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Coarse-graining in Liouville Space and Master Equation

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Résumé: On propose une définition précise de l'espace de LIOUVILLE dans lequel on peut plonger les états microscopiques d'un système quantique irréductible. Dans cet espace, l'opération de «coarse-graining» peut être décrite par un projecteur. On présente alors une déduction non perturbative des équations maîtresses généralisées. Ces équations décrivent l'évolution des termes intervenant dans une description macroscopique classique du système considéré.

1. Introduction

It seems natural to present statistical mechanics in the following terms: a physical system Σ is investigated by means of a collection of measurements; the quantities accessible to these effective measurements form a set $\tilde{M}$, the elements of which we will call *macroscopic observables*. If one describes Σ with $\tilde{M}$ only, it may happen that the evolution of the system presents some peculiar facts (for instance, irreversibility) which are contradictory with the laws of mechanics. A phenomenological study of these facts leads to thermodynamics. The aim of statistical mechanics is to restore the wonderful unity of mechanics by considering $\tilde{M}$ as being only a part (which is in general very small) of the whole set of all the measurements which could, *in principle*, be performed on the system Σ. We shall denote this new set by M and call its elements *microscopic observables*. One then supposes that the evolution of Σ, when described by means of M, is governed by the usual (classical or quantum) mechanical laws. For instance, if we consider a gas Σ, $\tilde{M}$ could be the measurements of p, V, T and of all the quantities related to them; M is much larger and comprises in particular the positions of the individual particles of the gas; there is no essential reason to forbid the measurement of such quantities; practical reasons however make these measurements so difficult to realise that one is well founded, in general, to exclude them from $\tilde{M}$. The difficult problem[1]) of how to determine in a natural way $\tilde{M}$ from an a priori given M will not be touched in this note.

Every macroscopic observable $\tilde{A}$ of $\tilde{M}$ is characterised by the discrete set of all its possible values $A(\Delta)$. Let $p(\Delta)$ denotes the *probability* that the value $A(\Delta)$ would be realised if the measurement of $\tilde{A}$ would be performed. The set of all the $p(\Delta)$ for all the $\tilde{A}$ of $\tilde{M}$ characterises than completely the macroscopic state of the system. The first problem is now to embed this macroscopic situation in a microscopic description.

At this point, let us introduce some restrictions on $\tilde{M}$ and on M in order to be able to give for the theory a mathematical frame which is precise, simple, sufficiently realistic and efficient. We will suppose that:

(i) the macroscopic observables form a *classical* set. By this assertion we mean that we will restrict our considerations to situations $(\Sigma, \tilde{M})$ for which the dispersion obtained when a macromeasurement is carried out is not affected by the simultaneous measurement of any other macroscopic observable. In other words, we will suppose that the operational measuring process for macroobservables is the one we are familiar with in classical physics.

(ii) the microscopic 'observables' form a *quantum* system; for simplicity, we shall further assume that M does not exhibit superselection rules.

We do not claim to have here the most general situation that one could imagine. We even do not claim that any more involved situation will never appear in practical problems. We however think that these assumptions are not too crude for the usual experimental needs; in fact, they correspond to the usual frame of quantum statistical mechanics. We hope then that they are quite sufficient to allow a clarification of the way how irreversibility enters in physics.

Let then $\mathfrak{H}$ be the Hilbert space attached to the *microscopic description*, M being the set of all (essentially) self-adjoint operators on $\mathfrak{H}$. We have supposed that $\tilde{M}$ is contained in M, that all the $\tilde{A}$ commute among themselves and have only discrete spectra; thus, $\tilde{M}$ induces in $\mathfrak{H}$ a partition in mutually orthogonal subspaces, such that every macroscopic observable can be written as:

$$\tilde{A} = \sum_{\Delta} A(\Delta)\, E_{\Delta} . \tag{1.1}$$

(We will denote by the same symbol E_{Δ} the subspaces and the corresponding projectors.)

Each (microscopic) state of Σ can be represented by a bounded self-adjoint positive operator W of unit trace; following the usual terminology, we shall call such operators: *density operators*; the expectation value of any observable A is then given, for the state W, by:

$$\langle A \rangle_W = \mathrm{Tr}\, W A \; ; \tag{1.2}$$

in particular, for macroscopic observables, one has:

$$\langle \tilde{A} \rangle_W = \sum_{\Delta} p(\Delta)\, A(\Delta) \; , \tag{1.3}$$

where:

$$p(\Delta) = \mathrm{Tr}\, W E_{\Delta} . \tag{1.3'}$$

The $p(\Delta)$'s define the 'macroscopic state' or better the 'macroscopic content' of the considered microscopic state.

If two (microscopic) states W and W' satisfy the condition:

$$\mathrm{Tr}\, W E_{\Delta} = \mathrm{Tr}\, W' E_{\Delta} \tag{1.4}$$

for every E_{Δ}, they lead to the same expectation value for every macroscopic observable; the converse is also true. We shall then call such states *macroscopically equivalent*; this is an equivalence relation and each *equivalence class* is characterised by the set of

the corresponding $p(\Delta)$'s. Let us now introduce the *supplementary condition* that all the E_Δ are finite-dimensional. We agree that this assumption seems at first sight to be of rather technical nature. However the reader will convince himself that it is very difficult to find an objection against it on the basis only of physical phenomenological arguments without inferring to a non-operational idealization. We emphasize that we do not fix any upper bound to the dimension of these subspaces. We can now associate with each E_Δ a density operator W_Δ, defined as:

$$W_\Delta = \frac{E_\Delta}{\mathrm{Tr}\, E_\Delta} \tag{1.5}$$

which describes an *uniform probability distribution* inside the subspace E_Δ. Each class of macroscopically equivalent states contains a density operator $\tilde{W}$ (representative of that class) of the form:

$$\tilde{W} = \sum_\Delta p(\Delta)\, W_\Delta\,; \tag{1.6}$$

we shall call *macroscopic states* these particular density operators $\tilde{W}$. Conversely, with any microscopic observable A, one may introduce an unique macroscopic observable $\tilde{A}$ defined as:

$$\tilde{A} = \sum_\Delta A(\Delta)\, E_\Delta\,, \tag{1.7}$$

where:

$$A(\Delta) = \mathrm{Tr}\, A\, W_\Delta\,. \tag{1.7'}$$

Again, two microscopic observables which lead to the *same* $A(\Delta)$ for every W_Δ are *macroscopically equivalent* in that sense that they lead to the same expectation values for every macroscopic state. In order to follow the familiar terminology we shall refer to the operation which transforms a microscopic observable A into its macroscopic equivalent $\tilde{A}$ as the *coarse-graining operation*. One remarks that this operation, applied on states, gives exactly the transition from a microscopic state W to the corresponding macroscopic state $\tilde{W}$.

We will now examine the problem of the evolution. Let us introduce explicitely the assumption announced in the beginning, i.e. that the time evolution of Σ is governed by a one-parameter symmetry[2]) group of the *microscopic* description. From WIGNER's theorem one has:

either $$A \to A^t = U^{-t}\, A\, U^t \tag{1.8 H}$$

or $$W \to W^t = U^t\, W\, U^{-t}\,, \tag{1.8 S}$$

respectively in HEISENBERG and in SCHRÖDINGER picture. This assumption has an immediate consequence which we would like to mention here. Let us first remark that the number $\mathrm{Tr}\, W^2$ can serve to measure the 'degree of mixture' of the state W. We want to relate this quantity with the negentropy (or information) contained in the state W. STUECKELBERG and collaborators[3]) already emphasized that the definition of this concept is by far not unique. Among all the possibilities, we propose the following special choice:

$$S = -k \ln \mathrm{Tr}\, W^2 \quad (\text{with } k > 0)\,. \tag{1.9}$$

This expression is a positive, continuous, monotonic decreasing function of Tr W^2; it reaches its minimum (zero) when W is a pure state (i.e. when $W^2 = W$). Moreover S, as defined by (1.9), is an extensive quantity. Nothing seems then to prevent us to call $(-S)$ the *microscopic negentropy* (or *information*) on Σ contained in the state W. Professor STUECKELBERG drew the author's attention to the fact that if all the above properties, *but* the extensivity of S, were required, then among all the possible definitions, the following choice could be very convenient:

$$S' = \mathrm{Tr}\,(W - W^2) = 1 - \mathrm{Tr}\,W^2\,. \tag{1.9'}$$

In particular, all the statements on the entropy made in this paper would remain true with the modified definition (1.9'), including those on the macroscopic entropy to be introduced below.

The assumption that the time evolution of W^t is governed by (1.8 S) leads directly to the conservation of the microscopic entropy S. This result can be regarded as the quantum analog of the classical Liouville theorem. In this context, it is important to remark that Tr W^2 (and thus S itself) is *not* a constant within an equivalence class of states. For any given equivalence class, the maximal value of S is precisely obtained with the macroscopic state $\tilde{W}$, characteristic of the class considered. (A quite simple proof of this statement will be given at the end of section 2.) We propose thus the introduction of a new quantity:

$$\tilde{S} = -k \ln \mathrm{Tr}\,(\tilde{W})^2\,. \tag{1.10}$$

This expression is characteristic of a class of macroscopically equivalent states. Through $\tilde{W}$, $\tilde{S}$ is directly related to the $p(\Delta)$'s (see definition 1.6) which express the whole macroscopic knowledge (see relation 1.3) obtained from any of the microstates W of a same equivalence class. We will thus call $(-\tilde{S})$ the *macroscopic negentropy* (or *macroscopic information*) on Σ when the system is in any of the microstates W that belong to the equivalence class of $\tilde{W}$. We mention that $\tilde{S}$ is a positive, continuous, monotonic decreasing function of Tr $(\tilde{W})^2$. There is however a profound difference between S and $\tilde{S}$: for S, one can infer from (1.8 S) that S is a constant of the evolution; this conclusion is no more true in general for $\tilde{S}$. The reason is that the equation which governs the time evolution of:

$$(W^t)^{\sim} \equiv \sum_{\Delta} p^t(\Delta)\, W_\Delta\,, \tag{1.11}$$

where:

$$p^t(\Delta) = \mathrm{Tr}\,W^t\,E_\Delta \tag{1.12}$$

is quite different from the relation (1.8 S); this equation shall be derived in section 3. It is perhaps worthwhile to indicate at this point that the typical form of the coarse-graining operation (as emphasized in section 2) allows an immediate proof of the following statement: if W^0 is a macrostate at time $t = 0$, then for any time $t \neq 0$ (i.e. either $t > 0$ or $t < 0$) one has:

$$\tilde{S}(t) \geqslant \tilde{S}(0)\,. \tag{1.13}$$

This is in complete agreement with the results obtained by STUECKELBERG et al.[3]). Incidentally this does *not* imply without further analysis any kind of *monotonic* increase of $\tilde{S}$ with time. This is due to the very peculiar role of the '*present*'. Later on the fact that W^0 is *assumed* to be a macrostate shall be refered to as the 'fundamental a priori assumption of statistical mechanics' (see below in this section).

Let us now consider the time evolution of the expectation values:

$$\langle A^t \rangle_{W^0} = \langle A \rangle_{W^t} = \mathrm{Tr}\, W^t A \,. \tag{1.14}$$

For macroscopic observables (1.14) reduces to:

$$\langle \tilde{A} \rangle_{W^t} = \sum_{\Delta} A(\Delta)\, p^t(\Delta) \,, \tag{1.15}$$

where $p^t(\Delta)$ is defined by (1.12). The probability of finding the value $A(\Delta)$ if one performs the measurement of the observable $\tilde{A}$ at time t is precisely $p^t(\Delta)$. These expressions contain therefore all the knowledge needed in order to be able to make experimentally verifiable predictions. Up to now we did not submit W^0 to any restriction. This is however too general for physical purpose, since W^0 can only be prepared by means of macroscopic observables. The most general state resulting from a maximal macroscopic preparation is of the form:

$$W^0 = \sum_{\Delta} E_\Delta\, \overline{W}^0\, E_\Delta \,, \tag{1.16}$$

where $\overline{W}^0$ is the density operator corresponding to the state of the system before the macroscopic preparation. We note that W^0 and $\overline{W}^0$ are macroscopically equivalent and that in general neither W^0 nor $\overline{W}^0$ are macrostates; this fact is well known in the theory of the measuring process (for a modern presentation of the orthodox point of view, see for instance ref. 4). The observer, who has at his disposal the macromeasurements only, can not descriminate two microscopic states belonging to the same class of macroscopic equivalence; however $p^t(\Delta)$ will depend in general on the choice of the microscopic state W^0 inside its equivalence class (see our Equation (3.13)). One way to get out with this difficulty would be to say that one has to perform a certain average on the results; this is however very imprecise. On the other hand, since one is dealing with a probability problem, one has to be aware of the fact that the problem is not defined as long as one has no 'a priori probabilities'. In our case, this definition amounts to a choice between all the possible initial microscopic states which are compatible with the results of measurements at time $t = 0$. The most natural choice is to take, as initial state, that state which corresponds to the most chaotic microscopic situation compatible with the macroscopic knowledge at time $t = 0$ (i.e. to attribute a uniform probability inside each subspace E_Δ). This special state is precisely the macroscopic state $\tilde{W}^0$ characteristic of the equivalence class of the initial states. We will call this supplementary condition the *fundamental a priori assumption of statistical mechanics*. It is, in fact, a reformulation of the customary 'initial random phase assumption', which is now adapted to our presentation where the coarse-graining is introduced from the beginning as an essential ingredient of the theory. We also can indicate that this later assumption is itself related with BOLTZMANN's hypoth-

esis; however we want to emphasize that we do not make any kind of *repeated* random phase assumption.

With our assumption $p^t(\Delta)$ reduces to:

$$p^t(\Delta) = \sum_{\Delta'} p^0(\Delta')\ P^t(\Delta, \Delta')\ , \tag{1.17}$$

with:

$$P^t(\Delta, \Delta') = \mathrm{Tr}\ W_{\Delta'}\ U^{-t}\ E_\Delta\ U^t\ . \tag{1.18}$$

For the experimental predictions it is then sufficient to know $P^t(\Delta, \Delta')$ for each pair (Δ, Δ'). In a previous publication[5]), we have given an evolution equation for that quantity, in analogy with VAN HOVE's treatment[6]) of the problem, but modified in the light of SWENSON's paper[7]). Our presentation had the advantages to be both coarse-grained and non-perturbative. However a difficulty, already present in VAN HOVE's works, remained in that paper: one did not succeed in deriving an equation for $P^t(\Delta, \Delta')$ itself, but only for an object $P^{E,t}(\Delta, \Delta')$ which is often refered as the 'spectral resolution' of $P^t(\Delta, \Delta')$. In the meantime a very nice paper by ZWANZIG[8]) appeared. One finds there an integro-differential *master equation* for the 'relevant part' of the density operator. The approach is non-perturbative, too. However the quantity investigated in that paper is a fine-grained operator.

The present note has two aims. First a physical aim, i.e. to present a slight generalization of ZWANZIG's paper, including coarse-graining. The second aim is of mathematical nature: by a rigorous treatment of the problem, one can throw off all doubts concerning questions such as: convergence in infinite dimensional space, existence of solutions, etc.; in particular, the use of tetradics notation is avoided by a sharpened definition of the Liouville space in which the Liouville operator acts as an hermitian operator on a Hilbert space. No reference to any (fine-grained) basis in $\mathfrak{H}$ is used.

2. Coarse-graining and Liouville Space

Let $\mathfrak{H}$ be the (finite or infinite) Hilbert space of the microscopic description, and $B(\mathfrak{H})$ the set of all bounded linear applications of $\mathfrak{H}$ to itself. As we already mentioned, every microscopic state can be uniquely represented by a density operator, i.e. a bounded, self-adjoint, positive operator W of unit trace, defined on $\mathfrak{H}$. Conversely to each such operator corresponds a state. Let us then consider the set:

$$C = \{W \mid W \in B(\mathfrak{H})\ ;\quad \mathrm{Tr}\ W = 1\ ,\ \ W^* = W\ ;\quad W > 0\}\ . \tag{2.1}$$

One can easily verify that C is a convex set, the extremal points of which are the pure states, i.e. the density operators satisfying the supplementary condition $W^2 = W$. One can furthermore define a functional Φ on $C \times C$ to the real interval $[0, 1]$:

$$\Phi(W_1, W_2) = \mathrm{Tr}\ W_1\ W_2\ , \tag{2.2}$$

Φ is symmetric and bilinear in the sense of convex sets. Moreover, it is positive definite, i.e. that $\Phi(W, W) = 0$ would imply $W = 0$.

This is a very interesting structure and FANO was, to the author's knowledge, one of the firsts to suggest to use it systematically for a representation of quantum

mechanics (for a recent pedagogical presentation of this point of view, see FANO's lecture notes[9]) and references quoted therein).

Since functional analysis is by far best known in the context of Hilbert spaces or Banach algebrae than in that of convex sets, it is technically very tempting to try to embed C in one of these more complete mathematical structures. This is achieved if one considers the set:

$$\mathfrak{L} = \{A \mid A \in B(\mathfrak{H}) ; \quad \mathrm{Tr}\, A^* A < \infty\} \tag{2.3}$$

equipped with the sesquilinear form:

$$(A_1, A_2) = \mathrm{Tr}\, A_1^* A_2 . \tag{2.4}$$

This form satisfies all the axioms of a scalar product on a complex Hilbert space; in particular it generates a (positive definite) norm:

$$\|A\|_{\mathfrak{L}} = +(\mathrm{Tr}\, A^* A)^{1/2} . \tag{2.5}$$

(This norm has not to be confused with the norm $\|A\|_{\mathfrak{H}}$ of A considered as an operator on $\mathfrak{H}$.) If one adds to this structure the multiplication law inherited from the multiplication of operators in $\mathfrak{H}$, $\mathfrak{L}$ becomes even a Hilbert algebra[10]). This will be used later on. It is this object (i.e. $\mathfrak{L}$ with its complete mathematical structure defined above!) that we will call, for shortness, the *Liouville space* attached to the Hilbert space $\mathfrak{H}$. C is then a convex set in $\mathfrak{L}$; moreover it is complete in $\mathfrak{L}$, i.e. that if A belongs to $\mathfrak{L}$, then $\mathrm{Tr}\, W A = 0$ for all W in C implies $A = 0$.

Let us first remark that the linear application $\mathfrak{V}$ of $\mathfrak{L}$ onto itself, defined for every A in $\mathfrak{L}$, as:

$$\mathfrak{V} A = U A U^{-1} , \tag{2.6}$$

where U is a unitary operator in $\mathfrak{H}$, is also unitary.

The time evolution can then be described by a one parameter group of unitary operators in $\mathfrak{L}$. We will assume that the expectation value of any observable is a continuous function of time. Remembering the definition of the scalar product on $\mathfrak{L}$, one sees that this means mathematically that we assume weak continuity for $\mathfrak{V}^t$ (In fact, since $\mathfrak{V}^t$ is unitary, this is equivalent to strong continuity.) Weak continuity itself is enough for STONE's theorem. $\mathfrak{V}^t$ admits then an infinitesimal generator L. Following the terminology adopted for instance by PRIGOGINE and BALESCU[11]) or by ZWANZIG[8]) we will call this operator the quantum *Liouville operator*. One can write for any W^t in the domain of L:

$$\frac{d}{dt} W^t = -i L W^t . \tag{2.7}$$

Coming back to the description in space $\mathfrak{H}$, one has:

$$\frac{d}{dt} W^t = -i (H W^t - W^t H) , \tag{2.8}$$

which is the usual von Neumann equation.

L and H are very closely related. In particular, if the hamiltonian H is a bounded operator in $\mathfrak{H}$, then the same is true for the Liouville operator L in $\mathfrak{L}$; one has in fact:

$$\|L\|_{\mathfrak{L}} \leqslant 2\|H\|_{\mathfrak{H}} . \tag{2.9}$$

We will further assume, as in our previous paper[5]), that H, and consequently L, are bounded operators. This circumstance will be discussed in the conclusion. This supplementary condition will be technically very useful and it will prove quite sufficient for a mathematically meaningful interpretation of the operations we shall performe in the next section; in particular, $\mathfrak{V}^t$ can now be written:

$$\mathfrak{V}^t = e^{-iLt} = \sum_n \frac{t^n}{n!} (-i\,L)^n \tag{2.10}$$

and $\mathfrak{V}^t$ is not only strongly continuous but even uniformly continuous. Conversely for the uniform continuity of $\mathfrak{V}^t$ (which will be used extensively later on) it is necessary that L is bounded (see for instance Reference 12, corollary to th. 11.4.1).

We want now to point out that the coarse-graining operation takes in $\mathfrak{L}$ a very remarkable form. Let us consider the application $\mathfrak{D}$ of $\mathfrak{L}$ into itself, defined for every A in $\mathfrak{L}$, as:

$$\mathfrak{D}\,A = \sum_{\Delta} (\mathrm{Tr}\,A\,W_{\Delta})\,E_{\Delta} = \sum_{\Delta} (\mathrm{Tr}\,A\,E_{\Delta})\,W_{\Delta} , \tag{2.11}$$

where $\{E_{\Delta}\}$ is a partition of $\mathfrak{H}$ in mutually orthogonal subspaces of finite dimension, and W_{Δ} is defined for each E_{Δ} as $E_{\Delta}/\mathrm{Tr}\,E_{\Delta}$; from the physical point of view (see section 1) we remember that this operation applied on observables or on states reduces to our coarse-graining. Considered now as an operator on $\mathfrak{L}$, $\mathfrak{D}$ is linear, idempotent and self-adjoint. We see then that $\mathfrak{D}$ is a projector in $\mathfrak{L}$. We shall call $\mathfrak{D}$ the *coarse-graining projector*. This property of the coarse-graining will be of central importance for the development of the next section. As a first application of this remarkable property let us consider the following inequality:

$$\|W\|_{\mathfrak{L}}^2 \geqslant \|\mathfrak{D}\,W\|_{\mathfrak{L}}^2 , \tag{2.12}$$

which is obviously valid for any state W, since $\mathfrak{D}$ is a projector. We remember that (because of definition 2.11):

$$\mathfrak{D}\,W \equiv \tilde{W} , \tag{2.13}$$

which is the macroscopic state (see definitions 1.3 and 1.6) characteristic of the equivalence class containing W. Since S (defined by 1.9 or 1.9′) is a monotonic decreasing function of:

$$\mathrm{Tr}\,W^2 = \|W\|_{\mathfrak{L}}^2 , \tag{2.14}$$

the above considerations prove the following assertion, announced in the introduction: 'For any given equivalence class of states, the maximal value of the entropy is precisely obtained with the macroscopic state characteristic of the class under consideration'. The inequality (1.13) has the same source: it is a consequence of the following sequence:

$$\|\mathfrak{D}\,W^t\|^2 \leqslant \|W^t\|^2 = \|\mathfrak{V}^t\,W^0\|^2 = \|W^0\|^2 = \|\mathfrak{D}\,W^0\|^2 . \tag{2.15}$$

3. The Coarse-grained Master Equation

As we pointed out in the introduction (see definition 1.11), the state:

$$(W^t)^{\sim} = \sum_{\Delta} p^t(\Delta)\, W_\Delta = \mathfrak{D}\, W^t\,, \tag{3.1}$$

contains all the useful informations for prediction on the expectation values at time t of the macroscopic observables when the initial state W^0 is given. At this point of the derivation, it is not necessary to impose any restriction to the initial state W^0. We will introduce our assumption $W^0 = \tilde{W}^0 = \mathfrak{D}\, W^0$ only after equation (3.13).

We want an evolution equation for the state $\mathfrak{D}\, W^t$ and the aim of this section is to satisfy this need. We shall obtain a coarse-grained master equation, i.e. an integro-differential equation entirely in terms of $\mathfrak{D}\, W^t$ without any reference to the state W^t itself. Our derivation shall run parallel with that of ZWANZIG[8]); in fact when all the E_Δ are one-dimensional projectors (fine-grained situation) we find ZWANZIG's equation as a particular case. Let us now transpose ZWANZIG's arguments to our case.

Using the notation of section 2, let L be the Liouville operator, $R(z; -i\,L)$ the resolvant of $(-i\,L)$, $\mathfrak{V}^t$ the one-parameter unitary group describing the time evolution of the system in space $\mathfrak{L}$. We already remarked that if the hamiltonian H is assumed to be bounded, L is also bounded and $\mathfrak{V}^t$ is uniformly continuous; one can then write (see th. 11.4.1 of reference 12):

$$R(z; -i\,L) = \int_0^\infty e^{-z\,t}\, \mathfrak{V}^t\, dt \tag{3.2}$$

and the representation is valid at least for $|z| > \|L\|_{\mathfrak{L}}$. $R(z; -i\,L)$ appears then for such values of z as the *Laplace transform* of $\mathfrak{V}^t$. Since z is outside the spectrum of L, one has:

$$(z + i\,L)\, R(z; -i\,L) = I\,, \tag{3.3}$$

or:

$$z\, R(z; -i\,L) - I = -i\,L\, R(z; -i\,L)\,. \tag{3.4}$$

By left multiplication with $\mathfrak{D}$ and $(I - \mathfrak{D})$ one receives respectively:

$$\mathfrak{D}\,(z\, R(z; -i\,L) - I) = -i\,\mathfrak{D}\,L\, R(z; -i\,L)\,, \tag{3.5.1}$$

$$z\,(I - \mathfrak{D})\, R(z; -i\,L) - (I - \mathfrak{D}) = -i\,(I - \mathfrak{D})\,L\, R(z; -i\,L)\,. \tag{3.6.1}$$

Let us introduce the trivial equation $I = (I - \mathfrak{D}) + \mathfrak{D}$ and the fact that $\mathfrak{D}\,L\,\mathfrak{D} = 0$ (due to the relation between L and H):

$$\mathfrak{D}\,(z\, R(z; -i\,L) - I) = -i\,\mathfrak{D}\,L\,(I - \mathfrak{D})\, R(z; -i\,L)\,, \tag{3.5.2}$$

$$\left.\begin{aligned}(z + i\,(I - \mathfrak{D})\,L\,(I - \mathfrak{D}))\,(I - \mathfrak{D})\, R(z; -i\,L) \\ = (I - \mathfrak{D}) - i\,L\,\mathfrak{D}\, R(z; -i\,L)\,.\end{aligned}\right\} \tag{3.6.2}$$

The left-hand side of equation (3.5.2) is the Laplace transform of the time derivative of $\mathfrak{D}\,\mathfrak{V}^t$, the operator of interest. In order to write the right-hand side of this equation

in a more convenient form, we shall extract $(I - \mathfrak{D})\ R(z; -i\,L)$ from equation (3.6.2) and use this in equation (3.5.2). Let us first write:

$$L^{(I-\mathfrak{D})} \equiv (I - \mathfrak{D})\ L\ (I - \mathfrak{D})\ , \tag{3.7}$$

we have:

$$\| L^{(I-\mathfrak{D})} \|_{\mathfrak{L}} \leqslant \| L \|_{\mathfrak{L}} < |z|\ . \tag{3.8}$$

This relation insures the existence of:

$$(z + i\ (I - \mathfrak{D})\ L\ (I - \mathfrak{D}))^{-1} = R(z; -i\ L^{(I-\mathfrak{D})})\ . \tag{3.9}$$

We shall use later that the representation of this operator as the Laplace transform of the unitary uniformly continuous one-parameter group (see reference 12, theorem 11.4.1 and its corollary):

$$\mathfrak{V}^t_{(I-\mathfrak{D})} \equiv e^{-i(I-\mathfrak{D})L(I-\mathfrak{D})t} \tag{3.10}$$

is valid because of condition (3.8).

Putting then together equations (3.5.2) and (3.6.2), one receives:

$$\left.\begin{aligned} \mathfrak{D}\ (z\ R(z; -i\ L) - I) = -i\ \mathfrak{D}\ L\ R(z; -i\ L^{(I-\mathfrak{D})})\ (I - \mathfrak{D}) \\ - \mathfrak{D}\ L\ R(z; -i\ L^{(I-\mathfrak{D})})\ L\ \mathfrak{D}\ R(z; -i\ L)\ . \end{aligned}\right\} \tag{3.11}$$

Taking the inverse Laplace transform of the two sides of the equation (3.11), one obtains:

$$\frac{d}{dt}\ \mathfrak{D}\mathfrak{V}^t = -i\ \mathfrak{D}\ L\ \mathfrak{V}^t_{(I-\mathfrak{D})}\ (I - \mathfrak{D}) - \int_0^t dt'\ \mathfrak{D}\ L\ \mathfrak{V}^{t'}_{(I-\mathfrak{D})}\ L\ \mathfrak{D}\ \mathfrak{V}^{t-t'}\ , \tag{3.12}$$

the last term of this expression looks like the ordinary convolution product in the Laplace transformation theory for complex-valued functions. The mathematical justification of the extension of this formula to our case can be found as a consequence of lemma (13.3.6) of reference 12. Applying the operator equation (3.12) to *any* state W^0, one finds:

$$\frac{d}{dt}\ (\mathfrak{D}\ W^t) = -i\ \mathfrak{D}\ L\ \mathfrak{V}^t_{(I-\mathfrak{D})}\ (I - \mathfrak{D})\ W^0 - \int_0^t dt'\ \mathfrak{D}\ L\ \mathfrak{V}^{t'}_{(I-\mathfrak{D})}\ L\ (\mathfrak{D}\ W^{(t-t')})\ . \tag{3.13}$$

The first term of the right-hand side of equation (3.13) vanishes if one requires the initial state W^0 to satisfy our fundamental a priori assumption (see section 1), i.e. if W^0 is a macrostate:

$$\mathfrak{D}\ W^0 = W^0 \quad \text{implies} \quad (I - \mathfrak{D})\ W^0 = 0\ . \tag{3.14}$$

With this supplementary condition (of physical nature), one is then left with an integro-differential evolution equation involving $(\mathfrak{D}\ W^t)$ only, and where any reference to W^t itself is avoided. This was precisely the aim of this section. We find ZWANZIG's result [8]) as a particular case if we impose to every E_Δ to be one-dimensional. Our coarse-graining operator $\mathfrak{D}$ reduces then to ZWANZIG's D and our equation (3.13) overlaps ZWANZIG's equation (30). We find then the fine-grained equation as a particular case of our coarse-grained equation.

One can even pursue a little further and show how our equation (3.13) generates an equation which can be considered as the non-perturbative coarse-grained generalization of PAULI's master equation. Let us consider:

$$p^t(\Delta) = \mathrm{Tr}\, E_\Delta\, W^t = (E_\Delta, \tilde{W}^t)\ . \tag{3.15}$$

From equation (3.13), one derives immediately:

$$\frac{d}{dt}\, p^t(\Delta) = -\int_0^t dt' \sum_{\Delta'} (E_\Delta, K(t')\, W_{\Delta'})\, p^{t-t'}(\Delta')\ , \tag{3.16}$$

where:

$$K(t') = L\, \mathfrak{W}^{t'}_{(I-\mathfrak{D})}\, L\ . \tag{3.17}$$

From the fact that L is an hermitian operator in $\mathfrak{L}$, related to H as indicated in section 2, it follows that:

$$\sum_{\Delta} (E_\Delta, K(t)\, E_{\Delta'}) = 0 = \sum_{\Delta'} (E_\Delta, K(t)\, E_{\Delta'})\ . \tag{3.18}$$

We have then derived here the coarse-grained analog of ZWANZIG's equation (42). It is also interesting to compare this result with the 'double normalization' used by STUECKELBERG et al.[3]) as an essential ingredient of their proof.

Let us now consider the integrand of equation (3.16) and let us denote by N_Δ the dimension of the projector E_Δ:

$$\sum_{\Delta'} (E_\Delta, K(t')\, E_{\Delta'})\, \frac{1}{N_{\Delta'}}\, p^{t-t'}(\Delta')$$

$$= \left[\sum_{\Delta' \neq \Delta} (E_\Delta, K(t')\, E_{\Delta'})\, \frac{1}{N_{\Delta'}}\, p^{t-t'}(\Delta')\right] + (E_\Delta, K(t')\, E_\Delta)\, \frac{1}{N_\Delta}\, p^{t-t'}(\Delta)\ . \tag{3.19}$$

Using there the second of equations (3.18), one can write:

$$(E_\Delta, K(t')\, E_\Delta) = -\sum_{\Delta' \neq \Delta} (E_\Delta, K(t')\, E_{\Delta'})\ . \tag{3.20}$$

Inserting this in equation (3.16), one obtains the desired equation:

$$\frac{d}{dt}\, p^t(\Delta) = -\int_0^t dt' \sum_{\Delta' \neq \Delta} (E_\Delta, K(t')\, E_{\Delta'}) \left[\frac{1}{N_{\Delta'}}\, p^{t-t'}(\Delta') - \frac{1}{N_\Delta}\, p^{t-t'}(\Delta)\right], \tag{3.21}$$

which again generalizes to the coarse-grained situation, the fine-grained equation obtained by ZWANZIG (see his equation (46)). The kernel $K(t)$ is defined by the relation (3.17), i.e. explicitely:

$$K(t) = L\, e^{-i(I-\mathfrak{D})L(I-\mathfrak{D})t}\, L\ . \tag{3.22}$$

Similar ideas have already been exploited by G. LUDWIG[16]). Our proof was given explicitely in order to emphasize the mathematical cares which are to be taken. The Laplace-transforms which were carried out are made rigourous (and not only formal) by the explicit assumption that L is a bounded operator in $\mathfrak{L}$. We want also to mention that LUDWIG's final equation is the Laplace-transform of an alternative form of our

equation (3.11). However this step would be only formal as long as the existence of the inverse of

$$[z + \mathfrak{D}\, L\, R(z; -i\, L^{(I-\mathfrak{D})})\, L\, \mathfrak{D}]$$

is not proved. Finally his results can be slightly simplified if one uses – as we did – the fact that $\mathfrak{D}\, L\, \mathfrak{D} = 0$.

4. Conclusions

Generalized *coarse-grained* master equations were derived with a mathematical method inspired from that of ZWANZIG[8]). These equations (equations (3.13) or (3.21)) describe the time evolution of the quantities which are of interest for a macro-observer. This approach is *non-perturbative* and the resulting equations can thus be regarded as exact.

The assumptions under which this derivation was possible are presented in sections 1 and 2. They are essentially:

a) The macroscopic observables form a classical system, whereas the microscopic description obeys the laws of ordinary quantum mechanics.

b) The macrocells E_Δ, which are the common maximal eigen subspaces of the macroscopic observables, are finite-dimensional; however the Hilbert space of the microscopic description is allowed to be infinite-dimensional. The reasons for this choice are explained in section 1.

c) The initial states satisfy an a priori probability assumption which is a generalization of the 'initial random phase assumption'. It could be remarked that equation (3.13) is also valid without this assumption. *No* kind of 'repeated random phase assumption' was needed at any place of our derivation, even for equation (3.21).

d) The hamiltonian of the system is bounded. We admit that this restriction was imposed mainly for technical reasons; strictly speaking our derivation is no more correct when this assumption is not satisfied. Were this assumption really not tenable for a given microscopic description, we have however still two possibilities at least to avoid a radical change of the method; one can either impose some further restriction on the admissible states or, in a more orthodox way, we can use the well-known formalism of the energy shells. Let us recall the main features of this formalism in connection with our problem. Let:

$$H = \int_0^\infty \lambda\, dE_\lambda \tag{4.1}$$

be the spectral resolution of the hamiltonian. Let us now consider a partition $\{I_a\}$ of the spectrum $S\,p(H)$ in finite intervals. For each of these intervals, let us construct the projector (possibly infinite-dimensional):

$$E_a \equiv \int_{I_a} dE_\lambda \tag{4.2}$$

to which we will refer as the *energy shell* corresponding to the interval I_a. Since the time-evolution operator leaves every energy shell invariant, we can split the evolution problem and treat each energy shell separately. Our assumption (d) is always satisfied in each shell and we can simply repeat our derivation for each shell separately. The

last point we want to mention in connection with this splitting of the problem is that we have to be careful to define the macroscopic observables in such a way that the macrocells become subspaces of the energy shells.

As a general remark, we want once more to emphasize that our derivation was made mathematically possible by an appropriate sharpened definition of the Liouville space as an Hilbert algebra in which the states form a convex complete set.

In his recent paper[8]), ZWANZIG was able to show the equivalence of his equation with all known master equations[13])[14])[15]) except that of VAN HOVE. We can then infer that the present method is a non-perturbative approach to the coarse-grained analog of all these equations. In an earlier paper, we did the same kind of approach for VAN HOVE's equation; we can then consider the problem of the non-perturbative deduction of generalized coarse-grained master equations as completely solved.

Finally, for such questions as: the definition of the interaction as the difference between the (microscopic) hamiltonian H and the coarse-grained operator describing the (macroscopic) energy $\tilde{H}$, the role of VAN HOVE's diagonal condition, etc., we refer to our previous paper[5]); its conclusions are easily transposed to the present derivation and remain valid.

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