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PROPERTIES OF QUANTUM MARKOVIAN MASTER EQUATIONS*

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ABSTRACT.

In this paper we give an essentially self-contained
account of some general structural properties of the dynamics
of quantum open Markovian systems. We review some recent
results regarding the problem of the classification of quantum
Markovian master equations and the limiting conditions under
which the dynamical evolution of a quantum open system obeys
an exact semigroup law (weak coupling limit and singular
coupling limit). We discuss a general form of quantum detailed
balance and its relation to thermal relaxation and to
microreversibility.

0. INTRODUCTION.

Recently, much work has been devoted to the rigorous study of the conditions under which memory effects can be neglected in the dynamical description of quantum open systems, thus leading to a time evolution obeying an exact semigroup law $\begin{bmatrix} 23,24,70,25-28,45,37,34,35,63 \end{bmatrix}$. This has gone parallely with an extended investigation of the problem of the classification of quantum Markovian master equations $\begin{bmatrix} 33,58,60,28 \end{bmatrix}$.

In this paper we present a short, organic and essentially self-contained review of those results in the field, of which we are aware and which we deem to be most representative. We make no claim to completeness, since the literature on the subject is growing very rapidly, and in writing the paper we have essentially confined ourselves to a discussion of those features of the theory which deal with general structural properties rather than with specific physical applications. For the latter, we refer to the review articles of Haake $\begin{bmatrix} 44 \end{bmatrix}$ and Agarwal $\begin{bmatrix} 5 \end{bmatrix}$.

The unified starting point for the rigorous study of the limiting conditions which lead to a Markovian reduced dynamics is the well known generalized master equation, which gives a formally exact description of the irreversible dynamical evolution of a quantum open system coupled to its surroundings. Therefore, we give in Section 1 a short review of this technique. In Section 2, we recall the property of complete positivity of a reduced dynamics and briefly touch upon the problem of automorphic extensions of families of completely positive maps. In Section 3, we discuss qualitatively the conditions under which a generalized master equation can be approximated by a Markovian master equation (weak coupling or van Hove limit and singular coupling limit) and we review the results obtained

so far concerning the structure of the generators of quantum
dynamical semigroups. In Section 4, we discuss the restrictions
implied by complete positivity on the Markovian dynamics of a
2-level system, this being, to our knowledge, the only case
so far in which such restrictions have been given an explicit
form in terms of observable parameters of the dynamical evol-
ution. In Section 5, we give a short summary of the rigorous
theory of the weak coupling limit, in the form which has
recently been given by Davies. Section 6 is devoted to an
exposition of a simple but fairly general model of singular
coupling. In Section 7, we study a quantum form of detailed
balance for a Markovian master equation, which turns out to
be characteristic of dynamical semigroups describing relax-
ation to thermal equilibrium, thus providing yet another
characterization of KMS states. Finally, we derive in Section
8 the implications of microreversibility (time reversal
invariance) on the generators of quantum dynamical semigroups
and we discuss their relation to analogous conditions which
have recently been proposed in the literature, and to detailed
balance.

The results of Sections 7 and 8 are mostly new, and will
be treated extensively in future publications.

1. GENERALIZED MASTER EQUATION.

The generalized master equation (GME) is a tool for
extracting the dynamics of a subsystem of a larger system,
by the use of projection techniques on Banach spaces [85, 86,
11, 33, 66, 67, 44, 8, 57, 64, 5, 30]. Although this technique is well

known, we shall briefly recall it, mostly in order to introduce
the notations needed in the following.

We are interested in a spatially confined quantum system S, with
underlying Hilbert space $\mathfrak{H}^S$ and algebra of observables $\mathcal{B}(\mathfrak{H}^S)$,
the algebra of bounded operators on $\mathfrak{H}^S$.
The "reservoir" R will be taken as an infinite quantum system,
with algebra of observables $\mathfrak{A}^R$ and Hilbert space $\mathfrak{H}^R_\omega$
determined by the GNS representation π_ω induced by a suitable
reference state ω^R on $\mathfrak{A}^R$, which we will assume to be stationary
under the free evolution of R. We assume π_ω to be faithful and
in our notation we will not distinguish between an element A of
$\mathfrak{A}^R$ and its representative $\pi_\omega(A)$.

S + R is considered to be isolated, so that its time evol-
ution is determined by a selfadjoint Hamiltonian H acting on
$\mathfrak{H}^S \otimes \mathfrak{H}^R_\omega$:

(1.1) $$H = H^S \otimes \mathbb{1}^R + \mathbb{1}^S \otimes H^R + \lambda H^{SR} = H^0 + \lambda H^{SR}$$

where H^S is the free Hamiltonian of S,

H^R is the free Hamiltonian of R in the representation
induced by the stationary state ω^R,

$H^{SR} = \sum_j V^S_j \otimes V^R_j$ is the interaction Hamiltonian,

with V^S_j selfadjoint on $\mathfrak{H}^S$ and V^R_j selfadjoint on $\mathfrak{H}^R_\omega$.

We denote by $\mathfrak{T}(\mathfrak{H}^S \otimes \mathfrak{H}^R_\omega)$ the Banach space of trace-class
operators on $\mathfrak{H}^S \otimes \mathfrak{H}^R_\omega$, which is homomorphic to the space of
normal functionals on $\mathcal{B}(\mathfrak{H}^S) \otimes \pi_\omega(\mathfrak{A}^R)''$ according to the map

$$\varphi : \mathfrak{T}(\mathfrak{H}^S \otimes \mathfrak{H}^R_\omega) \longrightarrow [\mathcal{B}(\mathfrak{H}^S) \otimes \pi_\omega(\mathfrak{A}^R)'']_*,$$

(1.2)

$$\varphi(W)[A] = \mathrm{Tr}^{S+R}[WA], \qquad \forall A \in \mathcal{B}(\mathfrak{H}^S) \otimes \pi_\omega(\mathfrak{A}^R)''.$$

In the following, we shall use the same notation for W and $\varphi(W)$.

We use capital scripts, and occasionally capital greek letters, to denote operators acting on the spaces $\mathcal{I}(\mathfrak{H}^S)$, $\mathcal{I}(\mathfrak{H}_\omega^R)$, $\mathcal{I}(\mathfrak{H}^S \otimes \mathfrak{H}_\omega^R)$. We denote the identity maps acting on these spaces by $\mathfrak{J}^S$, $\mathfrak{J}^R$ and $\mathfrak{J}$ respectively. The dynamics on $\mathcal{I}(\mathfrak{H}^S \otimes \mathfrak{H}_\omega^R)$ is induced by

$$(1.3) \qquad \mathcal{H} = \mathcal{H}^S \otimes \mathfrak{J}^R + \mathfrak{J}^S \otimes \mathcal{H}^R + \lambda \mathcal{H}^{SR} = \mathcal{H}^0 + \lambda \mathcal{H}^{SR}$$

with $\mathcal{H}^S = [H^S, .]$, $\mathcal{H}^R = [H^R, .]$, $\mathcal{H}^{SR} = [H^{SR}, .]$. We define two one-parameter groups of automorphisms of $\mathcal{I}(\mathfrak{H}^S \otimes \mathfrak{H}_\omega^R)$:

$$(1.4) \qquad t \longrightarrow \mathcal{U}_t^0 : \quad \mathcal{U}_t^0 W = \exp\left[-i\mathcal{H}^0 t\right]W ,$$

$$(1.5) \qquad t \longrightarrow \mathcal{U}_t \equiv \mathcal{U}_t^{(\lambda)} : \quad \mathcal{U}_t W = \exp\left[-i\mathcal{H}t\right]W , \; W \in \mathcal{I}(\mathfrak{H}^S \otimes \mathfrak{H}_\omega^R)$$

describing the uncoupled and coupled global time evolutions, respectively.

We are interested in the reduced dynamics of S, under the assumption that the initial state of S+R is of the form $W(0) = \rho \otimes \omega^R$, where ρ is any normalized positive element of $\mathcal{I}(\mathfrak{H}^S)$.

The operation of partial trace with respect to R is defined as

$$(1.6) \qquad \begin{aligned} &\mathrm{Tr}_R : \; \mathcal{I}(\mathfrak{H}^S \otimes \mathfrak{H}_\omega^R) \longrightarrow \mathcal{I}(\mathfrak{H}^S) , \\ &\mathrm{Tr}^S\left[\mathrm{Tr}_R[W]A\right] = \mathrm{Tr}^{S+R}\left[W(A \otimes \mathbf{1}^R)\right] \quad \forall \; A \in \mathcal{B}(\mathfrak{H}^S) . \end{aligned}$$

The "amplification" $\mathcal{A}$ [33] is the linear operator

$$(1.7) \qquad \begin{aligned} &\mathcal{A} : \; \mathcal{I}(\mathfrak{H}^S) \longrightarrow \mathcal{I}(\mathfrak{H}^S \otimes \mathfrak{H}_\omega^R) \\ &\mathcal{A}\rho = \rho \otimes \omega^R . \end{aligned}$$

Then

(1.8)
$$\rho = \alpha\, \mathrm{Tr}_R$$

is a bounded idempotent (a projection) on $\tilde{\mathcal{I}}(\mathfrak{H}^S \otimes \mathfrak{H}^R_\omega)$, which projects onto the subspace $\tilde{\mathcal{I}}(\mathfrak{H}^S) \otimes \omega^R$, isomorphic to $\tilde{\mathcal{I}}(\mathfrak{H}^S)$.

The reduced dynamics $t \longrightarrow \Lambda_t$ of S in the Schrödinger picture is defined as follows:

(1.9) $\mathrm{Tr}^S\big[(\Lambda_t\rho)A\big] = \mathrm{Tr}^{S+R}\big[\mathcal{U}_t(\rho \otimes \omega^R)(A \otimes \mathbf{1}^R)\big], \forall \rho \in \mathcal{I}(\mathfrak{H}^S), \forall A \in \mathcal{B}(\mathfrak{H}^S)$

namely

(1.10) $\Lambda_t\rho = \mathrm{Tr}_R\big[\mathcal{U}_t \alpha\rho\big]$ or $\alpha\Lambda_t\rho = \rho\,\mathcal{U}_t\alpha\rho$.

The dual Heisenberg dynamics $t \longrightarrow \Lambda_t^*$ is given by:

(1.11) $\mathrm{Tr}^S\big[\rho(\Lambda_t^*A)\big] = \mathrm{Tr}^{S+R}\big[(\rho\otimes\omega^R)\mathcal{U}_t^*(A\otimes\mathbf{1}^R)\big], \forall \rho\in\mathcal{I}(\mathfrak{H}^S), \forall A\in\mathcal{B}(\mathfrak{H}^S)$

that is

(1.12) $\Lambda_t^*A = \mathcal{E}\,\mathcal{U}_t^*(A\otimes\mathbf{1}^R), \forall A\in\mathcal{B}(\mathfrak{H}^S)$

where $\mathcal{E}$ is defined as

(1.13)
$$\mathcal{E} : \mathcal{B}(\mathfrak{H}^S)\otimes\pi_\omega(\mathfrak{A}^R)'' \longrightarrow \mathcal{B}(\mathfrak{H}^S)$$
$$\mathrm{Tr}^{S+R}\big[(\alpha\rho)A\big] = \mathrm{Tr}^S\big[\rho(\mathcal{E}A)\big] ,$$

and can be shown to be a conditional expectation [58,81,62] onto $\mathcal{B}(\mathfrak{H}^S)$.

Starting from the Liouville-von Neumann equation for the density operator of the global system S+R

(1.14)
$$\frac{d}{dt} W(t) = -i \mathcal{H} W(t)$$

one can formally derive an exact equation for the reduced density operator $\rho(t) = \text{Tr}_R W(t)$ of S, called the generalized master equation, which, under our assumption on the initial condition, has the form [41, 33]

(1.15)
$$\frac{d}{dt} \rho(t) = -i \mathcal{H}_{eff} \rho(t) + \lambda^2 \int_0^t ds\, \mathcal{K}(s)\, \rho(t-s)$$

where

(1.16)
$$\mathcal{H}_{eff} = [H_{eff}, \cdot] \quad,$$

$$H_{eff} = H^S + \lambda \sum_j \omega^R(v_j^R) v_j^S$$

and

(1.17)
$$\mathcal{K}(s) = -\text{Tr}_R[\mathcal{H}^{SR}(\mathbb{1} - \mathcal{P}) \mathcal{U}_s'(\mathbb{1} - \mathcal{P}) \mathcal{H}^{SR} \mathcal{R}]$$

where

(1.18)
$$\mathcal{U}_t' = \exp[-i \mathcal{H}' t] \quad; \quad \mathcal{H}' = (\mathbb{1} - \mathcal{P}) \mathcal{H} (\mathbb{1} - \mathcal{P})$$

By setting

(1.19)
$$\mathcal{H}^{SR}(t) = \mathcal{U}_{-t}^o \mathcal{H}^{SR} \mathcal{U}_t^o = [e^{iH_0 t} H^{SR} e^{-iH_0 t}, \cdot] = [H^{SR}(t), \cdot]$$

we see that the integral kernel $\mathcal{K}(s)$ admits a formal power series expansion in the coupling constant λ of the form

(1.20)
$$\mathcal{K}(s) = e^{-i \mathcal{H}^S s} \left[\mathcal{K}_0(s) + \sum_{n=1}^{\infty} (-i)^n \lambda^n \int_{0 \leq t_n \leq \ldots \leq t_1 \leq s} dt_1 \ldots dt_n\, \mathcal{K}_n(s|t_1 \ldots t_n) \right],$$

where

$$(1.21) \qquad \mathcal{K}_0(s) = - \text{Tr}_R \left[\mathcal{H}^{SR}(s)(\mathbb{1} - \mathcal{P}) \mathcal{H}^{SR} \mathcal{Q} \right] \, ,$$

$$(1.22) \qquad \begin{aligned} \mathcal{K}_n(s|t_1 \ldots t_n) &= \\ &= - \text{Tr}_R \left[\mathcal{H}^{SR}(s)(\mathbb{1} - \mathcal{P}) \mathcal{H}^{SR}(t_1)(\mathbb{1} - \mathcal{P}) \ldots (\mathbb{1} - \mathcal{P}) \mathcal{H}^{SR}(t_n)(\mathbb{1} - \mathcal{P}) \mathcal{H}^{SR} \mathcal{Q} \right] \end{aligned}$$

$\mathcal{K}_n(s|t_1 \ldots t_n)$ depends on the multi-time correlation functions $\omega^R(v^R_{j_1}(t_1) \ldots v^R_{j_k}(t_k))$ of the reservoir operators appearing in the interaction Hamiltonian, up to order $k = n+2$, the relevant times being $t_0 = s, \ t_1, \ldots, t_n, \ t_{n+1} = 0$.

The Born approximation of the GME (1.15) amounts to keeping only the term $e^{-i \mathcal{H}^S s} \mathcal{K}_0(s)$ in the expansion (1.20) of $\mathcal{K}(s)$. The term $\lambda \sum_j \omega^R(v^R_j) V^S_j$ is a modification to the free Hamiltonian due to the interaction with the reservoir. It vanishes when $\omega^R(v^R_j) = 0 \ \forall j$, which is the case in several applications [5,33,41] and will be assumed for simplicity in the following.

2. COMPLETE POSITIVITY OF THE REDUCED DYNAMICS.

Before taking up the problem of the conditions under which the GME (1.15) can be well approximated by a Markovian master equation and studying rigorous models thereof, we discuss a special feature displayed by the reduced dynamics, independently of the nature of the systems under consideration and of their interaction.

To this end, we first recall a definition. Let $\mathcal{A}$ and $\mathcal{B}$ be C^*-algebras, and denote by $M(n)$ (n integer ≥ 1) the algebra of $n \times n$ complex matrices. A linear map $\phi : \mathcal{A} \rightarrow \mathcal{B}$ is called n-positive if the map

$$\dot{\phi}_n : \mathfrak{A} \otimes M(n) \longrightarrow \mathfrak{B} \otimes M(n),$$

$$\dot{\phi}_n(A \otimes M) = \phi(A) \otimes M, \qquad A \in \mathfrak{A}, \quad M \in M(n),$$

is positive. ϕ is called <u>completely positive</u> if it is n-positive for all integers n. Two important classes of completely positive maps are the $*$-automorphisms and the conditional expectations [77, 61]. Also, if $\mathfrak{A}$ and/or $\mathfrak{B}$ is commutative, every positive map of $\mathfrak{A}$ into $\mathfrak{B}$ is completely positive [12,19,77,78]. On the other hand, there exist positive maps which are not 2-positive; an example is provided by the $*$-antiautomorphisms and more generally by the Jordan automorphisms which are not reduced to $*$-automorphisms [38].

There is an extensive mathematical literature on positive and completely positive maps [12,19,20,77-79].

The reduced dynamics in the Heisenberg picture $t \longrightarrow \Lambda_t^*$ of a system S coupled to a reservoir R has the remarkable property that Λ_t^* is completely positive for all t, since it is the composition of a $*$-automorphism and a conditional expectation. To our knowledge, the complete positivity of a reduced dynamics was first pointed out by Kraus [54,55] in the context of state changes produced by quantum measurements, and has been subsequently discussed by several authors [58,38,2] from different standpoints.

Conversely, Evans [31] has recently shown by construction that if $t \longrightarrow \phi_t$, $t \in \mathbb{R}_+$, is a family of completely positive maps of a (concrete) C^*-algebra $\mathfrak{A}$ into itself with $\phi_t(1) = 1$ $\forall$ t and $\phi_0 = 1$, then there exist a larger (concrete) C^*-algebra $\mathfrak{B}$, a group $\{\alpha_t\}$ of $*$-automorphisms of $\mathfrak{B}$ and a conditional expectation $\mathscr{E}$ from $\mathfrak{B}$ onto $\mathfrak{A}$ such that

$$\phi_t(A) = \mathscr{E}[\alpha_t(A)] \qquad \forall A \in \mathfrak{A}.$$

In this sense, all families of completely positive identity preserving maps of a C^*-algebra are similar to reduced dynamics. However this construction has no direct physical interpretation.

In the particularly interesting case when $\mathfrak{A} = \mathfrak{B}(\mathfrak{H}^S)$ and $t \rightarrow \phi_t$ is a norm- continous normal semigroup, there is an entirely different construction $[22, 32]$ of $\mathfrak{B}$, $\{\alpha_t\}$ and $\mathfrak{G}$ for which $\{\alpha_t\}$ is implemented by a strongly continous group of unitary operators on the Hilbert space on which $\mathfrak{B}$ acts. This construction suggests an interpretation of $\mathfrak{B}$ as the algebra of observables of a larger system whose global dynamics $\{\alpha_t\}$ induces the reduced dynamics $\{\phi_t\}$ on $\mathfrak{A}$. Remark however that $t \rightarrow \alpha_t$ is weakly*-continous, but not strongly continous, unless the generator of $t \rightarrow \phi_t$ is a derivation. Indeed, suppose that $\{\alpha_t\}$ is strongly continous with generator $i\mathfrak{K}$ and that the generator L of $\{\phi_t\}$ is the closure of its restriction to $\mathfrak{D}(\mathfrak{K}) \cap \mathfrak{A}$, then $L = i\overline{\mathfrak{G}\mathfrak{K}}$, which is again a derivation $[32]$.

We suspect that the construction of Refs. 22, 32 corresponds to a singular coupling of the system $\mathfrak{A}$ to a boson or fermion reservoir, in the sense of the models to be discussed in Section 6. However, we have not been able so far to give a proof of this statement.

3. MARKOV APPROXIMATION AND CLASSIFICATION OF DYNAMICAL SEMIGROUPS.

An evolution equation for the density operator of a subsystem S of a closed system S+R is said to be a Markovian master equation (MME) if it has the form

(3.1) $$\frac{d}{dt}\rho(t) = \mathcal{L}\rho(t) = -i\mathcal{H}_{eff}\rho(t) + \mathcal{L}_D\rho(t)$$

where $\mathcal{H}_{eff}$ is as in (1.16), and where the operator $\mathcal{L}_D$ contains all dissipative effects. Equations of the form (3.1) imply a semigroup law of evolution for the state of S, and are of common use in the phenomenological treatment of open systems (relaxation processes [1,11,13,14] , quantum theory of damping [3], Brownian motion [4], optical pumping [43], superradiance [16,17], theory of lasers [42]; for extensive lists of references, see [41] and [5]. For applications to the quantum theory of measurement and to the decay of unstable systems, see respectively [36] and [80,56]). However, it is in general impossible to derive an MME as an exact consequence of (1.15). Indeed, if $\mathcal{H}$ is such that $\mathcal{H}_{eff}$ and $\mathcal{K}(s)$ are well defined operators, and if (1.15) can be put in the form (3.1), it follows that $\mathcal{L}$ is trivially given by (see [29])

$$\mathcal{L}\rho = \left.\frac{d}{dt}\rho(t)\right|_{t=0} = -i\mathcal{H}_{eff} \quad .$$

Hence we do not expect (1.15) to reduce to the form (3.1) unless the global dynamics $\mathcal{U}_t$ of S+R has some "singular" character, corresponding to a limiting situation in which the memory effects which are present in (1.15) become negligible. From the structure of the kernel $\mathcal{K}(s)$ in (1.15), one expects that a situation of this kind will take place if the typical variation time τ_S of $\rho(t)$ is much longer than the decay time τ_R of the correlation functions of the reservoir. Then (1.15) should be well approximated by an MME (3.1) with

(3.2) $$\mathcal{L} = -i\mathcal{H}_{eff} + \lambda^2\int_0^\infty ds\,\mathcal{K}(s)$$

for times larger than τ_R. A similar argument applies to other

types of master equations, such as those satisfied by the coarse-grained density operator which describes the dynamics of the macroscopic observables of a large system[85,86,67,73,57,68,82,83].

Even though the importance of the separation of two time scales for the validity of the Markovian approximation to the GME has been recognized long ago [15,83,65] and made object of extensive studies [83,11,33] , rigorous treatments of the limiting procedure $\tau_S/\tau_R \longrightarrow \infty$ are rather recent.
Two possible limits can be taken:

1) the weak coupling limit $\lambda \to 0$, with rescaled time $\tau = \lambda^2 t$ [82,83]. In this case τ_R remains constant, while τ_S tends to infinity. Rigorous models thereof were studied by Davies [23,24] and Pulè [70] and a general rigorous treatment has been recently given by Davies [25-27], and will be discussed in Section 5. Roughly speaking, it turns out that in the limit $\lambda \to 0$ the expansion (1.20) reduces to the Born approximation and the integral extends to infinity due to the change in the time scale. In particular, this situation is approximately verified for a system which is not completely isolated from its surroundings and relaxes to thermal equilibrium with it;

2) the singular reservoir limit, in which $\tau_R \to 0$. As an example, this could be regarded as a drastic simplification of a situation like the one which takes place in a laser, where the system of interest is driven by the various pump and loss mechanisms.   To our knowledge, it was first explicit ly recognized by Hepp and Lieb. [45] that the condition $\tau_R = 0$ requires a singular coupling. In Refs. 37, 34, 35 , to be discussed in Section 6, we have shown on explicit models that this kind of limiting procedure allows one to derive all completely positive trace preserving semigroups of an N-level system. Briefly speaking, the Markovian behaviour is

achieved in the limit $\tau_R \to 0$ since $\mathcal{K}_0(s)$ tends to $\mathcal{K}_0 \delta(s)$ and the higher order corrections vanish.

Since the completely positive maps of a C^*-algebra form a convex cone which is closed in the bounded-weak topology [58], the property of complete positivity of the Heisenberg reduced dynamics is not destroyed by any of the limiting procedures which are employed to obtain a Markovian master equation.

From the above discussion, we conclude that the operator $\mathcal{L}$ in the MME (3.1) can be regarded as the generator of a strongly continous one-parameter semigroup of positive and trace preserving maps of $\mathcal{T}(\mathfrak{H}^S)$ whose dual maps are completely positive (and automatically ultraweakly continous and identity preserving): such semigroups are referred to as dynamical semigroups [49,38,58,47,28].

A classification of norm continous (or, equivalently, with a bounded generator) dynamical semigroups of $\mathcal{T}(\mathfrak{H})$, $\mathfrak{H}$ separable, has been recently given by Lindblad [58]. The general form of the generator of such a semigroup is the following:

$$\mathcal{L}\rho = -i[H,\rho] + \frac{1}{2}\sum_j \left\{ [v_j, \rho v_j^*] + [v_j \rho, v_j^*] \right\}$$

(3.3)

$$= -i[H,\rho] + \sum_j v_j \rho v_j^* - \frac{1}{2}\left\{ \sum_j v_j^* v_j, \rho \right\}, \quad \rho \in \mathcal{T}(\mathfrak{H})$$

where H is a bounded selfadjoint operator, $\{v_j\}_{j\in I}$ is a sequence of bounded operators, $\sum_j v_j^* v_j$ converges ultraweakly, and the r.h.s. converges in the trace norm.

The generator $\mathcal{L}^*$ of the dual semigroup $\{\Lambda_t^*\}$ in the Heisenberg picture is given by

$$\mathcal{L}^* A = i[H,A] + \frac{1}{2}\sum_j \left\{ [v_j^*, A] v_j + v_j^* [A, v_j] \right\}$$

(3.4)

$$= i[H,A] + \Psi_{\{v\}}(A) - \frac{1}{2}\left\{ \Psi_{\{v\}}(\mathbb{1}), A \right\}, \quad A \in \mathcal{B}(\mathfrak{H}),$$

where the convergence is ultraweak, and where

$$(3.5) \qquad \Psi_{\{V\}}(A) = \sum_j V_j^* A V_j$$

is the general form of a completely positive ultraweakly continous map of $\mathcal{B}(\mathcal{H})$ into itself [54,55]. This result has been successively extended to more general W^*-algebras under certain conditions on their cohomology groups [60].

The problem of the classification of unbounded generators is very difficult. A particularly simple case is obtained by allowing for the selfadjoint operator H in (3.3) to be unbounded. Some physically more meaningful classes of unbounded generators are discussed in [28,59].

In the case of an N-level system ($\dim \mathcal{H} = N$), (3.3) and (3.4) can be given the form [38]

$$(3.6) \qquad \mathcal{L}\rho = -i[H,\rho] + \frac{1}{2} \sum_{i,j=1}^{N^2-1} c_{ij}\left\{[F_i, \rho F_j^*] + [F_i \rho, F_j^*]\right\}$$

$$(3.7) \qquad \mathcal{L}^*A = i[H,A] + \frac{1}{2} \sum_{i,j=1}^{N^2-1} c_{ij}\left\{[F_j^*,A]F_i + F_j^*[A,F_i]\right\}$$

where $H = H^*$, $\mathrm{Tr}(H) = 0$, $\mathrm{Tr}(F_j) = 0$, $\mathrm{Tr}(F_i^* F_j) = \delta_{ij}$, and $\{c_{ij}\}$ is any positive matrix. For a given $\mathcal{L}$, H is uniquely determined by the condition $\mathrm{Tr}(H) = 0$, and $\{c_{ij}\}$ is uniquely determined by the choice of the F_j's. The conditions $\mathrm{Tr}(H)=0$, $\mathrm{Tr}(F_j)=0$ provide a canonical separation of the generator into a Hamiltonian plus a dissipative part. There is no general immediate criterion for an analogous separation when $\dim \mathcal{H} = \infty$. If the condition of complete positivity is replaced by the weaker requirement of simple positivity, the generator for an N-level system can again be written in the form (3.6), where the matrices $\{c_{ij}\}$ belong to a strictly larger convex cone

than the positive one.

For the proof. of (3.4) and (3.6), we refer to [58,38,53].

Still in the case of an N-level system, the knowledge of the general form of the generator has allowed Spohn to derive sufficient conditions for the existence of a unique stationary state [75,76]. With the generator $\mathcal{L}$ written in the form (3.3) (respectively,(3.6)) a sufficient condition for the uniqueness of the stationary state and for all states to relax to it in the limit $t \to \infty$ is given by

(3.8) $\text{lsp}\left\{v_j \mid j \in I\right\}$ is selfadjoint and $\left\{v_j \mid j \in I\right\}' = \mathbb{C}\mathbf{1}$,

where lsp denotes the linear span and

$\left\{\ \right\}'$ denotes the commutant in $\mathcal{B}(\mathfrak{H})$ (respectively, by the requirement that the multiplicity of the eigenvalue zero of the matrix $\left\{c_{ij}\right\}$ be less than N/2). Also the irreducibility condition given by [21] ensures the existence of a unique faithful stationary state. There is no apparent straightforward extension of the above results to the infinite-dimensional case. An example thereof where the stationary state is unique and approached by all states for long times is provided by the Brownian motion of a quantum harmonic oscillator [59].

4.   IMPLICATIONS OF COMPLETE POSITIVITY (2-LEVEL SYSTEMS).

In the case of an N-level system, the condition $\left\{c_{ij}\right\} \geqslant 0$ implicitly expresses inequalities to be satisfied among the physical parameters characterizing the dynamical evolution (such as relaxation times and components of equilibrium states), which would be weaker or even non-existing if just positivity

were required.

So far, we have only been able to make such inequalities explicit for a 2-level system [38,51]. In this case, let $\{t \longrightarrow \Lambda_t , t \geqslant 0\}$ be a positive trace preserving semigroup of $K(n)$, and let $\{\mathbb{1}\} \cup \{F_i\}_{i=1,2,3}$ be a complete orthogonal set of selfadjoint matrices, with $F_i F_j = \frac{1}{4} \delta_{ij} \mathbb{1} + \frac{i}{2} \sum_{k=1}^{3} \varepsilon_{ijk} F_k$. Then the polarization components $M_i(t) = \mathrm{Tr}\left[(\Lambda_t \rho) F_i\right]$ satisfy the Bloch equations:

$$(4.1) \qquad \frac{d}{dt} M_i(t) = \sum_{j,k=1}^{3} \varepsilon_{ijk} h_i (M_k(t) - M_k^0) - \gamma_i (M_i(t) - M_i^0)$$

where

$$\gamma_1 , \gamma_2 , \gamma_3 \geqslant 0,$$

$$h_i \text{ real},$$

$$M_i^0 = 0 \quad \text{if} \quad \gamma_1 \gamma_2 \gamma_3 = 0$$

and

$$\inf_{x_1^2 + x_2^2 + x_3^2 = 1} \left[\sum_{i=1}^{3} (\gamma_i x_i (x_i - 2M_i^0) + \sum_{j,k=1}^{3} 2 \varepsilon_{ijk} x_i h_j M_k^0) \right] \geqslant 0 \quad \text{if} \gamma_1 \gamma_2 \gamma_3 > 0.$$

$\vec{M^0}$ is a stationary state for the evolution (4.1) and it is the only stationary state iff $\gamma_1 \gamma_2 \gamma_3 > 0$; in this case every state approaches $\vec{M^0}$ as $t \to \infty$.

The condition of complete positivity, expressed by the positivity of the matrix $\{c_{ij}\}$, imposes further restrictions on the range of variation of $\vec{M^0}$ and implies the inequalities

$$(4.2) \qquad \gamma_1 + \gamma_2 \geqslant \gamma_3 ; \quad \gamma_2 + \gamma_3 \geqslant \gamma_1 ; \quad \gamma_3 + \gamma_1 \geqslant \gamma_2 .$$

Since the γ_i's are essentially inverse relaxation times, (4.2) shows that no two relaxation times can be much longer than the third. In particular, a completely positive non-Hamil_

tonian evolution of a 2-level system admits at most a one-dimensional manifold of stationary states.

As a special example, take $h_1 = h_2 = 0$ and the system to be axially symmetric about the direction of the "external magnetic field". In this case $M_1^o = M_2^o = 0$, $1/\gamma_1 = 1/\gamma_2 = 1/\gamma_\perp = T_\perp$ (transverse relaxation time), $1/\gamma_3 = 1/\gamma_\shortparallel = T_\shortparallel$ (longitudinal relaxation time). The necessary and sufficient condition for the dynamics to be completely positive is

(4.3)
$$T_\shortparallel \geqslant \tfrac{1}{2} T_\perp .$$

To our knowledge, this relation is satisfied experimentally in all known cases [1,13,44 and references quoted therein].

A further insight into the strong geometrical restrictions imposed by complete positivity on the reduced dynamics of a 2-level system is provided by a comparison of the structures of the extreme points of the convex sets $P(2)$ and $CP(2)$ respectively of the positive and the completely positive trace preserving linear maps of $M(2)$. Writing a density matrix as $\rho = \tfrac{1}{2}(\mathbb{1} + \vec{x} \cdot \vec{\sigma})$, $\|\vec{x}\| \leqslant 1$, where $\{\sigma_i\}_{i=1,2,3}$ are the Pauli matrices, the extreme points of $P(2)$ (respectively, of $CP(2)$) are the following [39] :

$$x_1' = x_1 \cos(\alpha - \beta)$$

$$x_2' = x_2 \cos(\alpha - \beta)$$

$$x_3' = x_3\cos(\alpha - \beta)\cos(\alpha + \beta) + \sin(\alpha - \beta)\sin(\alpha + \beta)$$

up to $O(3)$ transformations

(respectively,

$$x_1' = x_1 \cos(\alpha - \beta)$$

$$x_2' = x_2 \cos(\alpha + \beta)$$

$$x_3' = x_3\cos(\alpha - \beta)\cos(\alpha + \beta) + \sin(\alpha - \beta)\sin(\alpha + \beta)$$

up to $SO(3)$ transformations),

where $\rho' = \frac{1}{2}(\mathbb{1} + \vec{x}'\cdot\vec{\sigma}) = \Gamma\rho$, $\Gamma \in P(2)$ (respectively, $\Gamma \in CP(2)$) and the range of variation of α and β is given by

$$\begin{cases} \alpha = \beta = 0, \\ 0 \leq \beta \leq \alpha \leq \pi/4, \\ \pi/4 \leq \alpha \leq \pi/2, \quad 0 \leq \beta \leq \pi/2 - \alpha. \end{cases}$$

5. WEAK COUPLING LIMIT.

A rigorous justification of the reduction of the GME (1.15) to the MME (3.1) in the weak coupling limit has been given by Davies in a series of papers [25,26,27]. Here we present a short sketch of the simplest version of this method.

Assume that $\mathcal{H}^{SR}$ is bounded and $\mathrm{Tr}_R\, \mathcal{H}^{SR}\mathcal{U} = 0$ so that $\mathcal{H}_{eff} = \mathcal{H}^S$. In order to avoid domain problems, it is convenient to work with an integrated form of the GME. An elementary change of variables in the double integration yields

$$(5.1) \qquad \rho(t) = \mathcal{U}_t^S\, \rho(0) + \lambda^2 \int_0^t du \int_0^{t-u} dx\; \mathcal{U}_{t-x-u}^S \mathcal{K}(x)\, \rho(u),$$

where $\mathcal{U}_t^S = \exp[-i\mathcal{H}^S t]$.

We pass to the interaction picture and we rescale the time, setting $\lambda^2 t = \tau$ and $\lambda^2 u = \sigma$, with the purpose of letting λ go to zero. The use of the interaction picture can be interpreted as an averaging over "fast microscopic oscillations". We define

$$(5.2) \qquad \rho_I(\tau) = \lim_{\lambda \to 0} \mathcal{U}_{-\lambda^{-2}\tau}^S\, \rho(\lambda^{-2}\tau)$$

and find

$$\rho_I(\tau) = \rho_I(0) + \lim_{\lambda \to 0} \int_0^\tau d\sigma\, \mathcal{U}^S_{-\lambda^2\sigma} \left[\int_0^{\lambda^{-2}(\tau-\sigma)} dx\, \mathcal{U}^S_{-x}\, \mathcal{K}(x) \right] \mathcal{U}^S_{\lambda^2\sigma}\, \rho_I(\sigma).$$

We expect that in the limit $\lambda \to 0$ only the term $\mathcal{K}_0$ in the expansion (1.20) of $\mathcal{K}$ will give a nonvanishing contribution, so that

(5.3) $\qquad \rho_I(\tau) = \rho_I(0) + \lim_{\lambda \to 0} \int_0^\tau d\sigma\, \mathcal{U}^S_{-\lambda^2\sigma}\, K\, \mathcal{U}^S_{\lambda^2\sigma}\, \rho_I(\sigma)$

where

(5.4) $\qquad\qquad\qquad K = \int_0^\infty dx\, \mathcal{K}_0(x).$

Davies shows that this is indeed the case under the following conditions on $\mathcal{K}_0$, $\mathcal{K}_n$ ($n = 1, 2, \ldots$):

(5.5) $\quad \displaystyle\int_0^\infty dt\, \|\mathcal{K}_0(t)\| < \infty,$

$\quad \displaystyle\int_{0 \le t_n \le t_{n-1} \le \ldots \le t_1 \le t_0 \le t} dt_0 \ldots dt_n\, \|\mathcal{K}_n(t_0|t_1 \ldots t_n)\| \le a_n(t),$

with

(5.6) $\qquad\qquad a_n(t) \le c_n\, t^{n/2} \quad \text{for all } t \ge 0,$

where $\displaystyle\sum_n c_n z^n$ has infinite radius of convergence, and

(5.7) $\qquad\qquad a_n(t) \le d_n\, t^{n/2-\varepsilon} \quad \text{for some } \varepsilon > 0,\ d_n \text{ and all } t \ge 0.$

Since we are dealing with a spatially confined system S, the spectrum of $\mathcal{H}^S$ is purely discrete and the limit $\lambda \to 0$ in

(5.3) can be easily performed, to yield

$$(5.8) \qquad \rho_I(\tau) = \rho_I(0) + K^\sharp \int_0^\tau d\sigma \, \rho_I(\sigma)$$

where

$$(5.9) \qquad K^\sharp = \sum_\alpha Q_\alpha K Q_\alpha$$

the Q_α's being the spectral projections of $\mathcal{H}^S$ corresponding to distinct eigenvalues ω_α. Hence equivalently

$$(5.9') \qquad K^\sharp = \lim_{a \to \infty} \frac{1}{2a} \int_{-a}^a dx \, \mathcal{U}_{-x}^S \, K \, \mathcal{U}_x^S .$$

The differential form of (5.8) is the MME

$$(5.8') \qquad \frac{d}{d\tau} \rho_I(\tau) = K^\sharp \rho_I(\tau)$$

(now no domain problem arises, since $K^\sharp$ is bounded, as a consequence of the boundedness of $\mathcal{H}^{SR}$).

The rigorous result in [25] is

$$\lim_{\substack{\lambda \to 0 \\ \lambda^2 t = \tau}} \left\| \mathcal{U}_{-t}^S \, \mathrm{Tr}_R \mathcal{U}_t^{(\lambda)} \mathcal{A} \rho - \exp(K^\sharp \tau) \rho \right\|_1 = 0$$

uniformly on each interval $0 \leqslant \tau \leqslant \tau_4$.
More generally, one can release the assumption that $\mathcal{H}_{eff} = \mathcal{H}^S$ and that the spectrum of $\mathcal{H}^S$ is purely discrete, and find [26]

$$(5.10) \quad \lim_{\lambda \to 0} \left\{ \sup_{0 \leqslant t \leqslant \lambda^{-2}\tau} \left\| \mathrm{Tr}_R \mathcal{U}_t^{(\lambda)} \mathcal{A} - \exp\left(-it \mathcal{H}_{eff} + \lambda^2 K\right) \right\| \right\} = 0.$$

However, as K^4 is much simpler to use in place of K because it manifestly commutes with the free evolution, we shall restrict ourselves in the following to the case in which $\mathcal{H}_{eff} = \mathcal{H}^S$ and the spectrum of $\mathcal{H}^S$ is purely discrete.

We write the coupling between S and R as

$$(5.11) \qquad \lambda H^{SR} = \lambda \sum_\alpha v_\alpha^S \otimes v_\alpha^R$$

with v_α^S selfadjoint, v_α^R selfadjoint, and $\omega^R(v_\alpha^R) = 0$. If conditions $(5.5) - (5.7)$ are satisfied, the reduced dynamics is a semigroup whose generator K^4 is given by ($[25]$, with minor generalization and notational modifications)

$$(5.12) \qquad K^4 \rho = \sum_{\omega \in Sp \mathcal{H}^S} \sum_{\alpha\beta} \left\{ -i\, s_{\alpha\beta}(\omega) \left[v_\beta(\omega)^* v_\alpha(\omega), \rho \right] \right.$$
$$\left. + \hat{h}_{\alpha\beta}(\omega) \left(\left[v_\alpha(\omega)\rho, v_\beta(\omega)^* \right] + \left[v_\alpha(\omega), \rho\, v_\beta(\omega)^* \right] \right) \right\},$$

where $(2\pi)^{-1/2} \hat{h}_{\alpha\beta}(\omega)$ is the Fourier transform of $h_{\alpha\beta}(t) =$

$$= \omega^R(v_\beta^R v_\alpha^R(t)) = \omega^R(v_\beta^R e^{iH^R t} v_\alpha^R e^{-iH^R t}),$$

$$(5.13) \qquad s_{\alpha\beta}(\omega) = i \int_0^\infty dt\, e^{-i\omega t}\, h_{\alpha\beta}(t) - \tfrac{1}{2} \hat{h}_{\alpha\beta}(\omega) =$$
$$= \frac{1}{2\pi} \mathcal{P} \int_{-\infty}^\infty \frac{\hat{h}_{\alpha\beta}(\lambda)}{\lambda - \omega}\, d\lambda,$$

$\mathcal{P}$ denoting the principal part, and

$$v_\alpha(\omega) = \sum_{\varepsilon_m - \varepsilon_n = \omega} P_{nn} v_\alpha^S P_{mm} = \sum_{\varepsilon_m - \varepsilon_n = \omega} (v_\alpha)_{nm} P_{nm} = v_\alpha(-\omega)^*$$

$(P_{nm} = |n\rangle\langle m|, \quad H^S |n\rangle = \varepsilon_n |n\rangle, \quad (v_\alpha)_{nm} = \langle n | v_\alpha^S | m \rangle).$

Sufficient conditions for (5.5)-(5.7) to be satisfied are:

(i) $\sum_{-\infty}^{\infty} \|v_\alpha^S\|^2 < \infty$;

(ii) $\int_0^\infty |h_{\alpha\beta}(t)| (1+t)^\varepsilon \, dt < a$, with a independent of α, β ;

(iii) the reservoir is quasi-free, i.e. all truncated correlation functions $\omega^R(v_{\alpha_1}^R(t_1)\ldots v_{\alpha_k}^R(t_k))^T$ of order greater than two vanish.

The dual generator, written explicit ly in terms of the operators P_{mn}, is given by

$$
K^{b*} A = i \left[\sum_{\alpha\beta} \sum_{\varepsilon_i=\varepsilon_k} \sum_j s_{\alpha\beta}(\varepsilon_i-\varepsilon_j)(V_\beta)_{ij}(V_\alpha)_{jk} P_{ik}, A \right]
$$

(5.14)
$$
+ \sum_{\alpha\beta} \sum_{\varepsilon_i-\varepsilon_j=\varepsilon_k-\varepsilon_\ell} \hat{h}_{\alpha\beta}(\varepsilon_i-\varepsilon_j)(V_\beta)_{ij}(V_\alpha)_{\ell k}\left[P_{ij} A P_{\ell k}-\left\{\tfrac{1}{2} P_{ij}P_{\ell k}, A\right\}\right].
$$

We remark that $t \longrightarrow \sum_{\alpha\beta} \bar{x}_\alpha h_{\alpha\beta}(t)x_\beta$ is a function of positive type for all sequences $\{x_\alpha\}$ for which the expression converges, hence $\{\hat{h}_{\alpha\beta}(\omega)\}$ is a positive matrix for all ω, and its Hilbert transform $\{s_{\alpha\beta}(\omega)\}$ is selfadjoint. Therefore we recognize that K^{b*} is of the general form (3.5)

$$
K^{b*} A = i[H,A] + \psi(A) - \tfrac{1}{2}\{\psi(\mathbb{1}),A\}
$$

where $H = H^*$ and ψ is an ultraweakly continous completely positive map of $\mathcal{B}(\mathcal{H})$. Moreover H and $\psi(\mathbb{1})$ commute with the free Hamiltonian.

If the reference state of the reservoir is KMS at inverse temperature β, then the canonical state $\rho_\beta =\exp(-\beta H^S)/\text{Tr}[\exp(-\beta H^S)]$ is a stationary state for the reduced dynamics, as follows from the KMS condition on Fourier transforms

$$(5.15) \qquad \hat{h}_{\alpha\beta}(-\omega) = e^{-\beta\omega} \hat{h}_{\beta\alpha}(\omega).$$

This is a reflection of the stability property of KMS states, in the sense that for each perturbed evolution there exists a stationary state which is **KMS** with respect to the perturbed dynamics and approaches the **KMS** state for the unperturbed dynamics when the perturbation is removed $\left[10, 72 \right]$.

We shall see in Section 7 that the reduced dynamics (5.12) satisfies a quantum detailed balance condition as a consequence of (5.15).

6. MODELS OF SINGULAR RESERVOIRS.

The singular reservoir limit corresponds to a limiting situation in which the correlation functions

$$(6.1) \qquad h_{\alpha\beta}(t) = \omega^R(V_\beta^R V_\alpha^R(t))$$

of the operators V_α^R appearing in the interaction tend to $c_{\alpha\beta} \delta(t)$.

Before entering the discussion of specific models, we note that a correlation function (6.1) cannot tend to a δ-function if ω^R is KMS at some $\beta \neq 0$. In fact, by the continuity of the Fourier transform, $h_{\alpha\beta}$ tends to a δ-function if and only if its Fourier transform $\hat{h}_{\alpha\beta}$ tends to a constant almost everywhere. On the other hand, the KMS condition on

Fourier transforms (5.15) forbids $\hat{h}_{\alpha\beta}$ to approach a constant unless $\beta = 0$.

For a similar reason, if the reservoir is chosen to be a quasi-free Bose or Fermi gas and ω^R is the vacuum state, the limit of singular reservoir can only be performed if the one-particle energy spectrum is the whole real line. This is rather unphysical, but is necessary if one wants to reconstruct any dynamical semigroup as a reduced dynamics in the singular reservoir limit [37]. This feature is also shared by the models of Hepp and Lieb [45].

In [37] and [34] we have studied models which can account for all dynamical semigroups of an N-level system. The system S of interest is coupled to a quasi-free boson or fermion reservoir in the vacuum state or in the infinite temperature limit, by a linear coupling of the form

$$(6.2) \qquad H^{SR} = \sum_{\alpha=1}^{N^2} V_{\alpha}^{S} \otimes V_{\alpha}^{R} ,$$

where

$\{ V_{\alpha}^{S} | \alpha = 1, \ldots, N^2 \}$ can be conveniently chosen as a complete orthonormal set in $M(N)$, with $V_{N^2}^{S} = \mathbb{1}/\sqrt{N}$;

$$(6.3) \qquad V_{\alpha}^{R} = \varphi_{\alpha}(f^{\varepsilon}) = \sum_{\beta=1}^{N^2} \left[\sqrt{\mu_{\beta}} \bar{\lambda}_{\alpha}^{\beta} a_{\beta}(f^{\varepsilon}) + \sqrt{\mu_{\beta}} \lambda_{\alpha}^{\beta} a_{\beta}(f^{\varepsilon})^{*} \right] ,$$

where the $a_{\beta}(f)^{\#}$ are independent Bose or Fermi creation and annihilation operators, and

$$(6.4) \qquad \sum_{\alpha=1}^{N^2} \bar{\lambda}_{\alpha}^{\rho} \lambda_{\alpha}^{\sigma} = \delta_{\rho\sigma} ,$$

$$(6.5) \qquad f^{\varepsilon}(\omega) = (2\pi)^{-1/2} \exp\left[-\varepsilon^2 \omega^2/8 \right] ,$$

$$(6.6) \qquad f^{\varepsilon}(\omega) = \pi^{-1/2} \vartheta(\omega) \exp\left[- \varepsilon^2 \omega^2/8\right] \qquad \text{or}$$

$$(6.7) \qquad f^{\varepsilon,\beta}(\omega) = (2\pi)^{-1/2} \vartheta(\omega)(\beta\omega)^{1/2} \exp\left[- \varepsilon^2 \omega^2/8\right]$$

according to whether the reference state of the reservoir is the Fock vacuum, the infinite temperature fermion state, or a KMS boson state to be considered in the limit $\beta \to 0$.

The corresponding Fourier transforms of the correlation functions $h^{(\varepsilon)}_{\alpha\beta}(t)$ are respectively given by $[37, 34]$

$$(6.8) \qquad \hat{h}^{(\varepsilon)}_{\alpha\beta}(\omega) = C_{\alpha\beta}(2\pi)^{-1/2} \exp\left[- \varepsilon^2 \omega^2/4\right] ,$$

$$(6.9) \qquad \hat{h}^{(\varepsilon)}_{\alpha\beta}(\omega) = \left[C_{\alpha\beta}\vartheta(-\omega) + C_{\beta\alpha}\vartheta(\omega)\right] (2\pi)^{-1/2} \exp\left[- \varepsilon^2 \omega^2/4\right] ,$$

$$(6.10) \qquad \hat{h}^{(\varepsilon,\beta)}_{\alpha\beta}(\omega) = \left[C_{\alpha\beta}\vartheta(-\omega) + C_{\beta\alpha}\vartheta(\omega)\right] (2\pi)^{-1/2} \frac{e^{-\beta\omega}}{e^{-\beta\omega}-1} \exp\left[-\varepsilon^2 \omega^2/4\right],$$

where

$$(6.11) \qquad C_{\alpha\beta} = \sum_{\gamma=1}^{N^2} |\mu_\gamma|^2 \lambda^\gamma_\alpha \overline{\lambda^\gamma_\beta}$$

is the general form of a positive $N^2 \times N^2$ matrix.

As $\varepsilon \to 0$, (6.8) tends to the Fourier transform of $C_{\alpha\beta} \delta(t)$. This is also the case for (6.9) and (6.10), provided $\{C_{\alpha\beta}\}$ is chosen to be real and symmetric. As regards (6.10), one has to take at the same time the limit $\beta \to 0$.

The generator of the reduced dynamical semigroup is given by

$$(6.12) \qquad \mathscr{L}\rho = -i\left[H^S + H^1, \rho\right] + \frac{1}{2} \sum_{i,j=1}^{N^2-1} C_{ij} \left\{\left[V^S_i \rho, V^{S}_j\right] + \left[V^S_i, \rho V^{S}_j\right]\right\},$$

where $H^1 = -N^{-1/2} \sum_{k=1}^{N^2-1} \text{Im } C_{kN^2} V^S_k$. In $[37, 34]$, (6.12) was proved using the Dyson series expansion of $(x \otimes \Omega | \mathcal{U}^{0*}_{-t} \mathcal{U}^*_t (A \otimes 1^R) y \otimes \Omega)$,

$\omega^R = (\Omega \mid . \Omega)$. The same result has been obtained in [35] using the master equation approach. We give a short account of the latter technique.

From the expansion (1.20) of the integral kernel and with H^{SR} given by (6.2), we have

(6.13)
$$\mathcal{K}_0(s) = - \text{Tr}_R \left[\mathcal{H}^{SR}(s) \, \mathcal{H}^{SR} \mathcal{Q} \right]$$
$$= \sum_{\alpha\beta} \left\{ h^{(\varepsilon)}_{\beta\alpha}(-s) \left[v^S_\alpha(s), v^S_\beta \, . \right] - h^{(\varepsilon)}_{\alpha\beta}(s) \left[v^S_\alpha(s), \, . \, v^S_\beta \right] \right\}.$$

Hence, in the limit $h^{(\varepsilon)}_{\alpha\beta}(s) \rightarrow c_{\alpha\beta} \delta(s)$, the Born approximation yields

(6.14) $\frac{d}{dt} \rho(t) = -i \left[H^S, \rho(t) \right] + \frac{1}{2} \sum_{\alpha\beta} c_{\alpha\beta} \left\{ \left[v^S_\alpha \rho(t), v^S_\beta \right] + \left[v^S_\alpha, \rho(t) v^S_\beta \right] \right\}$

which is (6.12).

As regards the higher order terms, they give no contribution in the limit. Indeed, the series (1.20) is uniformly convergent on bounded ε-intervals, and all terms containing $\mathcal{K}_n$, $n = 1, 2, \ldots$, vanish as $\varepsilon \rightarrow 0$. We refer to [35] for the detailed proof of this statement, and confine ourselves here to the observation that in the expansion of the multitime correlation functions $\omega^R (v^R_{\alpha_0}(t_0) \ldots v^R_{\alpha_k}(t_k))$ appearing in $\mathcal{K}_n(t_0 \mid t_1 \ldots t_n)$ one is left only with those products in which some time arguments appear in "overlapping order", such as

$$h^{(\varepsilon)}_{\alpha\beta}(t_1 - t_3) \cdot h^{(\varepsilon)}_{\gamma\delta}(t_2 - t_4).$$

In the limit $\varepsilon \rightarrow 0$, such products do not yield any contribution under integration as in (1.20).

In the vacuum state case, (6.12) is the general form (3.6) of the generator for an N-level system. The restriction to real symmetric $\{C_{ij}\}$ in the infinite temperature case implies that the central state $\rho^o = \mathbb{1}/N$ is a stationary state for the reduced dynamics. This state is in thermal equilibrium with the infinite temperature reservoir, and the structure of the resulting semigroup is very similar to the one obtained in the weak coupling limit. Indeed, if we set $H^S = -\ln \rho^o = (\ln N)\mathbb{1}$ in (5.12), in the limit of weak coupling to an infinite temperature reservoir we obtain just (6.12) with $\{C_{ij}\}$ real and symmetric. In particular, (6.12) satisfies the detailed balance condition to be discussed in Section 7.

We remark that the singular reservoir limit at infinite temperature is equivalent to adding to H^S a purely random stochastic Gaussian Hamiltonian [37,69].

The foregoing models of singular coupling can be extended to system whose underlying Hilbert space is infinite-dimensional. However, in this case one needs some technical conditions which restrict the class of dynamical semigroups with bounded generators which can be obtained in the limit $\varepsilon \to 0$ [34].

We have just received a paper by Palmer [63], in which the author points out the mathematical similarity of the weak coupling and singular coupling limits, **the distinction of the two limits depending on which of two possible time scales is regarded as natural.**

7.   DETAILED BALANCE.

In this and the following Section, which contain results from [9] and from a work of ours in preparation [52] , we

discuss a quantum condition of detailed balance for a Markovian reduced dynamics, and its relation with the assumed invariance of the global dynamics under an operation of time reversal (microreversibility).

Since quantum dynamical semigroups are the analogues of classical discrete Markov processes [47, 50], a detailed balance condition for a Markovian master equation suggests itself as a natural generalization of the corresponding definition in the classical case. The Chapman-Kolmogorov equation for a discrete Markov process on $1, \ldots, N$

$$(7.1) \qquad \frac{d}{dt} \vec{p}(t) = \mathcal{L} \vec{p}(t) , \qquad \mathcal{L}_{ik} = D_{ik} - \delta_{ik} \sum_m D_{mi}$$

satisfies __detailed balance__ with respect to a stationary state $\vec{p}^0 = \{p^0_i\}_{i=1,\ldots,N}$, $p^0_i > 0$, $\sum_i p^0_i = 1$, if

$$(7.2) \qquad D_{ij} p^0_j = D_{ji} p^0_i .$$

The algebra of observables is the set $\mathfrak{A}$ of sequences $\vec{f} = \{f_i\}_{i=1,\ldots,N}$ and the state $\vec{p}^0$ defines on $\mathfrak{A}$ an inner product as

$$(7.3) \qquad \langle \vec{f}, \vec{g} \rangle = \sum_i p^0_i \bar{f}_i g_i .$$

It is straightforward to check that (7.2) is equivalent to

$$(7.4) \qquad \langle \vec{f}, L\vec{g} \rangle = \langle L\vec{f}, \vec{g} \rangle \qquad \forall \vec{f}, \vec{g} \in \mathfrak{A}$$

where $L = \mathcal{L}^* = \mathcal{L}^T$ is the generator of the dual "Heisenberg" dynamics.

Consider a strongly continous dynamical semigroup $\{\Lambda_t | t \in \mathbb{R}_+\}$ of $\mathcal{T}(\mathfrak{H})$ with a densely defined generator $\mathcal{L}$, admitting a faithful stationary state ρ^0. We can define, in analogy to (7.3), an inner product in $\mathcal{B}(\mathfrak{H})$ as

$$(7.5) \qquad \langle A,B \rangle = \mathrm{Tr}\left[\rho^0 A^* B\right]$$

and denote by $\mathcal{L}^2(\mathfrak{H}, \rho^0)$ the (separable) Hilbert space which is the completion of $\mathcal{B}(\mathfrak{H})$ with respect to (7.5) The elements of $\mathcal{L}^2(\mathfrak{H}, \rho^0)$ are of the form $X = B(\rho^0)^{-1/2}$, B a Hilbert-Schmidt operator.

The Heisenberg semigroup $t \to \Lambda_t^*$ is not, in general, strongly continous on $\mathcal{B}(\mathfrak{H})$, but it can be extended to a strongly continous contraction semigroup on $\mathcal{L}^2(\mathfrak{H}, \rho^0)$. Indeed, using Kadison's inequality [48,20] and the invariance of ρ^0, we have

$$\langle \Lambda_t^* A, \Lambda_t^* A \rangle = \mathrm{Tr}\left[\rho^0 (\Lambda_t^* A)^* (\Lambda_t^* A)\right]$$
$$\leq \mathrm{Tr}\left[\rho^0 \Lambda_t^*(A^* A)\right] = \mathrm{Tr}\left[\rho^0 A^* A\right] = \langle A,A \rangle.$$

The functions $t \to \langle A, \Lambda_t^* B \rangle = \mathrm{Tr}\left[\Lambda_t(\rho^0 A^*)B\right]$, $A, B \in \mathcal{B}(\mathfrak{H})$, are continous. Therefore, since $\mathcal{B}(\mathfrak{H})$ is dense in $\mathcal{L}^2(\mathfrak{H}, \rho^0)$, $t \to \Lambda_t^*$ is weakly measurable on $\mathcal{L}^2(\mathfrak{H}, \rho^0)$, hence strongly measurable and strongly continous [84].

We denote by L the densely defined generator of the extension of $\{\Lambda_t^*\}$ to $\mathcal{L}^2(\mathfrak{H}, \rho^0)$. In general $\mathcal{D}(L) \cap \mathcal{B}(\mathfrak{H})$ is not dense in $\mathcal{B}(\mathfrak{H})$ unless $t \to \Lambda_t^*$ is strongly continous on $\mathcal{B}(\mathfrak{H})$.

It would not do to generalize Definition (7.4) by asking L to be selfadjoint with respect to the inner product (7.5) (ρ^0-selfadjoint), since this would rule out the case of Hamil-

tonian dynamics. Indeed, if H is a selfadjoint operator on $\mathfrak{H}$ commuting with ρ^0, then $L_H = i[H, \ ]$ is skewadjoint with respect to (7.5) (ρ^0-skewadjoint). Hence we propose the following

Definition [52]: A quantum dynamical semigroup satisfies the detailed balance condition with respect to a faithful stationary state ρ^0 if L can be written as a sum

$$(7.6) \qquad\qquad L = L_a + L_s$$

where

(i) $L_a = i[H, .]$, H selfadjoint, $[H, \rho^0] = 0$ (then L_a is ρ^0-skewadjoint and generates a group of unitaries on $\mathcal{L}^2(\mathfrak{H}, \rho^0)$);

(ii) L_s is ρ^0-selfadjoint

Since ρ^0 is a faithful normal state on $\mathfrak{B}(\mathfrak{H})$, the set of functionals $\{\varphi_X , X \in \mathcal{L}^2(\mathfrak{H}, \rho^0)\}$, where

$$\varphi_X(A) = \langle X, A \rangle = Tr\left[(\rho^0 X^*)A\right],$$

is dense in the space of normal functionals on $\mathfrak{B}(\mathfrak{H})$ [71]. Therefore $\mathcal{U}_t$ and Γ_t defined as

$$Tr\left[\mathcal{U}_t(\rho^0 X^*)A\right] = \langle X, \exp(L_a t)A \rangle,$$

$$Tr\left[\Gamma_t(\rho^0 X^*)A\right] = \langle X, \exp(L_s t)A \rangle$$

$$X \in \mathcal{L}^2(\mathfrak{H}, \rho^0), \ A \in \mathfrak{B}(\mathfrak{H})$$

can be extended to dynamical semigroups of $\mathcal{T}(\mathfrak{H})$ with generators $\mathcal{L}_a = -i[H, .]$ and $\mathcal{L}_s$ such that

$$\text{Tr}\left[\mathscr{L}_a(\rho^0 x^\times)\Lambda\right] = \langle -L_a X, \Lambda \rangle,$$

$$\text{Tr}\left[\mathscr{L}_s(\rho^0 x^\times)\Lambda\right] = \langle L_s X, \Lambda \rangle \qquad\qquad A \in \mathscr{B}(\mathfrak{H}), \quad X \in \mathscr{D}(L)$$

and

(7.7)
$$\mathscr{L} = \mathscr{L}_a + \mathscr{L}_s.$$

If a decomposition of the form (7.7) exists, it is clearly unique, and it coincides in the finite-dimensional case with the one given by formula (3.6) [52]. Therefore it can be assumed in general as a criterion for the decomposition of generators satisfying detailed balance into a Hamiltonian plus a dissipative part.

ρ^0 is $\mathcal{U}_t$- and Γ_t-invariant and it can be shown [46, 74, 52] that $\mathcal{U}_t^*$ and Γ_t^* commute separately with the modular automorphism group Σ_t defined by

$$\Sigma_t A = (\rho^0)^{it} A (\rho^0)^{-it} \qquad A \in \mathscr{B}(\mathfrak{H}).$$

This implies that $\mathfrak{T}(\mathfrak{H}) \cap \{\rho^0\}'$ is stable under $\{\Lambda_t\}$. In particular, when the spectrum of ρ^0 is nondegenerate, all elements of $\mathfrak{T}(\mathfrak{H}) \cap \{\rho^0\}'$ can be diagonalized simultaneously, and the restriction of $\{\Lambda_t\}$ to $\mathfrak{T}(\mathfrak{H}) \cap \{\rho^0\}'$ determines a classical Markov process satisfying the detailed balance condition (7.2).

We note in passing that the foregoing definitions and results can all be easily extended to weakly$^\times$-continous semigroups of completely positive identity preserving normal maps of a $W^\times$-algebra, admitting a faithful normal stationary state. However, we have restricted ourselves to $\mathscr{B}(\mathfrak{H})$, since we are primarily

interested in dynamical semigroups of a spatially confined system. Moreover, we shall require in the following $t \to \Gamma_t$ to be norm continous, in order to be able to use the form (3.4) of the generator.

With the restriction that the dissipative part $t \to \Gamma_t$ is norm continous, it is possible to give the general form of the generator L of a dynamical semigroup satisfying detailed balance. This is provided by the following

Theorem [52]: In order for $\{\Lambda_t\}$ to be a dynamical semigroup of $\mathcal{T}(\mathfrak{H})$ satisfying detailed balance with respect to a faithful stationary state ρ^0 and having a norm continous dissipative part, it is necessary and sufficient that its Heisenberg generator L can be written in the form (7.6) with

$$(7.8) \quad L_a A = i[H, A] \qquad \text{and}$$

$$(7.9) \quad L_s A = w^* - \lim_{M \to \infty} \sum_{rr'ss'=1}^{M} c_{rr'ss'} \left[P_{rr'} A P_{s's} - \frac{1}{2}\{P_{rr'} P_{s's}, A\} \right],$$

where

(7.10) H is selfadjoint and commutes with ρ^0;

(7.11) $P_{rs} = |r\rangle\langle s|$, where $\{|r\rangle\}$ is a c.o.n.s. of eigenvectors of ρ^0, namely $\rho^0|r\rangle = \rho_r^0|r\rangle$;

(7.12) $\{c_{rr'ss'}\}$ is positive in the sense that

$$\sum_{rr'ss'} \bar{a}_{rr'} c_{rr'ss'} a_{ss'} \geqslant 0 \quad \text{for all } \{a_{rr'}\};$$

(7.13) $c_{rr'ss'} \, \rho_s^0 = c_{s'sr'r} \, \rho_{s'}^0 \quad$ or, equivalently,

$$c_{rr'ss'} \, \rho_r^0 = c_{s'sr'r} \, \rho_{r'}^0.$$

If $\mathfrak{H}$ is N-dimensional, Alicki [9] has proved that L_s can be

given a simple diagonal form as follows

$$(7.14) \qquad L_S A = \sum_{i,j=1}^{N} D_{ij} \left\{ X_{ij}^* [A, X_{ij}] + [X_{ij}^*, A] X_{ij} \right\},$$

where

$$(7.15) \qquad \text{Tr}[X_{ij}^* X_{k\ell}] = \delta_{ik} \delta_{j\ell} ;$$

$$(7.16) \qquad \rho^0 X_{ij} \rho^{0-1} = \rho_i^0 \rho_j^{0-1} X_{ij} ;$$

$$(7.17) \qquad X_{ij} = X_{ij} \ \text{for} \ \rho_i^0 = \rho_j^0 ; \quad X_{ij}^* = X_{ji} \ \text{for} \ \rho_i^0 \neq \rho_j^0 ;$$

$$(7.18) \qquad D_{ij} \geqslant 0 \ \text{for all} \ i,j; \quad D_{ij} \rho_j^0 = D_{ji} \rho_i^0 \ \text{for} \ \rho_i^0 \neq \rho_j^0 .$$

The profound meaning of the foregoing condition of detailed balance lies in the fact that it is satisfied with $\rho^0 = \rho_\beta$ by all dynamical semigroups obtained in the weak coupling limit for a system coupled to a reservoir in a KMS state at inverse temperature β , and that this is, in a sense, characteristic of this situation. Indeed, if the reference state of the reservoir is KMS at inverse temperature β , it is immediately seen by virtue of the KMS condition (5.15) that the dissipative part of (5.14) is of the form (7.9), (7.11)-(7.13), with $\rho^0 = \rho_\beta$. On the other hand, let a given reservoir R be in a reference state ω^R and let S be a spatially confined system with free Hamiltonian H^S interacting with R by a coupling $H^{SR} = \sum_\alpha V_\alpha^S \otimes V_\alpha^R$ and assume that

i) for all choices of S, H^S and H^{SR} for which Davies' conditions (5.5)-(5.7) are satisfied, there exists a faithful stationary state ρ^0, depending a priori on H^S and H^{SR} and

commuting with H^S, with respect to which the reduced dynamics of S in the weak coupling limit satisfies detailed balance;

ii) $\mathcal{U}^R$ is the closure of the vector span of the union of the identity $\mathbb{1}^R$ with the operators V_α^R for which (5.5)-(5.7) are satisfied.

Then there exists a $\beta > 0$ for which (5.15) holds. Hence ω^R is KMS for such β and $\rho^o = \exp(-\beta H^S)/Tr(\exp(-\beta H^S))$ [52].

In the case of an N-level system, it is also possible to write all matrices $\{c_{rr'ss'}\}$ satisfying the conditions (7.12)-(7.13) in the form $c_{rr'ss'} = \sum_{\alpha\beta} \hat{h}_{\alpha\beta} (\varepsilon_r - \varepsilon_{r'})(V_\beta)_{rr'}(V_\alpha)_{s's}$; for example, this can be done by applying the weak coupling limit to a fermion model like the one in Section 6 [52].

Finally, we remark that the semigroups satisfying detailed balance with respect to the central state are precisely those whose generator admits a diagonal expression in terms of selfadjoint operators. Such semigroups are exactly the ones which can be obtained by a singular coupling to a reservoir at infinite temperature.

8.   MICROREVERSIBILITY.

Recently, some interest has been devoted to the study of the conditions implied by time reversal invariance on the reduced dynamics of an open quantum system in the Markovian approximation and of their relations to detailed balance [6, 7,18]. In this Section, we derive a condition on the generator of a dynamical semigroup which follows from the invariance

under time reversal of the global dynamics $\mathcal{U}_t$ of S+R and
which holds in the weak coupling as well in the singular coup-
ling limit. This condition has a clear interpretation in terms
of microreversibility, but it does not depend on and makes no
reference to any particular stationary state, and therefore
it bears no relation in general to detailed balance. On the
other hand, the condition introduced by Agarwal in Ref. 6
(for later developments and applications, see [7,18]) is for-
mulated in terms of a time reversal invariant stationary state
ρ^o (assumed to exist) of the reduced dynamics of S and cons-
titutes actually a form of detailed balance.

We show that in the weak coupling limit Agarwal's condition
is a consequence of microreversibility if the reference
state ω^R of the reservoir is invariant under time reversal
and if $\rho^o \otimes \omega^R$ is stationary under the global dynamics in
the limit $\lambda \to 0$. This can be ensured if $\rho^o \otimes \omega^R$ has a
stability property which seems to be characteristic of KMS
states. However, in this case detailed balance is already im-
plied by weak coupling indipendently of time reversal invar-
iance. Similar conclusions have been drawn by Hepp [44] in
connection with the derivation of the Onsager relations.

We define a time reversal operation $\mathcal{C}$ on S+R as the tensor
product of the corresponding operations on S and R

$$\mathcal{C} (A^S \otimes A^R) = \mathcal{C}^S A^S \otimes \mathcal{C}^R A^R = \widetilde{A^S \otimes A^R}$$

where

$$\mathcal{C}^S A^S = T^S A^{S*} T^{S*} = \widetilde{A^S}, \quad \text{with} \quad T^S \text{ an antilinear}$$
unitary operator on $\mathcal{H}^S$;

$\mathcal{C}^R_A{}^R = \widetilde{A^R}$ with $\mathcal{C}^R$ a linear-antiautomorphism of $\mathfrak{A}^R$.

We request further that $(T^S)^2 = \mathbb{1}$.

We assume that the global and respectively the free evolution $\mathcal{U}_t$ and $\mathcal{U}^0_t$, as well as the reference state ω^R of the reservoir, are $\mathcal{C}$-invariant, namely

a) there exists a c.o.n.s. $\{|n\rangle\}$ in $\mathfrak{H}^S$ with
$T^S|n\rangle = |n\rangle$ and $H^S|n\rangle = \varepsilon_n|n\rangle \ \forall n$;

b) $\mathcal{U}^{R*}_t \mathcal{C}^R(A) = \mathcal{C}^R \mathcal{U}^{R*}_{-t}(A) \ \forall A \in \mathfrak{A}^R$, where $\mathcal{U}^R_t = \exp[-i\mathcal{H}^R t]$;

c) $H^{SR} = \widetilde{H^{SR}}$;

d) $\omega^R \cdot \mathcal{C}^R = \omega^R$.

Write the form (5.14) of the generator of a (Heisenberg) dynamical semigroup in the weak coupling limit as

$$\text{(8.1)} \quad LA = i\left[\sum_{\varepsilon_i = \varepsilon_k} B_{ik}P_{ik}, A\right] + \sum_{\varepsilon_i - \varepsilon_j = \varepsilon_k - \varepsilon_\ell} C_{ijk\ell}(P_{ij}AP_{\ell k} - \tfrac{1}{2}\{P_{ij}P_{\ell k}, A\})$$

where

$$\text{(8.2)} \quad B_{ik} = \sum_j \sum_{\alpha\beta} s_{\alpha\beta}(\varepsilon_i - \varepsilon_j)(V_\beta)_{ij}(V_\alpha)_{jk},$$

$$\text{(8.3)} \quad C_{ijk\ell} = \sum_{\alpha\beta} \hat{h}_{\alpha\beta}(\varepsilon_i - \varepsilon_j)(V_\beta)_{ij}(V_\alpha)_{\ell k}.$$

Noting that

$$\text{(8.4)} \quad C_{ijk\ell} = \int_{-\infty}^{+\infty} dt \cdot \text{Tr}^{S+R}\left[(P_{ki} \otimes \omega^R)H^{SR}(P_{j\ell} \otimes \mathbb{1}^R)H^{SR}(t)\right]$$

and using the time reversal invariance of the trace and the

assumption c), we have

$$(8.5) \quad c_{ijk\ell} = \int_{-\infty}^{+\infty} dt \ \mathrm{Tr}^{S+R}\left[\mathcal{C}((P_{ki} \otimes \omega^R) H^{SR}(P_{j\ell} \otimes \mathbb{1}^R) H^{SR}(t))\right]$$

$$= \int_{-\infty}^{+\infty} dt \ \mathrm{Tr}^{S+R}\left[\bar{H}^{SR}(-t)(P_{\ell j} \otimes \mathbb{1}^R) H^{SR}(P_{ik} \otimes \omega^R)\right] = c_{k\ell i j} \ .$$

Similarly, using (5.13), we find

$$(8.6) \quad B_{ik} = B_{ki} \ .$$

For the singular reservoir limit, the Heisenberg generator (6.12) can be given a form similar to (8.1)

$$(8.7) \quad LA = i \sum_{ik}\left[B_{ik}P_{ik}, A\right] + \sum_{ijk\ell} c_{ijk\ell}\left[P_{ij}AP_{\ell k} - \frac{1}{2}\{P_{ij}P_{\ell k}, A\}\right]$$

where

$$(8.8) \quad B_{ik} = \varepsilon_i \ \delta_{ik} \ ,$$

$$(8.9) \quad c_{ijk\ell} = \sum_{\alpha\beta} c_{\alpha\beta}(V_\beta)_{ij}(V_\alpha)_{\ell k} \ .$$

(8.4) and (8.5) still hold true, once the singular coupling limit is taken, and (8.6) is trivially satisfied. Then, in both cases, if we define the time reversed generator

$$(8.10) \quad \tilde{L} = \mathcal{C}^S L \mathcal{C}^S,$$

(8.5) and (8.6) can be equivalently written as

$$(8.11) \quad \tilde{L} = -L_H + L_D$$

where

(8.12)
$$L = L_H + L_D$$

is respectively decomposition (8.1) or (8.7). Hence, as expected, time reversal invariance tells us that the time reversed generator identifies with the generator of the reduced dynamics for negative times.

If a dynamics satisfying (8.11) admits a stationary state ρ^o which is $\mathcal{C}^S$-invariant [1], we can rewrite the condition

(8.13)
$$\langle e^{L\tau} A, B \rangle = \langle e^{L\tau} \tilde{B}, \tilde{A}^* \rangle$$

of Ref. 6 as

(8.13')
$$\langle LA, B \rangle = \langle A, \tilde{L}B \rangle$$

where the inner product is defined by (7.5). It is then easy to see that (8.11) implies the equivalence of (8.13') to detailed balance (7.6), with $L_a = L_H$ and $L_s = L_D$.

However, if one tries to derive (8.13) in the weak coupling limit from microreversibility, a further condition is needed which seems to be already an independent statement of detailed balance. To see this, note first that ρ^o can be chosen to be invariant under the free dynamics of S. Then, if we rewrite (8.13) as

(8.13")
$$\langle e^{L\tau} A, B \rangle = \langle A, e^{\tilde{L}\tau} B \rangle$$

we observe that it is equivalent to

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1) Note that this is by no means the case in general, as can be shown by explicit counterexamples.

(8.14) $\quad \lim\limits_{\lambda \to 0} \left| \langle \mathcal{U}^{S*}_{\tau/\lambda^2} e^{L\tau} A, B \rangle - \langle A, \mathcal{U}^{S*}_{-\tau/\lambda^2} e^{\tilde{L}\tau} B \rangle \right| = 0$

since the spectrum of $\mathcal{U}^{S*}_t$ is purely discrete and since $\left[\mathcal{U}^S_t, L\right] = 0$. Moreover, by thms. 1.2 and 1.4 of Ref. 26, we have

(8.15) $\quad \lim\limits_{\lambda \to 0} \left| \langle \mathcal{U}^{S*}_{\tau/\lambda^2} e^{L\tau} A, B \rangle - \mathrm{Tr}^{S+R}\left\{ (\rho^0 \otimes \omega^R)\left[\mathcal{U}^{(\lambda)*}_{\tau/\lambda^2}(A^* \otimes \mathbb{1}^R)\right](B \otimes \mathbb{1}^R) \right\} \right| = 0$

and similarly, using time reversal invariance,

(8.16) $\quad \lim\limits_{\lambda \to 0} \left| \langle A, \tilde{\mathcal{U}}^{S*}_{-\tau/\lambda^2} e^{\tilde{L}\tau} B \rangle - \mathrm{Tr}^{S+R}\left\{ (\rho^0 \otimes \omega^R)(A^* \otimes \mathbb{1}^R)\left[\mathcal{U}^{(\lambda)*}_{-\tau/\lambda^2}(B \otimes \mathbb{1}^R)\right] \right\} \right| = 0.$

By (8.15) and (8.16), (8.14) is equivalent to

(8.17) $\quad \lim\limits_{\lambda \to 0} \left| \mathrm{Tr}^{S+R}\left\{ (\rho^0 \otimes \omega^R)\left[\mathcal{U}^{(\lambda)*}_{\tau/\lambda^2}(A^* \otimes \mathbb{1}^R)\right](B \otimes \mathbb{1}^R) \right\} \right.$

$\qquad\qquad \left. - \mathrm{Tr}^{S+R}\left\{ (\rho^0 \otimes \omega^R)(A^* \otimes \mathbb{1}^R)\left[\mathcal{U}^{(\lambda)*}_{-\tau/\lambda^2}(B \otimes \mathbb{1}^R)\right] \right\} \right| = 0$

which is satisfied if $\rho^0 \otimes \omega^R$ is invariant under $\mathcal{U}^{(\lambda)}_t$ in the limit $\lambda \to 0$.[2] This can be ensured if for each $\lambda > 0$ there exists a state ψ_λ which is stationary for $\mathcal{U}^{(\lambda)}_t$ and approaches $\rho^0 \otimes \omega^R$ uniformly as $\lambda \to 0$. Such a stability property is possessed by KMS states [10,72] and seems to be characteristic thereof [40], and we know from the previous Section that the KMS condition already implies detailed balance, regardless of any property of invariance under time reversal.

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2) Even though it is not entirely clear from the context of their paper, it seems that this fact was also recognized by Carmichael and Walls in Ref. 18.

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