

On the Dynamical Basis of Macroscopic Theory

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A modification of the projection technique in convolutionless form is developed. The dynamical basis of macroscopic theory is discussed with the aid of this method in order to remove from it superfluous and artificial suppositions, in particular, those of a probability theory nature. It is shown that sufficient instability of the system with respect to the initial microstate naturally leads to the possibility of a macroscopic description, the latter proving to be closed, causal, and asymptotically exact. The objective sense of the theory and the principal questions of its interpretation are discussed.

KEY WORDS: Brussels school approach; contracted description; projection formalism; strictly Markovian master equation.

1. INTRODUCTION

Recent progress in the theory of irreversible processes has been accompanied by the steady weakening of suppositions of a probability theory nature, which long were considered as inalienable attributes of the theory. At present we can assert that suppositions of this kind are unnecessary for the foundation of the macroscopic theory: The necessary contraction of the exact dynamical description is provided by the system dynamics itself. More strictly, this assertion may be formulated as the alternative: Either the dynamical system has the properties that provide the possibility of its description in terms of macroscopic variables (on the coarsened time scale) *without using any statistical hypotheses*, or a macroscopic description is not possible at all.

The chief questions concerning the basis of the macroscopic theory have become more accessible following the work carried out by the Brussels group in the last decade,⁽¹⁻³⁾ and especially since the developed theory was translated into the projection formalism language.⁽⁴⁾ The present paper is

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devoted to the further development of this approach² both in its formal aspect and from the viewpoint of its physical interpretation.

In Section 2 we find a new representation of the Brussels formalism, which is intimately connected with the "Markovization" of the master equation. In contrast with previous ways of eliminating the memory,⁽⁷⁻¹⁰⁾ our method⁽¹¹⁾ is more suitable for practical calculations. The "Markovized" representation enables one to simplify essentially the proof of all the results of the theory because for the derivation of the asymptotic formulas (see Section 3) there is no necessity of using the Laplace transform, which leads to the cumbersome combinatorial calculations. Moreover, the present formalism provides a natural and straightforward proof of new and useful results and relationships. For instance, the generator of macroevolution is defined by a *linear* problem (see Section 3).

However, the main merit of the formalism is its physical obviousness. The starting point of the physical interpretation of the macroscopic theory is the assertion that the macrodescription must be adequate for a definite class of experiments, namely, those carried out with devices with finite time resolution. The consistent realization of this simple idea enables us to formulate (in Sections 2 and 3) common requirements for the dynamical system in order for its macroscopic description to be possible. Although we give no strict mathematical basis for the theory³ and limit ourselves to a qualitative discussion, the formalism is so transparent that the conditions found appear to be final. In other words, these requirements, being sufficient, are minimal at the same time.

Specifically, the adequacy idea is expressed in the fact that the macroscopic theory arises as the result of smoothing (averaging over time on a definite scale) of the dynamical picture. This natural interpretation turns out to be sufficient for an unambiguous answer to questions of the objective sense of the contracted description, the nature of irreversibility, the causality of the macrodescription, etc.

The formalism may be used not only in connection with perturbation theory for the Liouville (or von Neumann) equation, as is done in most work, but also for the description of any regime of physical interest (kinetic, hydrodynamic, turbulent), and even in situations beyond the theory of irreversible processes (scattering theory, theory of stochastic equations). The statement of the dynamical problem and the choice of the projector are peculiar in every specific case, but the common results of the theory are insensitive to them. Therefore, we limit ourselves to an abstract statement of

² An interesting and in some respects similar approach to the one presented here was initiated by Mori⁽⁶⁾ (see also Ref. 6); however, in that work the opportunities of the formalism have not been used completely.

³ For nondissipative systems some strict results were found by Kummer.⁽¹²⁾

the formalism, due to which the structure of the theory seems to be especially simple and lucid.

For completeness and to demonstrate the compactness of the formalism, we also give new proofs of known results, which in part are given in the appendix.

2. DYNAMICAL PROBLEM: FUNDAMENTAL SOLUTION

Let the closed dynamical system⁴ be described by the state vector $F(t)$ obeying the equation

$$(\partial_t - \mathcal{L})F(t) = 0 \tag{1}$$

and let the idempotent operators $P = P^2$ and $Q \equiv 1 - P = Q^2$ (conventionally called “projectors”) be defined over the state space so that the projector P separates out the macroscopic component of the state vector,⁵ $PF(t) \equiv f(t)$, while the component $QF(t) \equiv h(t)$ contains the irrelevant microscopic information. The choice of the operator P usually is limited only by the condition that the component $f(t)$ must be expressed in terms of macroscopic observables, which, in turn, are chosen from physical considerations. However, the theory allows us to verify, in principle, the correctness of this choice *a posteriori*.

The dynamical problem (1) is considered as the Cauchy problem, which is conveniently treated with the help of the fundamental (retarded) solution satisfying the equation

$$(\partial_t - \mathcal{L})U(t) = \delta(t), \quad U(t < 0) = 0 \tag{2}$$

Introducing special notations for the P and Q components of the dynamical operator,

$$\mathcal{L} = P\mathcal{L}P + P\mathcal{L}Q + Q\mathcal{L}P + Q\mathcal{L}Q \equiv \tilde{\mathcal{L}} + \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L} \tag{3}$$

and, analogously, for those of the fundamental solution,

$$U(t) = \tilde{U}(t) + U_1(t) + U_2(t) + \hat{U}(t) \tag{4}$$

we can write the components of Eq. (2) in the form

$$(\partial_t - \tilde{\mathcal{L}})\tilde{U}(t) = P \delta(t) + \mathcal{L}_1 U_2(t) \tag{5}$$

$$(\partial_t - \mathcal{L})U_2(t) = \mathcal{L}_2 \tilde{U}(t) \tag{6}$$

$$(\partial_t - \tilde{\mathcal{L}})U_1(t) = \mathcal{L}_1 \hat{U}(t) \tag{7}$$

$$(\partial_t - \mathcal{L})\hat{U}(t) = Q \delta(t) + \mathcal{L}_2 U_1(t) \tag{8}$$

⁴ The generalization to open systems with time-dependent dynamical operator $\mathcal{L}(t)$ offers no difficulties and was performed, for instance, by Demendy⁽¹³⁾ (in the conventional treatment).

⁵ In the general case the projector may be dependent on time (see, for instance, Ref. 6). However, this does not introduce serious difficulties, since the operator $P(t)$ always acts on the expression referred to the same moment t .

Using the elementary retarded Greenians

$$\tilde{G}(\tau) = \theta(\tau) \exp(\tau \mathcal{L}) P, \quad \hat{G}(\tau) = \theta(\tau) \exp(\tau \mathcal{L}) Q \quad (9)$$

and the basic fragments of the theory (also retarded)

$$\psi(\tau) = \mathcal{L}_1 \hat{G}(\tau) \mathcal{L}_2, \quad C(t) = \hat{G}(\tau) \mathcal{L}_2, \quad D(\tau) = \mathcal{L}_1 \hat{G}(\tau) \quad (10)$$

we can represent the formal solution of the system of Eqs. (5)–(8) as⁽¹⁴⁾

$$\begin{aligned} \tilde{U} &= \tilde{G} + \tilde{G} * \psi * \tilde{U} = (1 - \tilde{G} * \psi)^{-1} * \tilde{G} \\ U_1 &= \tilde{U} * D, \quad U_2 = C * \tilde{U}, \quad \hat{U} = \hat{G} + C * \tilde{U} * D \end{aligned} \quad (11)$$

where the “star” means the time convolution over the interval $(0, t)$. In this representation the component $\tilde{U}(t)$ plays the determining role.

On the basis of this solution one can easily obtain for the macroscopic component

$$f(t) = \tilde{U}(t)f(0) + U_1(t)h(0) \quad (12)$$

the well-known master equation with memory

$$(\partial_t - \mathcal{L})f(t) = \int_0^t d\tau \psi(\tau)f(t - \tau) + D(t)h(0) \quad (13)$$

In what follows, however, we diverge from the method of the Brussels group, having found a new representation for the component $\tilde{U}(t)$ which leads directly to the “Markovization” of Eq. (13).

The equation for $\tilde{U}(t)$, which is obtained by the elimination of $U_2(t)$ from Eqs. (5) and (6), is

$$(\partial_t - \mathcal{L})\tilde{U}(t) = P \delta(t) + \int_0^t dt'' \psi(t - t'')\tilde{U}(t'') \quad (14)$$

where it is taken into account that we look for the solution for $t > 0$ with the initial condition $\tilde{U}(0) = P$. However, since hitherto all the equations were exact and, consequently, causal (as is the original dynamical problem itself), we can define $\tilde{U}(t')$ for the intermediate time $(0 < t' < t)$ with the given $\tilde{U}(t)$. In that case, using the advanced Greenian

$$\tilde{G}^a(\tau) = -\theta(-\tau) \exp(\tau \mathcal{L}) P \quad (15)$$

we have

$$\begin{aligned} \tilde{U}(t') &= -\tilde{G}^a(t' - t)\tilde{U}(t) + \int_0^{t'} dt_1 \tilde{G}^a(t' - t_1) \int_0^{t_1} dt'' \psi(t_1 - t'')\tilde{U}(t'') \\ &\equiv -\tilde{G}^a \tilde{U}(t) + \tilde{G}^a * \psi * \tilde{U} = -(1 - \tilde{G}^a * \psi)^{-1} * \tilde{G}^a \tilde{U}(t) \end{aligned} \quad (16)$$

Inserting this in Eq. (14), we transform it to

$$[\partial_t - \Gamma(t)]\tilde{U}(t) = P \delta(t), \quad \Gamma(t) = \tilde{\mathcal{L}} + \gamma(t, t) \quad (17)$$

where (for arbitrary time arguments)

$$\begin{aligned} \gamma &= -\psi * (1 - \tilde{G}^a * \psi)^{-1} * \tilde{G}^a = -\Omega * \psi * \tilde{G}^a, \\ \Omega &= (1 - \psi * \tilde{G}^a)^{-1} \end{aligned} \quad (18)$$

Hence the equation for γ is

$$\gamma = -\psi * \tilde{G}^a + \psi * \tilde{G}^a * \gamma \quad (19)$$

Rewriting it in detail with the help of the definitions given above, we obtain after a sequence of transforms⁽¹⁵⁾

$$\gamma(t, t) = \int_0^t d\tau \psi(\tau) K(\tau/t) \quad (20)$$

where the operator K is defined by the linear integral equation (for $\tau > 0$)

$$K(\tau|t) = \exp(-\tau\tilde{\mathcal{L}}) - \int_0^\tau d\sigma \int_0^{t-\sigma} d\vartheta \{\exp[(\sigma - \tau)\tilde{\mathcal{L}}]\psi(\vartheta)K(\sigma + \vartheta|t)\} \quad (21)$$

Thus, we have obtained a new, somewhat more suitable, representation of the fundamental solution (11), in which, according to Eq. (17), the component $\tilde{U}(t)$ is expressed as

$$\tilde{U}(t) = \exp_+ \left\{ \int_0^t dt' \Gamma(t') \right\} P \quad (22)$$

where \exp_+ is time-ordered and we have omitted the factor $\theta(t)$ since in the following only times $t > 0$ will be considered.

Such a representation leads directly to the elimination of memory from the master equation (13). To show this with minimum labor, we have to repeat the previous construction for the component $U_1(t)$ defined by Eqs. (7) and (8). As a result,

$$U_1(t) = \int_0^t d\tau \exp_+ \left\{ \int_\tau^t dt' \Gamma(t') \right\} \Delta(\tau, 0) \quad (23)$$

where

$$\Delta = \Omega * D = D + \psi * \tilde{G}^a * \Delta \quad (24)$$

or, in more detail,

$$\Delta(\vartheta, 0) = D(\vartheta) - \int_0^\vartheta d\tau \int_{\vartheta-\tau}^t d\sigma \psi(\tau) \{\exp[(\vartheta - \tau - \sigma)\tilde{\mathcal{L}}]\Delta(\sigma, 0)\} \quad (25)$$

Inserting Eqs. (22) and (23) in the definition of macrocomponent (12), we find after time differentiation

$$[\partial_t - \Gamma(t)]f(t) = \Delta(t, 0)h(0) \quad (26)$$

If $\Gamma(t)$ achieves a definite limit with time, then, defining

$$\Gamma(t) = \Gamma^\circ + \delta\Gamma(t), \quad \Gamma^\circ = \lim_{t \rightarrow \infty} \Gamma(t) \quad (27)$$

we can rewrite Eq. (26) in the form

$$(\partial_t - \Gamma^\circ)f(t) = \delta\Gamma(t)f(t) + \Delta(t, 0)h(0) \quad (28)$$

where the right-hand side describes the difference of the dynamical picture from the macroscopic one.

3. ASYMPTOTIC SOLUTION

To this point we have been considering the exact dynamical relationships. Below we shall try to find the minimal conditions that provide the contraction of this description and the foundation of the macroscopic theory, i.e., the derivation of the closed equation for the component $f(t)$. First, as follows from Eq. (13), this can be achieved only when the contribution of the "initial correlations" $H(t) = D(t)h(0)$ damps with time sufficiently quickly, the damping having been provided for all $h(0)$, since in the macroscopic framework we cannot state any suppositions about the microstate [for instance, to suppose $h(0) = 0$ —"preparation of the system"], which are not controllable by the macroscopic experiment. If the characteristic time of damping of $H(t)$, τ_m , is much smaller than the characteristic evolution time of $f(t)$, τ_M , the macroscopic theory may be defined as the result of the averaging of the dynamical picture on some intermediate scale τ^* : $\tau_m \ll \tau^* \ll \tau_M$. The first strong inequality is necessary to exclude, with sufficient correctness, the contribution of the irrelevant microinformation; the second is necessary to preserve the differential-in-time character of the macrodescription. The main advantage of this simple interpretation⁶ consists in the fact that it is adequate to the real experimental situation—the observation with a device with finite time resolution τ^* . Moreover, there is no necessity of introducing into the theory of any artificial construction of the type of averaging either over the phase space or over the ensemble.

In practice, it is more convenient to use, instead of averaging on the scale τ^* , the limiting procedure, since the result of averaging coincides with the corresponding limit (in a strong sense), if the latter exists. One has to remember, however, that from the physical point of view we are interested

⁶ Of course, it is no more than a concretization of the idea of hierarchy of time scales, which was used by Chapman and Enskog and was clearly formulated by Bogoliubov.⁽¹⁶⁾

in the limit which is achieved on the finite time interval τ^* , so that all the slow dependences on t are preserved. In other words, it is the limit in the sense of the Tauberian theorems, and we use for it the special symbol τ^* -lim.

The microinformation enters in the theory not only due to the contribution of the initial correlations; therefore, we need other damping conditions, the totality of which will be subdivided in three groups:

$$A_1: \quad \tau^*\text{-lim}_t \psi(t) = \tau^*\text{-lim}_t \mathcal{L}_1[\exp(t\mathcal{L})]\mathcal{L}_2 = 0 \quad (29)$$

$$A_2: \quad \tau^*\text{-lim}_t D(t)h(0) = \tau^*\text{-lim}_t \mathcal{L}_1[\exp(t\mathcal{L})]h(0) = 0, \quad \forall h(0)$$

$$B: \quad \tau^*\text{-lim}_t C(t) = \tau^*\text{-lim}_t[\exp(t\mathcal{L})]\mathcal{L}_2 = 0 \quad (30)$$

$$C: \quad \tau^*\text{-lim}_t \hat{G}(t)h = \tau^*\text{-lim}_t[\exp(t\mathcal{L})]h = 0, \quad \forall h \quad (31)$$

Deferring the discussion of the physical justifiability of these conditions to the following section, let us find on their basis the asymptotics of the fundamental solution.

First, let us mention that if condition A_1 is fulfilled, the τ^* -lim of Eqs. (20) and (21) is well defined:

$$\gamma^\circ = \tau^*\text{-lim}_t \gamma(t, t) = \int_0^\infty d\tau \psi(\tau)K^\circ(\tau) \quad (32)$$

$$K^\circ(\tau) = \tau^*\text{-lim}_t K(\tau|t)$$

$$= [\exp(-\tau\mathcal{L})] - \int_0^\tau d\sigma \int_0^\infty d\vartheta \{\exp[(\sigma - \tau)\mathcal{L}]\psi(\vartheta)K^\circ(\sigma + \vartheta)\} \quad (33)$$

due to which the supposition (28) is justified, i.e.,

$$\begin{aligned} \tau^*\text{-lim}_t \Gamma(t) &= \Gamma^\circ = \mathcal{L} + \gamma^\circ, \\ \tau^*\text{-lim}_t \delta\Gamma(t) &= \tau^*\text{-lim}_t [\gamma(t, t) - \gamma^\circ] = 0 \end{aligned} \quad (34)$$

Using the conventional manipulations with the operator exponent (the interaction representation), one can represent the component $\tilde{U}(t)$ [(22)] in the form

$$\begin{aligned} \tilde{U}(t) &= [\exp(t\Gamma^\circ)] \cdot \exp_+ \left\{ \int_0^t dt' [\exp(-t'\Gamma^\circ)] \delta\Gamma(t') [\exp(t'\Gamma^\circ)] \right\} P \\ &\equiv [\exp(t\Gamma^\circ)] \cdot A(t) \end{aligned} \quad (35)$$

where the operator $A(t)$ also has the well-defined limit

$$A^\circ = \tau^*\text{-lim}_t A(t) = \exp_+ \left\{ \int_0^\infty dt' [\exp(-t'\Gamma^\circ)] \delta\Gamma(t') [\exp(t'\Gamma^\circ)] \right\} P \quad (36)$$

Since, as one can easily surmise, the operator Γ° describes the macroscopic (slow) evolution, we find for the asymptotic behavior of $\tilde{U}(t)$

$$\tilde{U}^\circ(t) = \tau^*\text{-lim}_t \tilde{U}(t) = [\exp(t\Gamma^\circ)]A^\circ \quad (37)$$

With the help of Eqs. (11) and (35), the component $U_1(t)$ may be represented as follows:

$$U_1(t) = \int_0^t d\tau \{\exp[(t - \tau)\Gamma^\circ]\} A(t - \tau) D(\tau) \quad (38)$$

Here the time integral converges quickly when the operator D damps; therefore, if conditions A_1 and A_2 are fulfilled,

$$U_1^\circ(t) = \tau^*\text{-lim}_t U_1(t) = \int_0^\infty d\tau \{\exp[(t - \tau)\Gamma^\circ]\} A^\circ D(\tau) = [\exp(t\Gamma^\circ)] A^\circ D^\circ \quad (39)$$

where⁷

$$\begin{aligned} D^\circ &= A^{\circ-1} \int_0^\infty d\tau [\exp(-\tau\Gamma^\circ)] A^\circ D(\tau) \\ &= \int_0^\infty d\tau [\exp(-\tau\Gamma^{\circ*})] D(\tau), \quad \Gamma^{\circ*} = A^{\circ-1}\Gamma^\circ A^\circ \end{aligned} \quad (40)$$

In the definition

$$U_2(t) = \int_0^t d\tau C(\tau) \{\exp[(t - \tau)\Gamma^\circ]\} A(t - \tau) \quad (41)$$

the convergence of the integral may be provided only by the damping of $C(\tau)$; therefore, if the conditions A_1 and B are fulfilled, the asymptotic behavior of $U_2(t)$ is given by

$$U_2^\circ(t) = \tau^*\text{-lim}_t U_2(t) = C^\circ [\exp(t\Gamma^\circ)] A^\circ \quad (42)$$

with

$$C^\circ = \int_0^\infty d\tau C(\tau) \exp(-\tau\Gamma^\circ) \quad (43)$$

Finally, for the existence of the well-defined asymptotic behavior of

$$\begin{aligned} \hat{U}(t) &= \hat{G}(t) + \int_0^t d\tau_1 \int_0^{t-\tau_1} d\tau_2 C(\tau_1) \\ &\quad \times \{\exp[(t - \tau_1 - \tau_2)\Gamma^\circ]\} A(t - \tau_1 - \tau_2) D(\tau_2) \end{aligned} \quad (44)$$

the fulfillment of all the conditions A_1 , A_2 , B , and C is required, and so

$$\hat{U}^\circ(t) = \tau^*\text{-lim}_t \hat{U}(t) = C^\circ [\exp(t\Gamma^\circ)] A^\circ D^\circ \quad (45)$$

Equations (37), (39), (42), and (45) are the basis of the "subdynamics"

⁷ The existence of the inverse operator $A^{\circ-1}$ is provided by the representation (36); $\Gamma^{\circ*}$ is the result of "star-transforming" Γ° (see appendix).⁽³⁾

due to Prigogine and co-workers, which reduces the original dynamical problem to the description of the evolution of the smoothed state vector

$$F^\circ(t) = U^\circ(t)F(0), \quad U^\circ(t) = (1 + C^\circ)[\exp(t\Gamma^\circ)]A^\circ(1 + D^\circ) \quad (46)$$

For its components we have

$$f^\circ(t) = PF^\circ(t) = [\exp(t\Gamma^\circ)]A^\circ[f(0) + D^\circ h(0)] \quad (47)$$

$$h^\circ(t) = QF^\circ(t) = C^\circ f^\circ(t), \quad F^\circ(t) = (1 + C^\circ)f^\circ(t) \quad (48)$$

Equation (48) exhibits the intimate connection of the subdynamics idea with that of synchronization suggested by Bogoliubov.⁽¹⁶⁾ From Eq. (47) the closed equation for the smoothed macrocomponent follows:

$$(\partial_t - \Gamma^\circ)f^\circ(t) = 0 \quad (49)$$

which has to be solved with the initial condition

$$f^\circ(0) = A^\circ[f(0) + D^\circ h(0)] \quad (50)$$

The same Equation (49) is obtained as the result of smoothing the master equation (28), since, as follows from Eq. (25), the operator $\Delta(t, 0)$ has the same damping property as $D(t)$. However, in this case the initial condition, instead of Eq. (50), is simply the smoothed value of $f(0)$. We defer the discussion of this point to the following section.

A special role in the Brussels approach belongs to the operator

$$\Pi = (1 + C^\circ)A^\circ(1 + D^\circ) \quad (51)$$

about which we can assert the following.

1. The operator Π is well defined if the operators A° , D° , and C° are defined, i.e., when the conditions A_1 , A_2 , and B in (29) and (31) are fulfilled. If, besides, the condition C is fulfilled, i.e., $U^\circ(t)$ [(46)] exists, then $\Pi = U^\circ(0)$.

2. As a consequence of the equality (A.4), the operator Π is idempotent^(17,18):

$$\Pi^2 = (1 + C^\circ)A^\circ(1 + D^\circ C^\circ)A^\circ(1 + D^\circ) = \Pi \quad (52)$$

3. The operator Π commutes with the dynamical propagator⁽¹⁹⁾ [see (A.13)]:

$$\Pi U(t) = U(t)\Pi = U^\circ(t) \quad (53)$$

These properties are important because, according to the definition (46),

$$F^\circ(t) = \Pi F(t) = U^\circ(t)F(0) = U^\circ(t)F^\circ(0) = U(t)F^\circ(0) \quad (54)$$

Thus, the smoothed state vector is obtained by the action of the operator Π on $F(t)$ (i.e., the operator Π plays in the calculation the role of a device in the experiment) and obeys the original dynamical equation, but with the

smoothed initial data. The latter, in particular, justifies the scheme suggested by Zubarev,⁽²⁰⁾ in which the nonequilibrium statistical operator is defined as the solution to the Liouville equation with the macroscopic initial condition.

To conclude this section, we mention that the equivalence of the results found above to those obtained by the Brussels group is almost obvious, and only two points connected with the new determinations of the operators A° [(36)] and $\Gamma^\circ = \mathcal{L} + \gamma^\circ$ [(32) and (33)] should be clarified. As for A° , the question is solved easily, since due to the equality (A.4) in both approaches it is represented in the form

$$A^\circ = (1 + D^\circ C^\circ)^{-1} \cdot P \quad (55)$$

For Γ° , with the help of iterations of Eq. (33), we directly obtain the expansion in powers of ψ :

$$\begin{aligned} \Gamma^\circ = & \mathcal{L} + \int_0^\infty d\tau \psi(\tau) [\exp(-\tau\mathcal{L})] - \int \int_0^\infty d\tau_1 d\tau_2 \int_0^{\tau_1} dt \\ & \times \psi(\tau_1) \{ \exp[(t - \tau_1)\mathcal{L}] \} \psi(\tau_2) \{ \exp[-(t + \tau_2)\mathcal{L}] \} + \dots \\ & + (-1)^{n-1} \int_0^\infty \dots \int d\tau_1 \dots d\tau_n \int_0^{\tau_1} dt_1 \dots \int_0^{\tau_{n-1} + t_{n-2}} dt_{n-1} \\ & \times \psi(\tau_1) \{ \exp[(t_1 - \tau_1)\mathcal{L}] \} \psi(\tau_2) \{ \exp[(t_2 - t_1 - \tau_2)\mathcal{L}] \} \dots \\ & \times \psi(\tau_n) \{ \exp[-(t_{n-1} + \tau_n)\mathcal{L}] \} + \dots \end{aligned} \quad (56)$$

which was found by Balescu and Wallenborn.⁽⁴⁾ Besides, as one can easily check by substitution, Eq. (33) is satisfied by the solution $K^\circ(\tau) = \exp(-\tau\Gamma^\circ)$, if, according to Eq. (32), Γ° obeys the nonlinear equation⁽²¹⁾

$$\Gamma^\circ = \mathcal{L} + \int_0^\infty d\tau \psi(\tau) \exp(-\tau\Gamma^\circ) \quad (57)$$

In our (linear) formulation of the problem one can be sure that the solution for Γ° (if it exists) is uniquely defined with its expansion of von Neumann type (56), which cannot be asserted on the basis of Eq. (57).

4. MACROSCOPIC DESCRIPTION

Let us now consider the extent to which we may count on the fulfillment of the damping conditions (29)–(31) in real many-particle systems. First, all the conditions are automatically satisfied if the condition (31) is fulfilled. This situation corresponds to the supposition about the regularity of the Laplace transforms of all the fragments of the theory at zero, used in the work of the Brussels school, so that condition C seems to play the fundamental role. However, it is just this condition (at least in the strong sense) in which we can be least sure.

Indeed, the contraction of the description has a sense only when the P subspace occupies a negligible volume in the full state space (usually of zero measure). Therefore, the spectrum of the operator $\hat{\mathcal{L}} = Q\mathcal{L}Q$ does not differ essentially from the spectrum of \mathcal{L} and, in particular, it is dense near zero. Due to this, the action of the propagator $\hat{G}(t)$ [(9)] does not lead to forgetting the arbitrary microscopic state $h(0)$. Besides, even for vectors that are not integrals of motion in the Q subspace, the convergence in the condition C may be nonuniform in the phase space [the latter is considered as the domain over which the vectors $F(t)$ are defined], which usually just takes place in the so-called “resonance” zones. It can be supposed that the “dangerous” domains (in the sense of the failure of condition C) of state space and phase space have zero measure; however, this can be justified only if we are interested in actually infinite times. Since for a reasonable physical interpretation of the theory damping on the finite time intervals is needed, these domains have finite measure and cannot be neglected on the basis of any physical considerations, since in the framework of macrotheory the microstate is not controllable.

There are rather less doubts about condition B [(30)], since in that case the propagator $\hat{G}(t)$ acts on the quite definite operator $\mathcal{L}_2 = Q\mathcal{L}P$, which describes the interactions in the system. Therefore, we may hope that the interactions characteristic of real many-particle systems do not prevent $C(\tau)$ from being damped.

Finally, if the set of macroobservables (i.e., the operator P) is chosen correctly, then, apparently, conditions A_1 and A_2 are definitely fulfilled. The thing is that the definitions of $\psi(\tau)$ and $D(\tau)$ include the operator $\mathcal{L}_1 = P\mathcal{L}Q$ which always contains the integration over the phase variables. Due to this, the contribution of the “dangerous” domains is integrally small and quickly decreases with time. In other words, the operator \mathcal{L}_1 realizes the mixing in the system, which in the end provides the elimination of the microinformation.

In connection with the foregoing, we should state one reservation. In many problems the dynamical equation (1) is formulated either in terms of distribution functions or in terms of dynamical observables, and in both cases it is not the state vector $F(t)$ [or $f(t)$] itself that is of interest, but the average values of observables. The latter are calculated by integrating the state vector over phase space either with the “gross observables” (such as energy, particle number, etc.) or with “good” distributions, due to which the same effect is achieved as in the action of the operator \mathcal{L}_1 —the elimination of the irrelevant microscopic information. In this situation the formalism may be treated in the “weak” sense, i.e., we may use all the obtained results, even those that require the fulfillment of conditions B and C, bearing in mind that they become of particular significance only after the calculation of the average values. When such integrations are not imposed by the demands

of the interpretation (for instance, in the theory of stochastic equations), the subdynamic formalism does not work in full measure.

The proper macroscopic description (49) has the strong sense in all cases, since for its basis only conditions A_1 and A_2 are required. However, an important point must be taken into account: As follows from Eqs. (40) and (57), the existence of the operators Γ° and D° is provided only by the exponentially quick damping of the fragments $\psi(t)$ and $D(\tau)$. Otherwise the corresponding time integrals are divergent due to the presence of slow exponential functions, since the operators Γ° and $\Gamma^{\circ*}$ have negative eigenvalues (although concentrated in small circle of radius $\sim \tau_M^{-1}$ around zero). Thus, in order to make the macroscopic description of the dynamical system possible, the latter must have the property of "exponential decay of correlations"⁽²²⁾ or even be a "Y (or C) system" in the sense of Anosov.^(22,23) However, this is not too strong a requirement, since real systems are usually extremely unstable with respect to the initial state (dynamically unstable). It is due to the instability that the existence of the time scale hierarchy is possible.

In the light of the above considerations the situation appears as follows. Having chosen some definite dynamical problem and the set of macroobservables of interest (i.e., the operator P), we settle on the microscopic scale τ_m on which the fragments $D(t)$ and $\psi(t)$ are damped. On the other hand, the operator P defines the macroscopic scale τ_M on which the macroobservables evolve. The scale τ^* on which the averaging of the dynamical picture occurs is fixed by experience. The macrotheory has objective sense only with the conditions $\tau_m \ll \tau^* \ll \tau_M$ and, thus, the macroscopic description is inevitably the asymptotic one with respect to the parameter $\epsilon \sim \tau_m/\tau_M$. The parameter usually enters in the dynamical operator explicitly, $\mathcal{L} = \mathcal{L}^\circ + \epsilon\mathcal{L}'$, which enables one to expand the generator of macroevolution Γ° in powers of ϵ . It is essential that due to the exponential damping of microinformation the macrotheory is *asymptotically exact*. Indeed, as one can readily check, for the simplest law of damping of $\psi(t)$ and $D(t)$, $\exp(-t/\tau_m)$, the error committed in the passage from the exact master equation (28) to the macroscopic equation (49) [i.e., the averaging of Eq. (28) on the scale τ^* due to which the contribution of the right-hand side is neglected] does not exceed $O[\exp(-\tau^*/\tau_m)]$. Choosing $\tau^* \sim \sqrt{\epsilon}\tau_M$, we obtain the exponentially small error $O[\exp(-1/\sqrt{\epsilon})]$, due to which, in particular, all the terms of the expansion of Γ° in ϵ are meaningful.

Let us now turn to the discussion of the initial condition for the macrotheory [see Eq. (50)],

$$f^\circ(0) = A^\circ[f(0) + D^\circ h(0)] \quad (58)$$

which contains, seemingly unexpectedly, the contribution of the initial micro-

information, whereas the direct averaging of Eq. (28) excludes this contribution. This circumstance represents in the most general form the situation known in hydrodynamics as the Hilbert paradox—the term is due to Uhlenbeck.⁽²⁴⁾ The point is that, using the methods of Chapman and Enskog or of Hilbert, we express the normal solution of the Boltzmann equation [$F^\circ(t) = (1 + C^\circ)f^\circ(t)$ in the given formalism] through the macroscopic variables, fully defining its time evolution by the initial values of these variables [$f(0)$]. The suspicion arises at once that the method gives too specific a solution and the correct result should contain the contributions from higher moments [$h(0)$]. More detailed investigation has induced some authors (see, for instance, Refs. 25 and 26) to include in the theory the so-called “initial slip,” i.e., to correct the initial value by taking into account the role of higher moments. Such corrections were calculated approximately up to the Barnett approximation, but we can show that the exact result is given by Eq. (58). For the model problem this was stated by Hauge.⁽²⁷⁾

As a matter of fact, this result is too formal and is not in the spirit of the macroscopic theory. Indeed, formulas (47) and (48) providing for the initial slip are obtained by the smoothing of the current solution without any restrictions on the initial state, so, although correct, they are not adequate to experience. The arbitrariness is removed if we take into account that the initial state (as well as the current state) is controlled only by the macroscopic experiment. In the process of measurement the initial state is smoothed and its only possible choice is defined, according to Eq. (48), by the relationships⁸

$$f(0) = f^\circ(0), \quad D^\circ h(0) = D^\circ h^\circ(0) = D^\circ C^\circ f^\circ(0) \quad (59)$$

Inserting these in Eq. (58) and using the identity (A.4), we have

$$f^\circ(0) = A^\circ(1 + D^\circ C^\circ)f^\circ(0) = f^\circ(0) \quad (60)$$

Thus, the Hilbert “paradox” is the result of incomplete physical consideration. The asymptotic solution $F^\circ(t)$ with the macroscopic initial condition is adequate to the real observation and, what is more important, the proper macroscopic theory (49) is *closed* and *causal*.

It is interesting to note that the solution of the macroscopic problem (49) gives information about the solution of the complete dynamical problem (although in the weak sense). This fact may be used for practical purposes. For instance, it is sometimes difficult in hydrodynamics to state the initial or boundary conditions for the macroscopic characteristics, while the corresponding conditions for the distribution function raise no doubts. In this case, in spite of the usual approach of dealing with the complete problem,

⁸ The combination $D^\circ C^\circ$ in Eq. (59) as well as $\mathcal{L}_1 C^\circ$ in Eq. (63), is well defined even if the operator C° does not exist.⁽¹⁵⁾

we may take advantage of the following simple recipe. If the conditions for the complete state vector (in symbolic form) are

$$W[F] = 0 \quad (61)$$

then the conditions for f° , which is consistent with the given level of description, are defined as follows:

$$W[(1 + C^\circ)f^\circ] = 0 \quad (62)$$

In conclusion, we mention that in cases when the damping condition C [(31)] is not fulfilled, the synchronization condition (48), as well as the subdynamics, has the weak sense. Actually, however, for the basis of the macrotheory it is sufficient to suppose the synchronization of $\mathcal{L}_1 h^\circ(t)$ [not of $h^\circ(t)$] with $f^\circ(t)$. But in such a form the supposition is fulfilled in the strong sense⁽¹⁵⁾:

$$\mathcal{L}_1 h^\circ(t) = \mathcal{L}_1 C^\circ f^\circ(t) = \gamma^\circ f^\circ(t) \quad (63)$$

5. CONCLUSION

The main inference from the above considerations is that in the dynamical foundation of the macroscopic theory we may, using a reasonable physical interpretation, avoid many speculations having no physical (experimental) basis—the suppositions of a probability theory nature, the concepts of ensembles, of coarse-graining in phase space, etc. In fact, if the dynamical system is sufficiently unstable [such as a “ $Y(C)$ system”] and the set of macro-observables is chosen correctly, we naturally come to the *closed, causal, asymptotically exact* macroscopic description without additional suppositions. The only trick we use is the smoothing (in time) of the dynamical picture, which mirrors a real observation with finite time resolution. From this, in particular, it follows that the *irreversibility* of the macrodescription, i.e., the presence of an odd with respect to \mathcal{L} component of the generator of macroevolution, $\Gamma^\circ(\mathcal{L}) \neq \Gamma^\circ(-\mathcal{L})$ is the *consequence of the observation*.

The foundation of this approach is reduced to a check of the sufficiently quick damping of the quantity $\mathcal{L}_1 \hat{G}(t)h$ for an arbitrary vector h in the micro-state space. For the present this assertion is not proved, but recent progress in methods of ergodic theory⁽²³⁾ enables us to hope that such a proof will be obtained in the near future (although the ergodic theory itself bears no relation to the foundation of the macrodescription). Actually, the problem is not too difficult: Although we deal, in essence, with the analysis of the complete dynamical problem, for the foundation of macrotheory it is sufficient to restrict ourselves to not too rough majorant estimations. At present

this damping condition may be verified, at least, by the perturbational method. By this method, in particular, one may check the choice of the projector P , which usually is made based only on physical considerations.

APPENDIX

Here we present simple proofs of the main relationships of the theory. We take into account that the operators $A^\circ = PA^\circ P$, $C^\circ = QC^\circ P$, $D^\circ = PD^\circ Q$, etc., have definite P and Q components and omit the operators P and Q in all cases where no misunderstanding can arise. For simplicity we consider all the damping conditions (29)–(31) to be fulfilled.

Taking advantage of the semigroup property of the fundamental solution

$$U(t_1)U(t_2) = U(t_1 + t_2) \quad (\text{A.1})$$

performing the limit $t_1, t_2 \rightarrow \infty$, and taking into account the definition

$$\Gamma^{\circ*} = A^{\circ-1}\Gamma^\circ A^\circ \quad (\text{A.2})$$

and the results of Section 3, we can calculate the PP component of Eq. (A.1):

$$\begin{aligned} [\exp(t_1\Gamma^\circ)]A^\circ A^\circ [\exp(t_2\Gamma^{\circ*})] + [\exp(t_1\Gamma^\circ)]A^\circ D^\circ C^\circ A^\circ \exp(t_2\Gamma^{\circ*}) \\ = [\exp(t_1\Gamma^\circ)]A^\circ \exp(t_2\Gamma^{\circ*}) \end{aligned} \quad (\text{A.3})$$

After the cancellation of common factors we obtain the identity^(17,18)

$$A^\circ(1 + D^\circ C^\circ)A^\circ = A^\circ, \quad A^\circ(1 + D^\circ C^\circ) = P \quad (\text{A.4})$$

We define

$$\Gamma^\circ = \tilde{\mathcal{L}} + \mathcal{L}_1 C^\circ, \quad \Gamma^{\circ*} = \tilde{\mathcal{L}} + D^\circ \mathcal{L}_2 \quad (\text{A.5})$$

[the first equality is the consequence of Eqs. (43) and (57); the second is the result of its “star-transformation”⁽³⁾] and calculate by partial integration the quantity

$$C^\circ \Gamma^\circ = \int_0^\infty d\tau [\exp(\tau \tilde{\mathcal{L}})] \mathcal{L}_2 [\exp(-\tau \Gamma^\circ)] \Gamma^\circ = \mathcal{L}_2 + \mathcal{L} C^\circ \quad (\text{A.6})$$

With the help of Eqs. (A.5) and (A.6) we have

$$\mathcal{L}(1 + C^\circ)P = \tilde{\mathcal{L}} + \mathcal{L}_2 + \mathcal{L}_1 C^\circ + \mathcal{L} C^\circ = (1 + C^\circ)\Gamma^\circ \quad (\text{A.7})$$

In addition, substituting Γ° of Eq. (A.5) in Eq. (A.6), we obtain the equation for C° :

$$\mathcal{L} C^\circ - C^\circ \tilde{\mathcal{L}} = -\mathcal{L}_2 + C^\circ \mathcal{L}_1 C^\circ \quad (\text{A.8})$$

Analogously (or using the “star-transformation”) we have for D°

$$\Gamma^{\circ*}D^\circ = \mathcal{L}_1 + D^\circ\mathcal{L} \quad (\text{A.9})$$

$$P(1 + D^\circ)\mathcal{L} = \Gamma^{\circ*}(1 + D^\circ) \quad (\text{A.10})$$

$$\tilde{\mathcal{L}}D^\circ - D^\circ\mathcal{L} = \mathcal{L}_1 - D^\circ\mathcal{L}_2D^\circ \quad (\text{A.11})$$

Now we can check the agreement of definitions (A.5) with Eq. (A.2), rewriting the latter in the form

$$\Gamma^{\circ*}(1 + D^\circ C^\circ) = (1 + D^\circ C^\circ)\Gamma^\circ \quad (\text{A.12})$$

Substituting in this equation $C^\circ\Gamma^\circ$ [(A.6)], $\Gamma^{\circ*}D^\circ$ [(A.9)], and (A.5), we find that it is an identity.

Finally, let us prove that the operator Π [(51)] commutes with $U(t)$. Taking into account Eqs. (A.2), (A.7), and (A.10), we have⁽¹⁹⁾

$$\begin{aligned} U(t)\Pi &= [\exp(t\mathcal{L})](1 + C^\circ)A^\circ(1 + D^\circ) \\ &= (1 + C^\circ)[\exp(t\Gamma^\circ)]A^\circ(1 + D^\circ) \\ &= (1 + C^\circ)A[\exp(t\Gamma^{\circ*})](1 + D^\circ) \\ &= (1 + C^\circ)A^\circ(1 + D^\circ)\exp(t\mathcal{L}) = \Pi U(t) = U^\circ(t) \quad (\text{A.13}) \end{aligned}$$

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