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On the Markov Character of Master Equations*)

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Abstract. The Markov assumption for the derivation of Master equations is discussed in the case of quantum statistical mechanics. The respective roles of coarse-graining and time-smoothing are analysed. It is emphasized that non-trivial Markov master equations, valid for all times, cannot be obtained unless time-smoothing is also introduced.

1. Introduction

In two previous papers[1)2)] we presented a systematic frame for the problem of the evolution equations of non-equilibrium statistical mechanics, and we proposed a mathematically rigorous derivation of these equations. In order to make the present note self-contained, let us first recall briefly the main line of our approach.

We consider a physical system Σ which is supposed to have a *microscopic quantum mechanical* description by means of a (complex) Hilbert space $\mathfrak{H}$. The evolution of Σ is therefore given by a one-parameter group $\{U^t\}$ of unitary operators whose generator H is refered to as the *microscopic hamiltonian*; H is supposed to be bounded, but no further restriction is imposed to its spectrum.

On the other hand we suppose that the *macroscopic observables* $\tilde{A}$ form a compatible set (i.e. they commute among themselves when represented as operators acting on $\mathfrak{H}$), and that they have discrete spectrum. Alltogether they therefore generate a partition $\{E_\Delta\}$ of $\mathfrak{H}$ into mutually orthogonal subspaces (which we refer to as *macrocells*), so that each of the macro-observable can be written as:

$$\tilde{A} = \sum_{\Delta} A(\Delta)\, E_\Delta \tag{I.1}$$

We further suppose that the E_Δ are of finite dimension (N_Δ).

For a justification of the above postulates the reader is refered for instance to reference [2)].

At time t the expectation value of any macroscopic observable $\tilde{A}$, taken for any (pure or mixture) state W^t is:

$$\langle \tilde{A} \rangle_W t = \sum_{\Delta} p^t(\Delta)\, A(\Delta)\,, \tag{I.2}$$

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where

$$p^t(\Delta) = \mathrm{Tr}\, W^t\, E_\Delta \tag{I.3}$$

The $p^t(\Delta)$ give nothing more or less than the *macroscopic information* contained in the state W^t. In order to make macroscopic (i.e. experimental) predictions it is therefore necessary and sufficient to know the evolution equations for the $p^t(\Delta)$'s and the initial conditions (i.e. the $p^0(\Delta)$'s), *provided* a kind of generalized *initial* random phase assumption is made; more precisely, instead of allowing any W to be an initial state, we only consider as possible initial states those which correspond to a uniform distribution inside each macrocell; this assumption means that we average over all the initial states compatible with the initial observed situation, giving to each of the corresponding pure state an equal a priori probability. Our initial states will therefore be of the form:

$$W^0 = \sum_\Delta p^0(\Delta)\, W_\Delta\,, \tag{I.4}$$

where

$$W_\Delta = \frac{E_\Delta}{N_\Delta}\,, \tag{I.5}$$

We will refer to this assumption as the *fundamental a priori assumption of statistical mechanics*. With this assumption the $p^t(\Delta)$ can be rewritten as:

$$p^t(\Delta) = \sum_{\Delta'} p^0(\Delta')\, P^t(\Delta, \Delta')\,, \tag{I.6}$$

where

$$P^t(\Delta, \Delta') = \mathrm{Tr}\, U^t\, W_{\Delta'}\, U^{-t}\, E_\Delta\,. \tag{I.7}$$

Several equations have been proposed as the evolution equations either for the occupation probabilities p^t or for the transition probabilities P^t. The first of them are the well-known PAULI's master equations[3]) which can be written as:

$$\frac{d}{dt}\, p^t(\Delta) = -\sum_{\Delta'} A(\Delta, \Delta')\, N_{\Delta'}\, p^t(\Delta) + \sum_{\Delta'} A(\Delta', \Delta)\, N_\Delta\, p^t(\Delta')\,, \tag{I.8}$$

where the $A(\Delta, \Delta')$ are symmetrical in (Δ, Δ') and proportional to:

$$\mathrm{Tr}\, W_\Delta\, V\, W_{\Delta'}\, V\,,$$

i.e. to the average of:

$$|\, <\alpha \mid V \mid \alpha'> \,|^2\,,$$

with α (respectively α') running over a complete orthonormal set of vectors in E_Δ (respectively $E_{\Delta'}$). V is the *interaction* which is supposed to be responsible for the approach to equilibrium. These equations are the result of a first order time-dependent perturbation calculus and rest upon an extra hypothesis, usually refered to as the *repeated* random phase assumption, which can be interpreted as the quantal analog of Boltzmann's Stosszahlansatz. As in the classical case however, this assumption is very hard (and even impossible in the general case) to justify from a physical point of view. It is the main merit of VAN HOVE's work[4]) to have removed this assumption; more-

over VAN HOVE gave a method to carry out the calculations to general order in V provided that this perturbation satisfies specific properties. He then derived an equation for a quantity $P^{E,t}$ related to P^t by:

$$P^t = \int_{-\infty}^{+\infty} P^{E,t}\, dE \tag{I.9}$$

and which can be interpreted as the "spectral resolution" of P^t with respect to the energy E. Generalizing to a coarse-grained situation a method initially proposed by SWENSON[5]) for a fine-grained situation, the present author[1]) rederived VAN HOVE's equations through a non-perturbative approach, making therefore no use of any property of the interaction. The last step was to obtain the equations for the p^t themselves. This was achieved, again through a non-perturbative approach, by ZWANZIG[6]) for a fine-grained situation, and by the present author[2]) for any coarse-grained situation. The fundamental a priori assumption of statistical mechanics is supposed to be valid, both in [1]) and in [2]); in this later however, the derivation is carried out without appealing to this assumption up to Equations 3.13. The final equations are [2]):

$$\frac{d}{dt}\, p^t(\Delta) = -\int_0^t \sum_{\Delta' \neq \Delta} K^{t'}(\Delta, \Delta') \left[\frac{1}{N_{\Delta'}}\, p^{t-t'}(\Delta') - \frac{1}{N_\Delta}\, p^{t-t'}(\Delta)\right] dt' \tag{I.10}$$

where the kernels

$$K^t(\Delta, \Delta')$$

are related to the hamiltonian in a way which can be more conveniently expressed with the help of the Liouville space $\mathfrak{L}$ associated with the Hilbert space $\mathfrak{H}$; for a definition of this space and its use in the present context see for instance reference [2]) where a derivation of (I.10) was carried out in $\mathfrak{L}$ itself rather than in $\mathfrak{H}$; we will simply recall here that $\mathfrak{L}$ is the complex Hilbert space

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

with the scalar product:

$$(A, B) = \mathrm{Tr}\, A^* B\,.$$

In $\mathfrak{L}$ the kernels $K^t(\Delta, \Delta')$ appear as matrix elements of the form:

$$K^t(\Delta, \Delta') = (E_\Delta, K(t)\, E_{\Delta'})\,, \tag{I.11}$$

where $K(t)$ is the operator:

$$K(t) = L\, e^{-i(I-\mathfrak{D})L(I-\mathfrak{D})t}\, L\,, \tag{I.12}$$

where $\mathfrak{D}$ is the coarse-graining projector[2]) and L is the well-known Liouville operator[2])[7]).

We are now in the position to come to the main concern of this note. Whereas PAULI's master equations are manifestly of Markov type, this is not the case (at least for every time) for any of their generalizations[1])[2])[4])[5])[6])[8]) with the only exception of the equations derived from probabilistic arguments by VAN KAMPEN[9]) and which are very similar in structure with those of PAULI. CHESTER[10]) raised in this connection the

following question, after having remarked that VAN KAMPEN's coarse-graining is much coarser than VAN HOVE's: "... Do we recover Markov master equations if we work with sufficiently coarse-grained functions? If we do so, then how coarse-grained must our variables be? ..." It is this question we intend to discuss in this note; the answer to the first part will turn out to be *no*, unless one makes explicite use of time-smoothing.

II. Markov processes

In this section we will recall the most elementary facts about Markov processes[11]) in order to make the connection with our problem.

Suppose that Σ is a concrete system (i.e. either a physical system or any probabilistic model) with a set $\{\Delta\}$ of possible "states" (to avoid any misunderstanding let us be more specific and say that Δ characterizes the outcome of a single experiment carried on Σ; for instance in the scheme of section I, when we say that the system is in the "state" Δ it means that we have measured, by a single macroscopic experiment, that the system is in cell E_Δ; repeating the same experiment on an ensemble will further fix the $p(\Delta)$'s.) Let us now denote by $z_t = \Delta$ the fact that the state Δ appears as the outcome of an experiment carried on Σ at time t. By definition, the evolution of Σ is a *Markov process* if the conditional probability:

$$P(z_t = \Delta \mid z_{t_1} = \Delta_1; z_{t_2} = \Delta_2; \ldots; z_{t_n} = \Delta_n) , \tag{II.1}$$

with

$$t_1 < t_2 < \ldots < t_n < t ,$$

only depends on the state at time t_n, i.e. is equal to:

$$P(z_t = \Delta \mid z_{t_n} = \Delta_n) . \tag{II.2}$$

We will later use the simpler notation (taking into account the Markov character of the evolution):

$$P(z_t = \Delta \mid z_s = \Delta') = P^{t,s}(\Delta, \Delta') . \tag{II.3}$$

If moreover:

$$P^{t,s}(\Delta, \Delta') = P^{t',s'}(\Delta, \Delta') , \tag{II.4}$$

whenever $t - s = t' - s'$, the evolution is said to be an *homogeneous* Markov process. In our case the transition probabilities are given by:

$$P^{t,s}(\Delta, \Delta') = \mathrm{Tr}\, U^{t-s} W_{\Delta'} U^{-(t-s)} E_\Delta = (\mathfrak{V}^{t-s} W_{\Delta'}, E_\Delta) = P^{t-s}(\Delta, \Delta') . \tag{II.5}$$

The second identity results from the passage to the Liouville space formalism developped in reference [2]). Equations (II.5) show that our processes, if Markovian, are also homogeneous.

As a consequence of the total probability theorem, a Markov process always satisfies the Chapman-Kolmogorov equations:

$$P^{u,s}(\Delta, \Delta') = \sum_{\Delta''} P^{u,t}(\Delta, \Delta'')\, P^{t,s}(\Delta'', \Delta') ,$$

whenever

$$s < t < u \tag{II.6}$$

For an homogeneous Markov process these equations reduce to:

$$P^{t_1+t_2}(\Delta, \Delta') = \sum_{\Delta''} P^{t_1}(\Delta, \Delta'')\, P^{t_2}(\Delta'', \Delta') \tag{II.7}$$

for all positive t_1 and t_2.

III. Coarse-graining and the Markov character of the evolution

Let us now consider a quantum statistical system Σ, described as in section I, and let us suppose that its evolution *is* a Markov process. We want to prove here that this assumption is not compatible with any non-equilibrium situation, how coarse the coarse-graining may be.

As mentionned in section II, the $P^t(\Delta, \Delta')$ have then to satisfy Equations (II.7); these can be written in Liouville space notation:

$$(\mathfrak{V}^{t_1+t_2} W_{\Delta'}, E_\Delta) = \sum_{\Delta''} (\mathfrak{V}^{t_2} W_{\Delta''}, E_\Delta)\, (\mathfrak{V}^{t_1} W_{\Delta'}, E_{\Delta''}). \tag{III.1}$$

Since the $E_\Delta/(N_\Delta)^{1/2}$ form a complete orthonormal set of vectors in the subspace $\mathfrak{D}$ of $\mathfrak{L}$, the Equations (III.1) are equivalent with the operator equations:

$$\mathfrak{D}\, \mathfrak{V}^{t_1+t_2}\, \mathfrak{D} = \mathfrak{D}\, \mathfrak{V}^{t_1}\, \mathfrak{D}\, \mathfrak{V}^{t_2}\, \mathfrak{D}\,. \tag{III.2}$$

Let us now form, making use of (III.2):

$$\frac{(\mathfrak{D}\, \mathfrak{V}^{t_1+t_2}\, \mathfrak{D} - \mathfrak{D}\, \mathfrak{V}^{t_2}\, \mathfrak{D})}{t_1} = \frac{(\mathfrak{D}\, \mathfrak{V}^{t_1}\, \mathfrak{D} - \mathfrak{D})\, \mathfrak{D}\, \mathfrak{V}^{t_2}\, \mathfrak{D}}{t_1} \tag{III.3}$$

In the limit where t_1 goes to zero, Equations (III.3) lead to:

$$-i\, \mathfrak{D}\, L\, \mathfrak{V}^t\, \mathfrak{D} = \frac{d}{dt}\, \mathfrak{D}\, \mathfrak{V}^t\, \mathfrak{D} = -i\, \mathfrak{D}\, L\, \mathfrak{D}\, \mathfrak{V}^t\, \mathfrak{D}\,. \tag{III.4}$$

We recall now the property[2]):

$$\mathfrak{D}\, L\, \mathfrak{D} = 0\,, \tag{III.5}$$

which is a direct consequence of the form of L and $\mathfrak{D}$ when expressed in $\mathfrak{H}$. Equations (III.4) reduce therefore to:

$$\frac{d}{dt}\, \mathfrak{D}\, \mathfrak{V}^t\, \mathfrak{D} = -i\, \mathfrak{D}\, L\, \mathfrak{V}^t\, \mathfrak{D} = 0 \text{ for all } t \tag{III.6}$$

we have then:

$$\mathfrak{D}\, L^n\, \mathfrak{D} = 0 \text{ for all } n \neq 0 \tag{III.7}$$

$$\mathfrak{D}\, \mathfrak{V}^t\, \mathfrak{D} = \mathfrak{D} \text{ for all } t \tag{III.8}$$

and therefore:

$$\frac{d}{dt}\, P^t(\Delta, \Delta') = 0\,, \tag{III.9}$$

$$P^t(\Delta, \Delta') = \delta_{\Delta\Delta'}\,. \tag{III.10}$$

If moreover the fundamental a priori assumption of statistical mechanics is postulated:

$$p^t(\Delta) = p^0(\Delta) \text{ for all } t\,. \tag{III.11}$$

All these results show that the evolution in quantum statistics cannot be a Markov process for all times, unless one restrict the interest to the trivial case of equilibrium situations. It is important to remark that up to here we have only introduced coarse-graining; our $\mathfrak{D}$ is however completely arbitrary; consequently the above conclusion remains valid as long as one uses coarse-graining arguments only, how coarse the coarse-graining may be.

IV. Introduction of time-smoothing

The above section shows that an essential ingredient has to be added to coarse-graining if one wishes to recover VAN KAMPEN's master equations. It is the purpose of the present section to emphasize the importance of time-smoothing in this connection; this concept is introduced in order to take into account the fact that the physical observations are not instantaneous; we moreover remark that, because of the incertainty relations between time and energy, time-smoothing and coarse-graining are not disconnected concepts.

From the physical point of view we are therefore not interested in the $p^t(\Delta)$ themselves, but rather in:

$$\bar{p}^t(\Delta) = \frac{1}{\tau} \int_t^{t+\tau} p^{t'}(\Delta)\, dt' , \tag{IV.1}$$

where τ is the non-vanishing duration of the experiments. Quite analogous with Equations (I.6) the $\bar{p}^t(\Delta)$ can be written as:

$$\bar{p}^t(\Delta) = \sum_{\Delta'} p^0(\Delta')\, \bar{P}^t(\Delta, \Delta') , \tag{IV.2}$$

with

$$\bar{P}^t(\Delta, \Delta') = \int_t^{t+\tau} \frac{P^{t'}(\Delta, \Delta')\, dt'}{\tau} \tag{IV.3}$$

In the Liouville space formalism these quantities can be rewritten as:

$$\bar{P}^t(\Delta, \Delta') = (\mathfrak{M}\, \mathfrak{V}^t\, W_{\Delta'}, E_\Delta) , \tag{IV.4}$$

with

$$\mathfrak{M} = \int_0^\tau \frac{\mathfrak{V}^t dt}{\tau} = \sum \frac{(-i\, L\, \tau)^n}{(n+1)!} . \tag{IV.5}$$

Further on $\mathfrak{M}$ will be refered to as the *time-smoothing operator*.

We will now ask whether it is possible to get a non-trivial result when imposing to the $\bar{p}^t(\Delta, \Delta')$ to satisfy Chapman-Kolmogorov equations of type (II.7), which read now as:

$$(\mathfrak{M}\, \mathfrak{V}^{t_1+t_2}\, W_{\Delta'}, E_\Delta) = \sum_{\Delta''} (\mathfrak{M}\, \mathfrak{V}^{t_2}\, W_{\Delta''}, E_\Delta)\, (\mathfrak{M}\, \mathfrak{V}^{t_1}\, W_{\Delta'}, E_{\Delta''}) . \tag{IV.6}$$

With the same arguments as used in section III one gets the operator equations:

$$\mathfrak{D}\, \mathfrak{M}\, \mathfrak{V}^{t_1+t_2}\, \mathfrak{D} = \mathfrak{D}\, \mathfrak{M}\, \mathfrak{V}^{t_1}\, \mathfrak{D}\, \mathfrak{M}\, \mathfrak{V}^{t_2}\, \mathfrak{D} . \tag{IV.7}$$

Incidentally we remark that these equations show that the $\bar{P}^t$ satisfy a Chapman-Kolmogorov equation if and only if the reduced evolution operators

$$\mathfrak{D}\,\mathfrak{M}\,\mathfrak{V}^t\,\mathfrak{D} \tag{IV.8}$$

form a one-parameter (semi-)group.

Following again section III, we deduce from Equations (IV.7) the differential equations:

$$\frac{d}{dt}\,\mathfrak{D}\,\mathfrak{M}\,\mathfrak{V}^t\,\mathfrak{D} = -i\,\mathfrak{D}\,\mathfrak{M}\,L\,\mathfrak{V}^t\,\mathfrak{D} = -i\,\mathfrak{D}\,\mathfrak{M}\,L\,\mathfrak{D}\,\mathfrak{M}\,\mathfrak{V}^t\,\mathfrak{D}\,, \tag{IV.9}$$

which evidently reduce to Equations (III.4) when $\tau = 0$, i.e. when $\mathfrak{M} = I$; we however have in general:

$$\mathfrak{D}\,\mathfrak{M}\,L\,\mathfrak{D} \neq 0 \tag{IV.10}$$

instead of the identity (III.5). This fact is crucial in insuring a generally non-trivial result in presence of time-smoothing. Expressed in the matrix form, Equations (IV.9) lead then to:

$$\frac{d}{dt}\,\bar{P}^t(\Delta, \Delta') = \sum_{\Delta''} K(\Delta, \Delta'')\,\frac{\bar{P}^t(\Delta'', \Delta')}{N_{\Delta''}} \tag{IV.11}$$

where

$$K(\Delta, \Delta') = i(\mathfrak{M}\,L\,E_{\Delta'}, E_{\Delta})\,. \tag{IV.12}$$

Using furthermore the property:

$$\sum_{\Delta'} K(\Delta, \Delta') = 0 = \sum_{\Delta} K(\Delta, \Delta')\,, \tag{IV.13}$$

which is an immediate consequence of the definition of K by (IV.12), one can write Equations (IV.11) in the form:

$$\frac{d}{dt}\,\bar{P}^t(\Delta, \Delta') = \sum_{\Delta'' \neq \Delta} K(\Delta, \Delta'')\left[\frac{\bar{P}^t(\Delta'', \Delta')}{N_{\Delta''}} - \frac{\bar{P}^t(\Delta, \Delta')}{N_{\Delta}}\right] \tag{IV.14}$$

i.e. with the help of Equations (IV.2):

$$\frac{d}{dt}\,\bar{p}^t(\Delta) = \sum_{\Delta' \neq \Delta} K(\Delta, \Delta')\left[\frac{\bar{p}^t(\Delta')}{N_{\Delta'}} - \frac{\bar{p}^t(\Delta)}{N_{\Delta}}\right], \tag{IV.15}$$

which, together with (IV.12) is the central result of this section.

The master Equations (IV.15) are Markovian by hypothesis and they have been deduced without any further assumption than our fundamental a priori assumption. They therefore constitute an exact result; it may still be interesting to note that the $K(\Delta, \Delta')$ reduce in first approximation (for $\Delta \neq \Delta'$) to:

$$K(\Delta, \Delta') = \mathrm{Tr}\,(V\,E_{\Delta}\,V\,E_{\Delta'})\,\tau\,, \tag{IV.16}$$

where the operator V (acting in $\mathfrak{H}$, and usually refered to as the "interaction responsible for the approach to equilibrium") is defined here as the difference of the total microscopic hamiltonian and the macroscopic energy operator:

$$V = H - \mathfrak{D}\,H = H - H_0\,. \tag{IV.17}$$

This result enforces the analogy of Equations (IV.15) and (I.8), giving to our equations the meaning of the greatest Markovian generalization of the master equations derived by PAULI. We emphasize that Equations (IV.15) have been derived without any use of perturbation methods, and are consequently valid to general order in V.

V. Conclusions

We started from the assumption that certain quantum statistical systems can present an evolution which is a Markov process. We proved that this condition does not contradict the fact that the system evolves in a non-equilibrium situation, *provided* that time-smoothing is used (in addition to coarse-graining) as an essential ingredient of the macroscopic description.

With this assumption we derived a generalization to all order in V of PAULI's master equations; the equations so obtained are therefore of a generality intermediary between the original PAULI's equations and the generalized master equations derived for instance in [2]). We emphasize moreover that the Markov master equations necessarily become trivial when time-smoothing is disregarded.

We know however that the Markov assumption, how pleasant or simple it may be, is also difficult to justify for general physical systems. It would therefore seem quite natural to try first to introduce time-smoothing (at least formally through the operator $\mathfrak{M}$ acting in $\mathfrak{L}$) in general derivations such as that of reference [2]), and then only, to look for their possible relations with Markov processes. We want finally to mention that an interpretation of the time parameter τ in terms of the structure of Σ itself is desirable, since $\mathfrak{M}$ (and therefore τ) will appear through the coefficients of the master equations in the expressions of the physical quantities related to the approach to equilibrium. We think therefore that further considerations on the possible relations between $\mathfrak{D}$, $\mathfrak{V}^t$ and $\mathfrak{M}$ could be of some help for a definitive solution of the master equations problem; we would like to hope that this note would at least have served to show the importance of an investigation along this line.

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