparatus, – but the occurrence of quantal phenomena at the macroscopic level allows us to establish indirect connexions, involving more than one classical measurement, between quantal parameters and classical quantities, and thereby to determine with arbitrary accuracy the numerical values of the quantal parameters.\*)

\*) Thus, Millikan’s determination of Planck’s constant from the study of the ejection of electrons from metallic surfaces by light of various frequencies involves essentially two measurements: that of the light frequency and that of the corresponding kinetic energy of the ejected electrons.

## 4. Observation of individual atomic processes

### 4.1. The consistency problem of quantum mechanics

Quantum mechanics presents essentially two epistemological problems. The one, just recalled, concerns the consistency of the rules of interpretation by which the formalism is brought into relation with macroscopic observation, the other the relations of complementarity between different conditions of observation. There is nothing to add to Bohr's analysis of these relations, and we shall therefore confine ourselves to a comment, from the point of view developed in this paper, of the consistency problem. Briefly restated, this problem arises from the fact that the basic concepts used in the formulation of the laws governing individual atomic processes necessarily belong to the classical modes of description of direct macroscopic observation, which it is the aim of atomic theory to relate to the very laws of atomic behaviour. This means, as mentioned above, that these basic concepts must be regarded, from a strictly logical point of view, as "primitive". However, there is nothing to prevent us from describing on the atomic scale the process of measurement by which a value of the physical quantity denoted by any of these concepts is ascribed to an atomic system, as a dynamical process involving interactions between the atomic system observed and all the atomic constituents of the measuring apparatus, and obeying the laws of quantum mechanics. Such an analysis will only lead to the same conclusion as that resulting from the direct application of the rules of interpretation of the formalism if these rules are consistent. A test of this consistency is especially desirable with respect to the rule usually designated as the "reduction" of the wave function representing the initial state of the observed atomic system, i.e. its replacement after the measurement by another wave function expressing the information obtained by this observation. Although such a rule is obviously consonant with the statistical form of causality inherent in quantum mechanics, its relation with the dynamical process of measurement can only be

elucidated by a careful consideration of the specific function of the measuring apparatus and its implications for the course of the measuring process.

The decisive step was made by N. BOHR,<sup>1)</sup> who pointed out that any measurement is essentially the codified registration of some characteristic signal arising from the interaction between the observed atomic system and a suitable recording device of macroscopic dimensions. Indeed, he emphasized that the very definition of a phenomenon must contain a specification of the experimental conditions under which it is observed, including the apparatus recording some kind of permanent mark allowing us to identify the process observed. Until the process has not been terminated by the registration of its permanent record, we have no basis for the use of the classical concepts corresponding to such record, and accordingly no possibility of giving any well-defined account of the process. In other words, it is precisely the recording by the apparatus which establishes the necessary link between the behaviour of an atomic system and its description in terms of concepts referring to our possibilities of observing it. Now, it is clear that the formation of a permanent mark on a recording device is an irreversible macroscopic process, retaining no other trace of the original state of the atomic system than the specific feature corresponding to the construction of the apparatus; this information modifies the conditions of observation upon which statistical predictions about the behaviour of the atomic system must henceforth be based, and it is precisely this modification which is expressed in the formal language of the theory by the assignment to the atomic system, according to the rule of "reduction", of a new wave-function, appropriate to the new conditions of observation.

Once it is realized that the wave-function of the atomic system after the measurement is a component factor in an expression representing the asymptotic state of the whole system including the measuring apparatus, it can hardly be doubted that it will have the form prescribed by the reduction rule, since the latter precisely corresponds to this asymptotic situation. As already mentioned, we are only concerned with the consistency of the use of the small set of classical concepts we have called "primitive". In quantum mechanics, these are the complementary sets defining space-time localization and momentum-energy exchange; the completion of the above argument in this case only requires, as BOHR showed, the consideration of simple dispositions of fixed or moving diaphragms. It is sufficient to discuss these, as he did, by the methods of classical optics, since the latter use an idealized representation of diaphragms which directly accounts for the irreversible modification of a wave pattern arising from its interaction with such material



bodies.\*) In this connexion, it must be remembered that, although the apparatus fixing the conditions of observation, like any other macroscopic bodies, may in principle be described as large quantal systems, they must be kept outside such a description in order to fulfil their special function (otherwise, they would become themselves objects of observation); it is for this deep-lying reason that their intervention is represented in the formalism of quantum mechanics by parameters denoting "external" forces and prescriptions for the selection of appropriate solutions of the fundamental equations – among them the reduction rule. Disregard of this circumstance is the most frequent source of misunderstanding concerning the foundations of quantum mechanics.

The general theory of large quantal systems obviously offers another possibility of dealing with the consistency problem: one has only to apply this theory to the system formed by the atomic system under observation and the measuring apparatus described as a large assembly of atoms. This was done by the Italian physicists<sup>4)</sup> on the basis of the form of quantal ergodic theory they had previously developed:<sup>8)</sup> \*\*) their result is, of course, in full harmony with BOHR's argument.<sup>5)</sup> The kinetic approach outlined in the preceding sections allows us to discuss the issue in a more direct and simpler manner and to throw further light on the role of the measuring process in the epistemological analysis of physical theory.

#### 4.2. Discussion of the measuring process

In order to analyse the course of a measuring process, we may use the schematization discussed in detail in ref.<sup>5)</sup>. The main point is to arrive at a sufficiently simple and general formulation of the restrictions that have to be imposed upon the structure and dynamical behaviour of a macroscopic body in order that it may fulfil its function of measuring a specific property of a given atomic system. Its mode of interaction with the atomic system must be such as to bring it into a state observable at the macroscopic level and uniquely related (at least approximately) to the specific atomic state of interest. Without loss of generality, we avoid unessential complications by assuming

\*) Somewhat less elementary is the case of quantum electrodynamics, owing to the necessity of taking account of all retardation effects in the measurement of a field component; in this case also, the consistency of the formalism could be established by a detailed analysis,<sup>2)</sup> in which advantage was taken of the smallness of the coupling between electro-magnetic fields and distributions of electric charge and current.

\*\*) More recently, they have given some consideration to the problem from the point of view of their own kinetic theory, but made no attempt at a detailed examination of the issues involved.<sup>26)</sup>

that the interaction between the atomic system and the measuring apparatus only lasts for a time short enough to allow us to disregard any dynamical change of the atomic system as a result of this interaction. The apparatus, on the other hand, reaches, at the termination of the interaction, a dynamical state which must be such as to fix the ultimate outcome of the measurement. For from the moment the interaction ceases, the two parts of the total system evolve independently, and we expect the apparatus to settle down, at the macroscopic level of observation, into a situation providing a “permanent” record\*) of its specific interaction with the atomic system. This requirement imposes essential restrictions upon the constitution of the measuring apparatus and upon the interactions of its constituent elements with the atomic system under investigation. If the aim of the measurement is to ascertain whether the atomic system is in an eigenstate  $|\varphi_s\rangle$  of the operator representing some physical quantity attached to the system, there must exist a complete orthogonal basis  $|sm\rangle$  of dynamical states of the measuring apparatus such that (i) only a definite set  $\{|sm\rangle\}$  of such states (denoted by a common index  $s$ ) interacts with the atomic system when the latter is in a definite state  $|\varphi_s\rangle$ ; (ii) the correlations between any two states  $|sm\rangle, |s'm'\rangle$  are much weaker when they belong to different such sets ( $s \neq s'$ ) than when they belong to the same set ( $s = s'$ ). (As an example, we may think of the formation of a particle “track” in a bubble chamber or a photographic emulsion.\*\*\*)

In order to show how these conditions ensure the desired functioning of the measuring device, let us examine the asymptotic time-evolution of its density supervector in its own superspace. We define the subspace  $P_o$  by the projector

$$P_o = \sum_s P_o^{(s)}, \quad P_o^{(s)} = \sum_m P_{sm} \times P_{sm},$$

and, accordingly, the correlation subspace by the projector

$$P_c = \sum_{ss'} P_c^{(ss')}, \quad P_c^{(ss')} = \sum_{mm'} P_{sm} \times P_{s'm'},$$

the summation  $\sum'$  extending over all values of  $m$  and  $m'$  if  $s \neq s'$  and all different values of  $m$  and  $m'$  if  $s = s'$ . The superoperator  $\Psi(t)$  given by eq. (21) and the asymptotic superoperators  $\theta, \eta$  derived from it by eqs. (20)

\*) By “permanent” we do not imply that the state in question is one of actual thermodynamic equilibrium, but only that it lasts long enough for macroscopic observation.

\*\*) The interaction of a particle with the medium gives rise at a certain point (corresponding to a state  $|\varphi_s\rangle$  in which the particle has a definite “position”) to a local fluctuation (represented by the set  $\{|sm\rangle\}$ ) around which a bubble or a spot develops (leading to the asymptotic density  $\hat{\rho}_s(\mathbf{M})(t)$  defined on p. 37). The condition (ii) expresses the requirement that the successive bubbles or spots formed by the passage of the particle through the medium be sufficiently distinct from each other for a recording of the corresponding positions of the particle.



will essentially effect transitions from any subspace  $P_o^{(s)}$  to the same subspace: for other transitions, on account of the condition (ii) above, will be much less probable. Moreover, if we consider the mutually orthogonal subspaces defined by the projectors  $P^{(ss')} = P_o^{(s)}\delta_{ss'} + P_c^{(ss')}$ , the leading terms of the superoperators of destruction and creation of correlations will be those linking any subspace  $P^{(ss)}$  with itself (i.e. the subspace  $P_o^{(s)}$  with the correlation subspace  $P_c^{(ss)}$ ); next in importance will be the links between subspaces  $P^{(ss')}$  and  $P^{(ss'')}$  for values of  $s'$  and  $s''$  in a small interval around  $s$ . Therefore, if we start from any initial density supervector  $\varrho^{(M)}$  of the measuring apparatus, and only retain the leading terms, the asymptotic time-evolution of its projection  $P^{(ss')} \varrho^{(M)}$  will take the form

$$\tilde{\Sigma}(t)P^{(ss')} \varrho^{(M)} = \delta_{ss'} P^{(ss)} \tilde{\varrho}^{(M)}(t) \equiv \delta_{ss'} \tilde{\varrho}_s^{(M)}(t): \quad (66)$$

this formula expresses a clear-cut asymptotic trend of the measuring system towards definite states  $\tilde{\varrho}_s^{(M)}(t)$  uniquely associated with the eigenstates  $|\varphi_s\rangle$  which are the objects of the measurement.\*)

After this preparation, the discussion of the measuring process is readily performed. Let the initial state of the atomic system be represented by a superposition  $\sum_s c_s |\varphi_s\rangle$  of the eigenstates  $|\varphi_s\rangle$ ; the resulting density supervector

$$\varrho^{(S)} = \sum_{ss'} \varrho_{ss'}^{(S)}, \quad \varrho_{ss'}^{(S)} = c_s c_{s'}^* |\varphi_s\rangle \langle \varphi_{s'}|$$

exhibits the correlation between the states  $|\varphi_s\rangle$  arising from definite phase relations between the coefficients  $c_s, c_{s'}^*$ . The initial form of the density supervector of the total system formed by the atomic system and the apparatus (i.e., let us recall it, the form this supervector takes immediately after the two constituents of the total system have interacted) is easily set up in conformity with our condition (i): to each component  $\varrho_{ss'}^{(S)}$  there corresponds a component  $P^{(ss')} \varrho^{(M)}$  of the apparatus density supervector. The total density supervector is thus initially

\*) It should be stressed that the approximation (66) is sufficient for the analysis of the most general measuring process of physical interest. The case envisaged by Wigner's theorem<sup>27)</sup>, in which the system formed by the atomic object and the measuring apparatus has an additive invariant, only occurs if the quantity to be measured is precisely such an invariant, or commutes with it, and an idealization of the type (66) is then in accordance with the theorem. If, however, the quantity to be measured does not commute with the additive invariants, Wigner's theorem has no relevance, for it is an obvious physical requirement that any such invariance should be destroyed by coupling the apparatus to a suitable external system of infinite extension. For instance, while a momentum measurement of infinite accuracy may be performed by means of an elastic collision of the atomic object with a freely moving test-body, the spatial localization of the object requires the test-body to be rigidly attached to some body of infinite mass serving as a spatial system of reference. It is worth pointing out how well adapted the  $\tilde{H}$ -space representation is to a concise and general account of the process of measurement.



$$\sum_{ss'} \varrho_{ss'}^{(S)} \cdot P^{(ss')} \varrho^{(M)},$$

and each factor evolves independently in its own superspace: the time-evolution of the atomic system is governed by its Liouville superoperator  $T^{(S)}(t) = \exp \{-iL^{(S)}t\}$ ; as to the apparatus, we are interested in its evolution at the macroscopic level, described in its asymptotic subspace by the superoperator  $\tilde{\Sigma}(t)$ . Adopting the idealized situation expressed by eq. (66), we therefore obtain at time  $t$  the total density supervector

$$\sum_s T^{(S)}(t) \varrho_{ss}^{(S)} \cdot \tilde{\varrho}_s^{(M)}(t).$$

From this expression a density supervector making explicit reference only to the atomic system may be derived by averaging it over the apparatus superspace, i.e. by taking its trace with respect to the apparatus basis; we may simply ascribe the same limiting value to all the  $\text{tr } \tilde{\varrho}_s^{(M)}(t)$  and normalize it to unity:

$$\lim_{t \rightarrow \infty} \text{tr } \tilde{\varrho}_s^{(M)}(t) = 1.$$

This gives us for the density supervector of the atomic system, after a time sufficient for the recording of a permanent mark on the apparatus, the expression

$$\sum_s |c_s(t)|^2 |\varphi_s\rangle \langle \varphi_s|, \quad (67)$$

from which every explicit reference to the apparatus has disappeared, and whose form agrees with the prescription of the reduction rule.

The way in which this result has been derived makes its meaning quite clear. In the first place, it is essentially an asymptotic result, and there is no question of its contradicting any consequence of the time-dependent Schrödinger equation. Secondly, the only interactions involved in the whole process are the specific interaction of short duration between the atomic system and the apparatus and the long sequence of interactions it triggers off between the constituent atoms of the apparatus; there is no question whatsoever of any non-physical intervention of any kind upon the atomic system: the whole measuring process is a purely automatic registering operation, obeying only the laws of quantum mechanics, and its outcome is accordingly in full harmony with these laws. Let us here emphasize again that the treatment of the measuring apparatus as a quantal system we have performed has no other purpose than exhibiting the consistency of the conceptual framework of quantum mechanics, in which formalism and rules of interpretation in terms of classical concepts form an inseparable whole. Thirdly, the difference between the "reduced" density (67) and that of the system before the

measurement simply reflects the change in our information about the system brought about by this measurement; the occurrence of such a difference is no peculiarity of quantum mechanics (though the particular form it takes is of course a specifically quantal one) – it is common to all statistical situations and in fact an essential component of the concept of probability.

#### 4.3. The role of the observer

Statistical causality has often been misrepresented as implying the intrusion of a “subjective” element into the description of the phenomena; this epistemological error (which was not made by the founders of the theory of probabilities) arises from an insufficient analysis of the conditions under which knowledge of the phenomena is obtained. The inclusion of a specification of the conditions of observation into the account of the phenomena is no arbitrary decision, but, as we have insistently stressed, a necessity imposed by the very laws governing the course of these phenomena and the mechanism of their observation, and thereby an indispensable part of their objective description, since it ensures that such a description will be common to all observers placed in the specified conditions. It is in order to make this objectivity quite apparent that we have analysed, in the preceding subsection, the observation process as a purely physical one, limited to the automatic registration of a record, which need not even be read.

Obviously, such an analysis touches only one side of the process of acquisition of objective knowledge. This process is not complete until a reading of the record has actually occurred, i.e. until the information it contains has been stocked into the brain of some observer. This “psychological” side of the cognitive process is obviously just as objective as the other, since it is the same for any conceivable observer, but the question arises whether it can legitimately be separated as sharply as we have done from the purely physical registration process. It would seem that our understanding of the fundamental biological processes has now reached a stage allowing us to give a definite answer to this question.

We must above all realize that there is a large class of physical and chemical dissipative processes, occurring far from the thermodynamic equilibrium conditions, which present structural inhomogeneities quite foreign to the familiar physical phenomena observed at or near equilibrium, but analogous to typical features of biological systems.<sup>28, 29)</sup> It has been shown, for example, that chemical reactions essential for the metabolism of living systems, as well as for the regulation of genetic and evolutionary processes, can be treated in detail in terms of usual chemical kinetics, and involve branches of the solution of the non-linear kinetic equations which do not



belong to the classical thermodynamic description of near-equilibrium situations, but only appear under conditions far from equilibrium.<sup>30, 31)</sup> Now, thermodynamics, both in its classical and its more general form just mentioned, is a mode of description adapted to the behaviour of macroscopic systems in the asymptotic  $\tilde{II}$  subspace; indeed, it has been explicitly established<sup>32)</sup> that the thermodynamic description can be derived from the kinetic equation associated with the time-evolution operator  $\tilde{\Sigma}(t)$ . It is natural to conclude from these considerations that the distinction between “living” and “non-living” systems appears to be part of their description in  $\tilde{II}$ -space, and accordingly cannot be based on any quantal description on the atomic scale. An analogy which may perhaps clarify the significance of this remark is the distinction between laminar and turbulent motion, which correspond to two types of solution of the Navier-Stokes equation: as this equation belongs to the macroscopic level – it is a consequence of the kinetic equation – we cannot characterize the difference between these two types of flow by means of the formalism of quantum mechanics. Likewise, it would seem that the characteristics of “life” cannot be formulated at the atomic level but are essentially macroscopic. Incidentally, this circumstance is sufficient to dismiss all “paradoxical” situations (such as the famous example ascribed to Schrödinger) which one would allegedly encounter when attempting to treat living systems by the methods of quantum mechanics. In such cases, just as in the general problem of observation, a correct epistemological analysis can only be developed at the macroscopic level of description.

If we accept this general inference from our present knowledge of biology, we do not see any special role to be attributed to a “living” observer in the discussion of the consistency problem of quantum mechanics: the only condition the intervention of such an observer has to fulfil is to be amenable to physical description at the macroscopic level. Now, we may confidently assume that the sense organs of an animal register signals from the physical environment in essentially the same way as material apparatus, and that the storage of these signals and their incorporation into sensory-motor schemes is also the result of physical and chemical processes of the type commonly observed in biology.<sup>\*)</sup> Since all the organs involved are of macroscopic order of magnitude, their activity can in principle be entirely described in the asymptotic subspace  $\tilde{II}$  of the appropriate superspace, like the functioning of any physical measuring apparatus.

\*) Of great interest in this respect is the experimental evidence showing that the memory of a specific sensory-motor scheme can be stored in the form of a coded macromolecule.



## 5. General conclusion

Perhaps the most significant general result of our approach is the introduction of generalized projection superoperators, made possible through the consideration of superspace. This generalization involves the concept of time-reversal invariance which replaces the usual one of self-adjointness, to which it reduces in the absence of dissipation. These new projectors allow us to give a precise characterization of the macroscopic level of description of general quantal systems, and to formulate quantitatively the conditions under which a given system will exhibit the properties belonging to this level: a formulation obviously susceptible to experimental test (for example, we may verify whether a system is in thermodynamical equilibrium). These questions actually amount to an extension of the scope of quantum mechanics, which has only been outlined in this paper and deserves a more detailed treatment. In a sense, the question of the definition of a macroscopic level of quantum mechanics may be considered as a simple illustration of this general method, which applies as well to a large class of other problems.

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## Appendix

### Matrix representation in superspace

Although we have not made use in the text of any explicit matrix representation of supervectors and superoperators, such a representation might be helpful in concrete applications. We therefore collect in this appendix simple practical rules for writing down such matrix components.

A supervector  $A$  is represented by its matrix elements in the form

$$A = \sum_{mm'} P_m A P_{m'} = \sum_{mm'} \langle m | A | m' \rangle P_{mm'}$$

where

$$P_{mm'} = |m\rangle\langle m'|, \quad P_{mm'}^+ = P_{m'm}.$$

In this notation, any superoperator  $O$  is a sum of factorizable superoperators:

$$O = \sum_{\substack{mm' \\ nn'}} O_{mm',nn'} P_{mn} \times P_{n'm'},$$

and with the adopted order of the indices one has

$$\begin{aligned} \langle m | O A | m' \rangle &= \sum_{nn'} O_{mm',nn'} \langle n | A | n' \rangle, \\ (OQ)_{mm',nn'} &= \sum_{pp'} O_{mm',pp'} Q_{pp',nn'}. \end{aligned}$$

The components of the adjoint superoperator are

$$O_{mm',nn'}^\dagger = O_{nn',mm'}^*$$

and the transposition gives

$$\langle m | A O | m' \rangle = \sum_{nn'} \langle n | A | n' \rangle O_{n'n,m'm}.$$

The adjoint symmetry of the superoperator  $O$  implies the relations

$$O_{mm',nn'} = O_{m'm,n'n}^*$$

between its components.