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On the existence of quantum subdynamics

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Abstract. It is shown, using only elementary operator algebra, that an open quantum system coupled to its environment will have a subdynamics (reduced dynamics) as an exact consequence of the reversible dynamics of the composite system only when the states of system and environment are uncorrelated. Furthermore, it is proved that for a finite temperature the KMS condition for the lowest-order correlation function cannot be reproduced by any type of linear subdynamics except the reversible Hamiltonian one of a closed system. The first statement can be seen as a particular case of a more general theorem of Takesaki on the properties of conditional expectations in von Neumann algebras. The concept of subdynamics used here allows for memory effects, no assumption is made of a Markov property. For dynamical systems based on commutative algebras of observables the subdynamics always exists as a stochastic process in the random variable defining the open subsystem.

1. Introduction

The problem considered here is how the dynamics of a small quantum system interacting with its environment (the heat bath or reservoir) can be given a reduced description involving only the degrees of freedom of the small system. It is assumed that the closed system (composed of the observed small system and the reservoir) has a reversible, deterministic Hamiltonian dynamics, while the evolution of the small system is expected to have irreversible and random properties. Various names, like *subdynamics* or *reduced dynamics*, are in use for this concept. Often they are understood to mean that the dynamics is governed by a master equation containing parameters describing the reservoir, but acting only on the dynamical variables of the small system.

Here a more general concept of subdynamics is used which allows for memory effects. The mathematical construction is inspired by the classical theory of stochastic processes. It is based on the physical assumption that the experimentally accessible correlation functions for the small subsystem can be expressed as averages over its initial partial state. The standard models used in this field, like those defined by master equations, are all of this type, but they often have additional simplifying features, e.g. a Markov property, which will not be assumed here.

In the commutative case there is *always* a subdynamics in the sense used here. This is due to the properties of marginal distributions (partial states) and conditional expectations in commutative probability. The subdynamics is a stochastic process for the random variables defining the small subsystem, and the correlation functions can be written as expectations involving only these variables. The precise form of the expectations will, of course, depend on the properties of the reservoir. This classical framework is sketched in section 2 in order to put the basic ideas into a form suited to the physical picture.

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The basic result shown in section 3 is that, when the probability measures are replaced by quantum density operators and the measurable functions by quantum observables, an analogous construction is possible only in rather trivial cases. When the algebra of observables for the open system is $B(\mathcal{K})$ (all bounded operators in a Hilbert space $\mathcal{K}$) the conditional expectation we need will exist precisely when the initial state of the composite system is a tensor product of the partial states. This product form must then be preserved by the evolution in order that a properly defined subdynamics shall exist for any choice of initial time.

This result can also be derived from a theorem of Takesaki which restricts the existence of conditional expectations for non-commutative operator algebras which leave invariant a faithful normal state [1]. Takesaki's theorem causes long-known difficulties in extending the concept of a stochastic process to a non-commutative setting [2–5], and one can see the problem considered here as a particular instance. Takesaki's theorem, which also applies to strictly infinite systems, is based on the theory of von Neumann algebras and modular Hilbert algebras and demands a formidable mathematical apparatus. However, the main idea behind it is elementary, and here we will use only the basics of operator algebras which are sufficient to deal with finite systems. In the appendix a simplified version of Takesaki's theorem is sketched.

If a subdynamics exists it does (by definition) reproduce the correlation functions of all orders. In section 4 we ask if there can exist a subdynamics satisfying the less restrictive condition of reproducing only the lowest-order correlation function for all values of the time parameter. If we assume the KMS condition for the time dependence of this function, we find that the answer is negative unless either the small system is closed or the temperature is infinite.

In section 5 there are references to some earlier work on similar problems. It is argued that the subdynamics picture can only be expected to hold as an approximation with restrictions on the time scales involved. There is a brief discussion on possible consequences in applications to physical relaxation processes.

2. The commutative case

We will first outline how the subdynamics is introduced in the classical (commutative) case. This is a well known part of the theory of stochastic processes, but the standard formalism does not relate to the physical picture of open systems. Here this scheme will be reformulated to make it similar to that used in the quantum physics context. In order to keep this as short as possible the standard measure theory disclaimer 'for almost all. . . ' will be skipped.

The observed open system is here called $\mathcal{S}_1$ and the reservoir $\mathcal{S}_2$. The composite system $\mathcal{S} = \mathcal{S}_1 + \mathcal{S}_2$ is described by a direct product phase space $\Omega = \Omega_1 \times \Omega_2$, and a direct product algebra of observables $\mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2$ which are measurable functions on the phase space (with respect to a given reference measure). The intrinsic and reversible dynamics of the composite system is represented by maps

$$T : \omega = (\omega_1, \omega_2) \mapsto T(\omega) = (\omega_1', \omega_2').$$

The states on the composite system are probability measures on Ω which we write as

$$\mu = \int_\Omega \mathrm{d}\mu(\omega)\delta_\omega.$$

Let a fixed reference measure μ be given as an initial state which defines the observable probability distributions. It is not necessarily stationary under the dynamics, but we must assume that the total probability is preserved

$$\int_\Omega \mathrm{d}\mu(T(\omega)) = \int_\Omega \mathrm{d}\mu(\omega) = 1.$$

The partial states for the two subsystems are the marginal distributions μ_1, μ_2 obtained by partial integration. Then there is for each $\omega_1 \in \Omega_1$, which is in the support of μ_1, a conditional probability measure on Ω_2, called $\mu_2(\cdot|\omega_1)$, defined in such a way that the state μ on the composite system is recovered by partial integration

$$\int_\Omega \mathrm{d}\mu(\omega) f(\omega) = \int_{\Omega_1} \mathrm{d}\mu_1(\omega_1) \int_{\Omega_2} \mathrm{d}\mu_2(\omega_2|\omega_1) f(\omega_1, \omega_2).$$

For every state ρ of the system $\mathcal{S}_1$, the support of which is contained in that of μ_1, we can define a state of the composite system

$$J(\rho) = \int_\Omega \mathrm{d}\rho(\omega_1)\, \mathrm{d}\mu_2(\omega_2|\omega_1)\delta_\omega. \tag{2.1}$$

Clearly the map J is uniquely defined by a faithful state μ and it holds that $J(\mu_1) = \mu$. For any state ρ of $\mathcal{S}_1$, the state $\mu' = J(\rho)$ defines a map J' which is equal to J or a restriction of it. When the state μ is not stationary then the map J will also be time dependent, but this will not appear explicitly in the notation.

It is convenient to introduce a notation (R) for the map which is the partial integration over Ω_2. The relations above can then be written in the following form, where $\circ$ denotes the composition of maps:

$$R \circ J = I := \text{the identity map} \tag{2.2}$$

$$J \circ R(\mu) = \mu \qquad \text{if } J \text{ is defined by } \mu. \tag{2.3}$$

The symbol $\mathbb{1}_2$ denotes the function which is equal to 1 everywhere on Ω_2, and we can then identify $\mathcal{A}_1 \otimes \mathbb{1}_2$ with $\mathcal{A}_1$ as a subalgebra of $\mathcal{A}$. For any $Y \in \mathcal{A}_1$ the partial integration map clearly satisfies $R((Y \otimes \mathbb{1}_2)\mu) = YR(\mu)$ and (2.1) gives the corresponding relation for J:

$$(Y \otimes \mathbb{1}_2)J(\rho) = J(Y\rho). \tag{2.4}$$

We also introduce a positive map $K : \mathcal{A} \to \mathcal{A}_1$ which is uniquely defined by the following relation for all states ρ of $\mathcal{S}_1$ and all $X \in \mathcal{A}$:

$$J(\rho)[X] = J(\rho)[K(X)] = \rho[K(X)]. \tag{2.5}$$

This relation restricted to $\mathcal{A}_1$ and (2.2) says that

$$K(Y \otimes \mathbb{1}_2) = Y \otimes \mathbb{1}_2 \tag{2.6}$$

for all $Y \in \mathcal{A}_1$, which implies that $K \circ K = K$. From (2.4) we find that for all $Y \in \mathcal{A}_1$, $X \in \mathcal{A}$

$$K[(Y \otimes \mathbb{1}_2)X] = (Y \otimes \mathbb{1}_2)K(X). \tag{2.7}$$

The relations (2.6) and (2.7) mean, by definition, that K is a *conditional expectation* [1].

The dynamical maps are defined on the states of the composite system as follows,

$$T^*(\mu) = \int_\Omega \mathrm{d}\mu(\omega)\delta_{T(\omega)}$$

and we can define reduced dynamical maps on the states of $\mathcal{S}_1$ as follows:

$$T_1^*(\rho) = R \circ T^* \circ J(\rho). \tag{2.8}$$

The maps T^* on the space of states are related to the corresponding dynamical maps T on the observables through the standard duality

$$T^*(\mu)[X] = \mu[T(X)].$$

The definition (2.8) is then equivalent to the relation

$$K \circ T(Y) = T_1(Y) \otimes \mathbb{1}_2 \tag{2.9}$$

for all $Y \in \mathcal{A}_1$, and together with (2.5) and (2.7) it implies that the lowest-order correlation function satisfies

$$\mu[X^\dagger T(Y^\dagger Y)X] = \mu_1[X^\dagger T_1(Y^\dagger Y)X] \tag{2.10}$$

for all $X, Y \in \mathcal{A}_1$. Thus this expectation value is reduced to an expression involving only the initial state and observables of the subsystem $\mathcal{S}_1$.

The multitime correlation functions are defined by combining the actions of observables in $\mathcal{A}_1$ with the dynamics. The observable $Y \in \mathcal{A}_1$ in (2.10) is replaced by a product of time translates of elements in $\mathcal{A}_1$

$$Y = T^n(X_n) \cdot T^{n-1}(X_{n-1}) \cdots T(X_1)$$

which is not, of course, itself in $\mathcal{A}_1$ in general. However, there is a unique positive operator $T_1(Y^\dagger Y) \in \mathcal{A}_1$ defined by (2.9) and satisfying (2.10). The map J (or K) then defines a *subdynamics*, by which we mean precisely that all the correlation functions can be expressed as expectations defined by the initial partial state of $\mathcal{S}_1$ as in equation (2.10). A stochastic process is defined by the set of all correlation functions (the Kolmogorov construction), so we can identify it with the subdynamics. If μ is stationary, then J is independent of time, and the subdynamics on $\mathcal{S}_1$ will be a stationary stochastic process.

What conditions will J have to satisfy in order that the process shall be Markovian? A sufficient condition is the following stronger version of (2.8):

$$J \circ T_1^* = T^* \circ J. \tag{2.11}$$

Then all probability distributions for sequences of observations of the subsystem $\mathcal{S}_1$ can be constructed using only the state μ_1, the map T_1 and the maps E defining the observations. Here each map E consists of a multiplication by a positive element in $\mathcal{A}_1$ and it is clear from (2.7) that all such maps commute with K (their duals commute with J). The proof then follows by the following induction argument. Consider the correlation function (probability for a sequence of n observations with given outcomes)

$$\mu[E_1 \circ T \circ E_2 \cdots \circ T \circ E_n(I)].$$

Rewrite this as

$$T^* \circ J \circ E_1^*(\mu_1)[E_2 \circ T \cdots \circ T \circ E_n(I)]$$

and use (2.11) to obtain that this expression equals

$$\begin{aligned} J \circ T_1^* \circ E_1^*(\mu_1)[E_2 \circ T \circ E_3 \circ \cdots \circ T \circ E_n(I)] \\ = T^* \circ J \circ E_2^* \circ T_1^* \circ E_1^*(\mu_1)[E_3 \circ \cdots \circ T \circ E_n(I)] \end{aligned}$$

and finally, by iteration, this is equal to

$$\mu_1[E_1 \circ T_1 \circ E_2 \cdots \circ T_1 \circ E_n(I)] \tag{2.12}$$

which is the form of the probability for the Markov chain generated by the stochastic operator T_1. If the system is irreducible, in the sense that is uniquely defined by the observations on the subsystem, then (2.11) is also a necessary condition on J.

To sum up, we find from the construction above that a subdynamics always exists in the commutative case, it is an exact consequence of the dynamics of the composite system and it is non-trivial if this dynamics does not leave the subsystem $\mathcal{S}_1$ invariant. Furthermore, it is stationary if it is constructed from a stationary state of the composite system, but the Markov property is satisfied only under very restrictive conditions.

3. The quantum case

The picture given in the previous section can be extended to the quantum case in a straightforward manner. The resulting quantum subdynamics has the structure introduced earlier as *quantum stochastic processes* in [6, 7], but we will not need the details given there. It is shown below that such a subdynamics will exist as an exact consequence of the dynamics of the composite system only when the correlations in the state of the composite system vanish.

For quantum mechanical systems we use a Hilbert space $\mathcal{K} = \mathcal{K}_1 \otimes \mathcal{K}_2$ for the composite system and an algebra of observables

$$\mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2$$

where we let the small system be fully quantum mechanical

$$\mathcal{A}_1 = B(\mathcal{K}_1)$$

while the algebra $\mathcal{A}_2$ can be arbitrary, possibly commutative. We let $\mathbb{1}$ denote the unit operator and consider only (normal) states which are defined by density operators. It is no real restriction to consider only finite-dimensional spaces as the simple operator algebra methods used are those relevant for finite systems. Note that the restriction map R of a state to $\mathcal{A}_1$

$$R(\rho)[X] = \rho[X \otimes \mathbb{1}_2]$$

is a partial trace on the density operators, which is a completely positive (CP) map. For the definitions and mathematical properties of CP maps see, for example, Paulsen [8], for the physical relevance see Kraus [9, 10] or Lindblad [11].

Assume that there is a projection $K : \mathcal{A} \to \mathcal{A}_1 \otimes \mathbb{1}_2$ satisfying (2.7), now in the non-commutative version where Y acts either on the right or on the left. Such conditional expectation maps always exist in finite dimensions and they are necessarily CP [1, 12]. Let J be defined by (2.5), which means that it will satisfy (2.2), and that it is a CP map. Now assume, in addition, that there is a faithful state μ satisfying (2.23).

The statement to be proved is that under these assumptions J must be of the form

$$J(\rho) = \rho \otimes \mu_2 \tag{3.1}$$

for all states ρ of $\mathcal{S}_1$; hence the state μ satisfying $J \circ R(\mu) = \mu$ is of product form $\mu = \mu_1 \otimes \mu_2$. The proof is quite straightforward. From (2.7) follows directly that

$$K(X \otimes Y) = (X \otimes \mathbb{1}_2) \cdot K(\mathbb{1}_1 \otimes Y) = K(\mathbb{1}_1 \otimes Y) \cdot (X \otimes \mathbb{1}_2).$$

As this holds for all $X \in \mathcal{A}_1$, it is clear that $K(\mathbb{1}_1 \otimes Y) \in \mathcal{A}_1$ commutes with all operators in $\mathcal{A}_1$, hence in the quantum case this operator must be a multiple of the unit operator, and consequently

$$K(\mathbb{1}_1 \otimes Y) = \mu_2(Y)\mathbb{1}$$

which means that J is of the form (3.1).

As we have already noted in the introduction, this statement is a simple version of a celebrated result by Takesaki about the lack of non-trivial conditional expectations in non-commutative operator algebras [1]. A translation of his statement to the present much simplified set-up will now be given in order to show the relation with the argument above.

Given a faithful state μ on the tensor product Hilbert space, consider the linear maps $K : \mathcal{A} \to \mathcal{A}_1$ which satisfy, for all $X, Z \in \mathcal{A}_1$, $Y \in \mathcal{A}$,

$$\mu[XYZ] = \mu[XK(Y)Z] = \mu_1[XK(Y)Z]. \tag{3.2}$$

If such a map exists it satisfies (2.6) and (2.7), i.e. it is a conditional expectation, and $\mu \circ K = \mu$. It is clear that the map will be uniquely defined by μ, if it exists at all. Furthermore, it must be completely positive due to the positive definiteness relation satisfied by the correlation functions; for instance, for all sequences $\{X_j \in \mathcal{A}_1, Y_j \in \mathcal{A}\}$

$$\sum_{j,k} \mu_1[X_j^\dagger K(Y_j^\dagger Y_k)X_k] \geqslant 0. \tag{3.3}$$

This follows from the corresponding relation for the first element in (3.2). The theorem of Takesaki then says that the map K exists precisely when $\mathcal{A}_1$ is left invariant by the group of unitaries (the modular automorphism group) generated by the self-adjoint operator $A = \ln \mu$,

$$\exp(\mathrm{i}tA)\mathcal{A}_1 \exp(-\mathrm{i}tA) = \mathcal{A}_1$$

which is equivalent to $[A, X] \in \mathcal{A}_1$ for all $X \in \mathcal{A}_1$. When $\mathcal{A}_1 = B(\mathcal{K}_1)$, it is clear that A is determined only up to an arbitrary self-adjoint element in $\mathcal{A}_2$. Furthermore, every group of automorphisms of $\mathcal{A}_1$ is implemented by a group of unitary maps in $\mathcal{K}_1$, and this is generated by a self-adjoint operator in $\mathcal{A}_1$. Consequently, the most general solution for A is of the form $A = A_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes A_2$, which means that the state μ is of tensor product form.

Up until now the construction of the subdynamics is based on a particular choice of reference state μ of product form. When this state is not stationary under the dynamics of the composite system there is also a choice of a preferred initial time for the correlation functions. If we demand that the construction of a subdynamics shall be possible for all initial times, then it is clear that the time translates of μ must also be of product form:

$$T^*(\mu_1 \otimes \mu_2) = \mu_1' \otimes \mu_2'.$$

Whether the state is stationary or not, the dynamics which can satisfy this condition is severely restricted. The invariance of the spectrum of the density operators under the reversible dynamics means that the transformation can act only in the degeneracy subspaces of the product state. There are two extreme cases. First, the non-interacting case where T is a product of transformations acting on the factor spaces. Secondly, the fully degenerate case where the quantum state μ is a trace and is invariant under all unitaries. This case can be interpreted as a model involving a heat bath of infinite temperature. There are also intermediate situations, but they are really as non-generic as the rest. The general conclusion is that there are few situations in which there can be a subdynamics as an exact consequence of the reversible dynamics of the composite quantum system. Defining a subdynamics nearly always involves an approximation scheme which neglects the correlations between observed system and reservoir.

It is clear that (3.2) is consistent with (2.10) and (2.9), but it is possible that there is a map $T_1 : \mathcal{A}_1 \to \mathcal{A}_1$ which satisfies (2.10) even when there is no map E satisfying (3.2). This possibility will be considered in the next section. What we can say is that if T_1 exists as a linear map (by which we mean that it is defined on the whole of $\mathcal{A}_1$), then the positive definiteness of the correlation functions (3.3) does imply that it must be CP. It is impossible to have for quantum systems a situation such as (2.10) defined by maps which are linear but not CP.

Note that in papers such as [11, 13], where the CP property of the dynamical maps is a crucial element, it is assumed as a mathematical starting point that there exists a (Markovian) dissipative dynamics defined by linear maps on the full state space of the small system. It is certainly always possible to construct a reservoir and a dynamics of the composite system which will realize this process as a subdynamics, but such a construction need not have all the physical properties we could ask for [14]. Similarly, in [6, 7] where a general non-Markovian subdynamics constructed from CP maps was introduced, the existence of such maps was part of the definition.

4. The KMS condition and subdynamics

The correlation functions (with a continuous time parameter) of quantum systems in thermal equilibrium satisfy the KMS condition (4.3). If this condition is satisfied for all operators in the composite system it implies the characteristic stability properties of canonical equilibrium states (see Bratteli and Robinson [15], ch 5.4). It will be shown that it is not possible to choose a subdynamics on the observables of $\mathcal{S}_1$ in such a way that the lowest-order correlation function satisfies the KMS condition, excepting two cases: when the dynamics on $\mathcal{S}_1$ is conservative (that of a closed system) and when the 'inverse temperature' $\beta = \hbar/k\Theta$ is zero.

Consider the correlation functions of the form (2.10), with the time parameter included:

$$R(X, Y; t) = \mu[X^\dagger T_t(Y)] = \mu_1[X^\dagger T_{1,t}(Y)]. \tag{4.1}$$

Here we assume that $X, Y \in \mathcal{A}_1$ as before, and that $T_{1,t}$ exists as a linear map on $\mathcal{A}_1$ defined for $t \geqslant 0$. We extend the relation to negative values of t through

$$R(X, Y; -t) = R(Y, X; t)^*.$$

This is actually a part of the following positive definite property of the correlation function: for all $X_k \in \mathcal{A}_1$ and complex λ_k

$$\sum_{k,l} \lambda_k^* R(X_k, X_l; t_k - t_l)\lambda_l \geqslant 0 \tag{4.2}$$

which is a straightforward generalization of (3.3), again coming from the correlation functions of the closed composite system.

The KMS condition reads ([15], ch 5.3): the correlation function has an analytic continuation in the time parameter into the strip $0 \leqslant \operatorname{Im} z \leqslant \beta$ such that for all real t

$$R(X, Y; t) = R(Y^\dagger, X^\dagger; -t + \mathrm{i}\beta). \tag{4.3}$$

Note that in the form it is used in [15] the arguments $X, Y \in \mathcal{A}$, but here it is essential that they are restricted to $\mathcal{A}_1$. The conclusions we can draw are inevitably weaker.

We now use some ideas and facts from the theory of modular Hilbert algebras ([15], ch 2.5). As long as it is enough to consider algebras $\mathcal{A}_1 = B(\mathcal{K}_1)$ in finite-dimensional Hilbert spaces the derivations are quite elementary. If the assumption on the existence of $T_{1,t}$ is correct and μ is a faithful state, then the correlation function can be represented in the Hilbert space $\mathcal{L} = \mathcal{H}_1 \otimes \mathcal{H}_1$ in the following way. There is a vector Ω in $\mathcal{L}$ such that for all $X \in \mathcal{A}_1$

$$\langle \Omega | X \otimes \mathbb{1} | \Omega \rangle = \mu_1(X).$$

Furthermore, the vector is cyclic and separating for $\mathcal{A}_1$, which means that every vector $\psi \in \mathcal{L}$ can be written in the form $\psi = (X \otimes \mathbb{1}|\Omega\rangle$ for a unique element $X \in \mathcal{A}_1$. The choice of Ω is not unique, but if the density operator is

$$\mu_1 = \sum_k \mu_k |k\rangle\langle k|$$

for some complete orthonormal set $\{|k\rangle\}$ and strictly positive eigenvalues $\{\mu_k\}$, one choice is

$$|\Omega\rangle = \sum_k \sqrt{\mu_k}|k\rangle \otimes |k\rangle$$

and it is then easy to check the correctness of the statements above. Other choices are unitarily equivalent. We also find the relation

$$(X \otimes \mathbb{1})|\Omega\rangle = [\mathbb{1} \otimes (\mu_1^{-1/2} X \mu_1^{1/2})^{\mathrm{T}}]|\Omega\rangle \tag{4.4}$$

where T stands for matrix transpose in the orthonormal basis defining Ω.

From the sesquilinear structure of the correlation function (4.1), it follows that there is a unique one-parameter family $V(s)$ of linear maps in $\mathcal{L}$ such that $V(0) = 1$ and

$$R(X, Y; t) = \langle\Omega|X^\dagger V(t) Y|\Omega\rangle.$$

Furthermore, the positive definite property (4.2) and Bochner's theorem imply that there is a normalized positive-operator-valued measure $E(\cdot)$ such that

$$V(t) = \int_{-\infty}^{\infty} \mathrm{d}E(u) \exp(-\mathrm{i}ut).$$

The analytic continuation in the complex parameter t can now be made inside this integral (the operator will be unbounded in the general case of an infinite-dimensional Hilbert space, of course). From the KMS condition we then find

$$\langle\Omega|X^\dagger V(t + \mathrm{i}\beta) Y|\Omega\rangle = \langle\Omega|T_{1,t}(Y) X^\dagger|\Omega\rangle.$$

But the right-hand side can be rewritten as follows, using the relation (4.4) twice

$$\langle\Omega|X^\dagger D T_{1,t}(Y)|\Omega\rangle = \langle\Omega|X^\dagger D V(t) Y|\Omega\rangle$$

where we have introduced the positive operator

$$D = \mu_1 \otimes \mu_1^{-1}.$$

The cyclic and separating property of Ω implies that we can identify the operators

$$D V(t) = V(t + \mathrm{i}\beta)$$

and each Fourier component

$$D\, \mathrm{d}E(u) = \exp(\beta u)\, \mathrm{d}E(u).$$

But D is a self-adjoint operator, its eigenspaces are orthogonal and consequently $V(t) = D^{-\mathrm{i}t/\beta}$ which means that

$$T_{1,t}(X) = \mu_1^{-\mathrm{i}t/\beta} X \mu_1^{\mathrm{i}t/\beta}.$$

Thus $T_{1,t}$ represents a Hamiltonian dynamics on $\mathcal{A}_1$; it is the modular automorphism group associated with the state μ_1.

These arguments used above fail precisely when $\beta = 0$. Then D is proportional to the unit operator and the KMS relation says that the state defining the correlation function is a trace. For $T_{1,t}$ we can have any family of CP maps satisfying

$$\mu_1 \circ T_{1,t} = \mu_1$$

and correlation functions generated by it will then have the required positive definite property.

5. Discussion

In the introduction we noted that the deep mathematical reason for the difficulties considered here has already been approached in pure mathematics [1] and in the context of quantum stochastic processes [2, 4, 5]. Recently the relation between the product form of the initial state and the existence of CP dynamical maps describing relaxation processes was also pointed out by Pechukas [16]. Pechukas suggested that the dynamical maps could be properly defined on a subset of initial states for the open system even when the initial state of the composite system is correlated. With the methods based on the correlation functions used in this paper, one option is to restrict the observables $\mathcal{A}_1$ of the open system to a smaller subalgebra. Takesaki's theorem will then allow a larger set of initial states. This procedure would restrict the quantum observables and introduce by fiat some classical property of the open system, but this line of thought has not been followed here.

A 'solution' which appears more physical is to accept that the description of relaxation processes by any kind of subdynamics involves an approximation. Of course, it is an old and established idea that a separation of time scales is necessary in describing dissipative processes on the basis of reversible microscopic dynamics. What is not so well established is the choice of quantities to be approximated. In the present formalism a natural choice is the correlation functions up to some finite order and up to some finite resolution of the time scale. A justification of such a procedure could only be given a firm foundation by the solution of particular models. Here we can only give a few general arguments why the choice of time scale is an essential ingredient. In a companion article the quantum analogue of Gaussian stochastic processes, the quasifree processes on the CCR algebra, are investigated [18]. There the conditions for having an exact subdynamics and for obtaining a good approximation of the correlation functions can be given in some greater detail.

Describing equilibrium thermal fluctuations in a quantum system always involves a natural time scale $\beta = \hbar/k\Theta$ defined by the heat bath. From section 4 we know that there is no exact reproduction of even the lowest-order correlation function by any subdynamics, but this does not exclude that there can be a good approximation on longer time scales. Note that the standard weak coupling limit, often used to derive master equations, involves a rescaling of the time parameter which will generally destroy the information about the intrinsic time scales of the reservoir [19, 20].

In applications the type of subdynamics most often considered is that of the Markovian kind. To be more precise, one generally assumes that the relaxation is given by a semigroup of dynamical maps. Strictly speaking the semigroup property does not imply that the higher-order correlations are given by the CP maps in analogy with the formula (2.12); the Markov property is stronger than that of having a semigroup. (An exception to this general statement is provided by the quasifree processes on the CCR algebra [7, 18].) The convergence of the multitime correlation functions to the form suggested by (2.12) has been proved in the appropriate limit [21]. Without such a result the higher-order correlation functions cannot be found from the semigroup, and there is a weaker sense of the subdynamics reproducing the exact dynamics of the composite system.

It has long been known that already the semigroup (exponential) relaxation cannot hold strictly when the reservoir has a finite temperature, and this is again due to the non-zero value of β [17, 22–25]. The failure is evident already at the lowest-order correlation function. At sufficiently low temperatures relaxation processes in quantum systems will always display some non-exponential effects, and the same holds for any finite temperature at a sufficiently short time scale. It has also been shown that the thermal correlation functions at a finite temperature has a deterministic property which is completely at variance with the randomness associated with Markov processes [14].

It could be an interesting open problem whether the effects of correlations in the initial state and the consequent lack of a subdynamics can be seen in some experimentally accessible quantities. One candidate suggested by [16] is as follows. It is known that the properties of the dynamical semigroups of CP maps imply the following simple relation between the longitudinal or population (T_1) and transversal or phase (T_2) relaxation times of a spin in a heat bath:

$$2T_1 \geqslant T_2 \tag{5.1}$$

(see e.g. [13]). Experimental manifestations of a breakdown of (5.1) are not known to me. In recent years there has been a series of papers where models are shown to depart from this expected relation when the weak coupling limit is abandoned [26–29]. However, the derivation of (5.1) depends on having a semigroup of CP maps where the generator is independent of time. Thus, there is an underlying assumption much stronger than that of having a subdynamics of a general type. It would be interesting to have realistic situations where the dynamical effects of the correlations in the initial state could be displayed without depending on extra assumptions about stationarity and a semigroup evolution. That such effects must exist is clear, the problem is whether they can be identified in the experimentally observable properties of the correlation functions.

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Appendix

We will give a simplified proof of Takesaki's theorem which works for finite quantum systems without using any deep results from operator algebra theory. We start from a set-up similar to that in section 4. The composite system is represented by an algebra $\mathcal{A} = B(\mathcal{K})$ which acts on the first factor in the Hilbert space $\mathcal{L} = \mathcal{K} \otimes \mathcal{K}$. Again there is a vector $\Omega \in \mathcal{L}$ which is cyclic and separating for the algebra $\mathcal{A}$ with $\mu(X) = \langle\Omega|X \otimes \mathbb{1}|\Omega\rangle$, and a positive operator Δ satisfying

$$\langle\Omega|X\Delta Y|\Omega\rangle = \langle\Omega|YX|\Omega\rangle \tag{A.1}$$

for all $X, Y \in \mathcal{A}$, where we identify X with $X \otimes \mathbb{1}$ wherever appropriate. Assume that there is a conditional expectation $E : \mathcal{A} \to \mathcal{A}_1$ with the desired properties. As $\langle\Omega|E(Y)|\Omega\rangle = \langle\Omega|Y|\Omega\rangle$ and $E(XE(Y)) = E(X)E(Y)$, it must hold for all $X, Y \in \mathcal{A}$ that

$$\langle\Omega|E(X)Y|\Omega\rangle = \langle\Omega|XE(Y)|\Omega\rangle = \langle\Omega|E(X)E(Y)|\Omega\rangle. \tag{A.2}$$

Let $P_1 \in B(\mathcal{L})$ be the projection onto the subspace $\mathcal{L}_1 \subset \mathcal{L}$ which is the closed linear span of the set $(\mathcal{A}_1 \otimes \mathbb{1})|\Omega\rangle$. Clearly $P_1|\Omega\rangle = |\Omega\rangle$. The defining relation for E (3.2) is then equivalent to the following identity for all $X, Y \in \mathcal{A}$:

$$\langle\Omega|XE(Y)|\Omega\rangle = \langle\Omega|XP_1Y|\Omega\rangle \tag{A.3}$$

and hence to the relation $E(Y) = P_1YP_1$. Combining (A.1)–(A.3) and the fact that $\Delta(X \otimes \mathbb{1})\Delta^{-1} = \mu X\mu^{-1} \otimes \mathbb{1}$ (cf (4.4)) it is found that

$$\langle\Omega|XE(Y)|\Omega\rangle = \langle\Omega|YP_1\Delta X|\Omega\rangle = \langle\Omega|E(X)Y|\Omega\rangle = \langle\Omega|Y\Delta P_1X|\Omega\rangle.$$

From the cyclic property of Ω it follows that $P_1\Delta = \Delta P_1$. Hence P_1 commutes with the spectral resolution of Δ and it follows that

$$\Delta^{-\mathrm{i}t} P_1 \Delta^{\mathrm{i}t} = P_1$$

and finally that

$$\Delta^{-\mathrm{i}t} \mathcal{A}_1 \Delta^{\mathrm{i}t} = \mathcal{A}_1$$

which is the statement of the theorem.

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