The Failure of the Quantum Regression Hypothesis

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The Markovian description of open quantum systems, which conventionally is defined by the quantum regression hypothesis, is investigated. We show that for a system staying in thermal equilibrium with its environment this hypothesis leads to a violation of the KMS condition, the fluctuation dissipation theorem, and under certain conditions to a violation of the principle of detailed balancing. This implies that quantum Markovian processes do not allow for basic physical principles. Also its quantitative predictions are not reliable in general.

1. INTRODUCTION

There are various physical phenomena which result from an interplay of a truly quantum mechanical behavior of a system with a few degrees of freedom and of the interaction with its environment causing an exchange of energy and a partial or even total destruction of phase relations within the considered system. We only mention a few examples: an initially excited atom interacting with the electromagnetic field [1, 2], nuclear spin relaxation in condensed matter [3], a laser [4], the movement of Frenkel excitons in a molecular crystal [5], tunneling centers in ionic crystals [6], phase slips of the macroscopic wave function in a superconducting interference device (SQUID) [7], the dynamics of collective nuclear coordinates in nuclear reactions [8], Schrödinger's cat [9], etc.

Classical physics provides different methods to deal with the influence of the environment on a system. Phenomenological deterministic equations represent the coarsest way of description of an irreversible time evolution. On a finer level the irregular action of the environment on the system must be taken into account. This goal was first achieved by Einstein [10]. The therefrom emerging theory of stochastic processes has gained steadily increasing importance since then. As a review of the first 40 years of this development [11] may serve, for the modern trends, see [12–18].

Statistical mechanical considerations have shown that within the framework of continuous Markovian processes the problem of stochastic modelling can be solved uniquely for equilibrium systems and for certain nonequilibrium systems [19–23].

Various attempts have been made to describe damping phenomena within a quantum mechanical framework.

Time-dependent and nonlinear Schrödinger equations have been proposed to describe friction in quantum systems ([24] may serve as a review). However, these modified Schrödinger equations yield different results for the same simple models [25]. Moreover, the description of an open system by a pure state is doubtful.

In principle it is always possible to apply usual quantum mechanics to the system combined with its environment. Radiation damping of a charged harmonic oscillator [26] and of an atom [1] are early examples. The treatment of elementary excitations and quasiparticles in many-particle systems by Green's functions [27] has to be mentioned in this context, too.

There exist different reduced descriptions in which the explicit appearance of the environment is eliminated. In one description the Heisenberg equations are modified in a way analogous to classical Langevin equations [4, 28–30]. For another description the Schrödinger picture is used and the Liouville von Neumann equation is modified by additional terms which cannot be cast in the form of a commutator with a Hamiltonian [31]. Feynman's path integral formulation of quantum mechanics can be generalized by an additional term in the action which cannot be written as a time integral of a Lagrange function [32, 33].

In the framework of the first two methods it is straightforward how to make a Markovian assumption. Because classical Markov processes are both of particular simplicity, compared with general processes, and, as already mentioned, have proved to be very useful, their transfer to quantum mechanics is very tempting and has been performed by several authors [34–36]. The assumption of a quantum Markov process is known under the term quantum regression hypothesis, too.

However, the confirmation of this hypothesis from microscopic models [4, 34, 31] relies on assumptions which are not very convincing, as the repeated random-phase approximation and the assumption of a thermodynamically unstable environment. Rigorous proofs are lacking. The semigroup dynamics of the density matrix which must hold for a quantum Markov process can be proved only on the basis of the rather restrictive assumption of weak coupling, and, in general, only holds for the dynamics averaged over the free (i.e., undamped) motion of the system [37].

It is the aim of the present paper to investigate the quality of the quantum regression hypothesis thoroughly. For this purpose we ask whether equilibrium correlation functions obtained from the quantum regression hypothesis obey those general symmetries following from statistical mechanics. In the case of an affirmative answer, we could hope that these properties would provide powerful means for a phenomenological modelling, as, e.g., in the classical case the Onsager Casimir relations do, which are implied by the principle of detailed balance. However, it comes out that none of these general physical properties are obeyed, and hence the quantum regression hypothesis fails in describing open systems in thermal equilibrium. Because in general nonequilibrium systems contain equilibrium situations as limiting cases one must expect the failure of this hypothesis in these cases, too.

The paper is organized as follows. We begin the next section with some

preparatory remarks on classical Markov processes, then formulate the quantum regression hypothesis, and discuss its general properties. In Section 3 we derive the class of stationary Gauss Markov processes of a single quantum oscillator by purely phenomenological considerations. For various other treatments of a damped harmonic oscillator see Ref. [38]. Mainly for this special class of processes we investigate in Sections 4, 5, and 6 the principle of detailed balancing, the KMS condition, and the fluctuation dissipation theorem, respectively, however, with a negative result in each case. Because there are only two assumptions from which the considered class of models follows, namely, the Gaussian assumption and the regression hypothesis, and because the Gaussian assumption is known not to be in any conflict with general physical properties, this failure must be due to the quantum regression hypothesis, as already mentioned above. In Section 7 we compare the quantum regression hypothesis with other different approaches and, finally, find that this hypothesis also yields quantitatively wrong results under most circumstances.

2. Regression Hypothesis

2.1. *Classical Markov Processes*

A stochastic process $x(t)$[1] can be characterized by its multitime joint probabilities $W^{(n)}(x_1, t_1; x_2, t_2; \ldots x_n, t_n)\, dx_1\, dx_2 \ldots dx_n$, $n = 1, 2, \ldots$, for finding the process at the different instants of time $t_1, t_2, \ldots, t_n$ in the intervals $(x_1, x_1 + dx_1)$, $(x_2, x_2 + dx_2), \ldots$, $(x_n, x_n + dx_n)$, respectively. From these the conditional probabilities are determined, e.g.,

$$P(x, t \mid x_1, t_1; x_2, t_2; \ldots x_n, t_n) = W^{(n+1)}(x, t; x_1, t_1; \ldots x_n, t_n)/W^{(n)}(x_1 t_1; x_2 t_2; \ldots x_n, t_n). \tag{2.1}$$

If the observation time t is later than all times t_i, by definition, for a Markov process the conditional probability depends on the condition at the latest time, say, t_1, only

$$P(x, t \mid x_1, t_1; \ldots x_n, t_n) = P(x, t - t_1 \mid x_1) \qquad \text{for} \quad t \geqslant t_1 \geqslant \ldots. \tag{2.2}$$

For the sake of simplicity we consider time-homogeneous processes only, i.e., processes for which the conditional probabilities are invariant under time translations.

For a Markov process any joint probability can be represented as a product of conditional probabilities with the one-time probability $W^{(1)}(x_n, t_n)$ at the earliest

[1] We consider scalar real processes only. Generalisations to more complicated cases are straightforward.

time of observation. Moreover the conditional probability determines the time evolution of the one-time probability $W^{(1)}(x, t) \equiv W(x, t)$:

$$W(x, t) = \int P(x, t-s \mid y)\, W(y, s)\, dy, \tag{2.3}$$

and, hence, it is the kernel of the propagator G_t defined by

$$G_t h(x) = \int P(x, t \mid y)\, h(y)\, dy \tag{2.4}$$

with an arbitrary integrable function h. Using the adjoint propagator $G_t^\dagger$ the mean value of an arbitrary function f of the process $x(t)$ reads

$$\langle f_t \rangle = \int W(x, 0)\, G_t^\dagger f(x)\, dx. \tag{2.5}$$

Multitime correlations of functions $f, g, \ldots$ of the process $x(t)$ are given by $G_t^\dagger$, too, e.g.,

$$\begin{aligned} \langle f_t g_s \rangle &= \int W(x, s)\, g(x)\, G_{t-s}^\dagger f(x)\, dx \\ &= \int W(x, 0)\, G_s^\dagger g G_{t-s}^\dagger f(x)\, dx. \end{aligned} \tag{2.6}$$

Consequently, G_t determines the complete dynamics of a Markov process. Because G_t itself is known from the dynamics of all mean values, the whole dynamics of a Markov process is already determined by the time evolution of the mean values. This fact is known as the regression theorem [34]. For a stochastic process with linear dynamics, as, e.g., an Ornstein Uhlenbeck process, this theorem implies that the regression of fluctuations is governed by the macroscopic equations [19].

There are some general properties of the generator which are important for quantum mechanical Markov processes, too:

(i) The propagator is a linear operator, which maps positive on positive functions.

(ii) The integral of a function is invariant under the propagator (conservation of total probability)

$$\int G_t f(x)\, dx = \int f(x)\, dx. \tag{2.7}$$

(iii) The propagator at $t = 0$ is the identity

$$G_0 = \mathbf{1}. \tag{2.8}$$

(iv) The propagators G_t, $t \geqslant 0$, form a semigroup:

$$G_t G_s = G_{t+s}, \qquad t, s \geqslant 0. \tag{2.9}$$

The adjoint propagator $G_t^\dagger$ has the same properties except for (ii) which is replaced by

(ii′) $G_t^\dagger$ maps the constant function onto itself:

$$G_t^\dagger 1 = 1. \tag{2.10}$$

Under weak additional assumptions concerning the continuity of G_t and the function space on which G_t acts, it follows from the properties (i), (ii), and (iv) that the propagator G_t and consequently the single-event probability obey linear equations of motion of first order in time [39]:

$$\dot{G}_t = \Gamma G_t, \tag{2.11}$$

$$\dot{W}(t) = \Gamma W(t). \tag{2.12}$$

Γ is the generator of the considered Markov process. It is defined by

$$\Gamma = \lim_{t \to 0^+} t^{-1}(G_t - \mathbf{1}). \tag{2.13}$$

Equation (2.12) is the master equation, and (2.11) is the equation for the respective Green's function from which the foreward and (by adjoining) the backward equations for the conditional probability follow. The integration of Eq. (2.11) with the initial condition (2.8) yields a solution with the semigroup property (iv) provided Γ obeys certain regularity conditions [39].

2.2. *Quantum Mechanical Markov Processes*

In the following we will always assume that the observables of the considered open quantum system S act as hermitian operators on a Hilbert space $\mathscr{H}_S$ and, vice versa, that all hermitian operators of $\mathscr{H}_S$ are observables of S.

As in the classical case the time evolution of an open system is completely determined only if both the dynamics of the mean values and the dynamics of the correlation functions of its observables are known. Again a quantum process will be called Markovian if the dynamics of all mean values determines already the dynamics of the correlation functions. This fact is known as quantum regression hypothesis. Again, as a consequence of this hypothesis for a linear process the regression of fluctuations is governed by the macroscopic equations. The precise meaning of the regression hypothesis in the general case is stated in Section 2.2.2 after some preparatory comments in Section 2.2.1 about the dynamics of the mean values.

2.2.1. *Dynamics of Mean Values*

In the following we shall assume that the Hilbert space of the system is separable. Then every state of the system is uniquely characterized by a density matrix ρ which is a positive operator with unit trace [40]. As is well known the mean value of an observable u of the system in the considered state is then given by

$$\langle u \rangle = \operatorname{tr} u\rho. \tag{2.14}$$

Because classically the observables correspond to functions on the state space, ρ is the quantum analogue of the single-time probability $W(x, t)$ at a fixed time t, and the trace corresponds to the state space integral. In analogy to the classical master equation (2.12) the dynamics of a quantum Markov process is given by a first-order differential equation in time

$$\dot{\rho}(t) = \Gamma\rho(t), \tag{2.15}$$

where Γ is called the dissipative Liouville operator. Γ is a linear superoperator, i.e., it acts on operators in the Hilbert space $\mathscr{H}_S$.

Because of its linearity the solution of the quantum master equation (2.15) can be written as

$$\rho(t) = G_t\rho(0), \tag{2.16}$$

where the propagator G_t is the solution of

$$\dot{G}_t = \Gamma G_t \tag{2.17}$$

with the initial condition

$$G_0 = \mathbf{1}. \tag{2.18}$$

$\mathbf{1}$ is the unit superoperator.

Obviously the quantum propagator G_t has corresponding properties as the classical one:

(i) G_t is a linear operator, which maps positive on positive Hilbert space operators.[2]

(ii) The trace is invariant under the propagator

$$\operatorname{tr} G_t\rho = \operatorname{tr} \rho. \tag{2.19}$$

(iii) G_0 is the unit operator (2.18).

(iv) The propagators G_t, $t \geqslant 0$, form a semigroup

$$G_tG_s = G_{t+s}. \tag{2.20}$$

[2] There are good arguments that this requirement of positivity must be replaced by the stronger requirement of complete positivity [42]. However, we do not want to go into these technical details.

For a discussion of the mathematical aspects of the semigroup theory of open quantum systems we refer to the literature [41, 42]. Mean values of observables at time t follow from (2.14) and (2.16),

$$\begin{aligned}\langle u_t \rangle &= \operatorname{tr} u G_t \rho(0) \\ &= \operatorname{tr} \rho(0)\, G_t^\dagger u,\end{aligned} \tag{2.21}$$

where the adjoint propagator $G_t^\dagger$ is defined with respect to the functional $\langle u | \rho \rangle = \operatorname{tr} u\rho$, u being bounded and ρ of the traceclass [41].

$G_t^\dagger$ shares the properties with G_t except for (ii), which is replaced by (ii'):

$$\text{(ii')} \qquad G_t^\dagger 1 = 1, \tag{2.22}$$

where 1 is the unit Hilbert space operator.

As an example of a semigroup we mention the time evolution of a closed Hamiltonian system. Then Γ is the Liouville von Neumann operator

$$\Gamma^H \cdot = -\frac{i}{\hbar}[H, \cdot], \tag{2.23}$$

where H is the Hamiltonian of the system. G_t^H and $G_t^{H\dagger}$ govern the dynamics in the Schrödinger and Heisenberg pictures, respectively:

$$G_t^H \rho = e^{-(i/\hbar)Ht} \rho e^{(i/\hbar)Ht}, \tag{2.24a}$$

$$G_t^{H\dagger} u = e^{(i/\hbar)Ht} u e^{-(i/\hbar)Ht}. \tag{2.24b}$$

In this particular case G_t is a unitary group.

In the following we will call $G_t^\dagger u$ a Heisenberg operator even if the dynamics is dissipative and, consequently, $G_t^\dagger u$ is no longer unitarily equivalent to u. The classical analogue of a Heisenberg operator is the conditional expectation of a random variable $f(x)$ evaluated at time t for known x at time $t_0 = 0$:

$$f_t(x) = \int P(y, t|x) f(y)\, dy = G_t^\dagger f(x).$$

2.2.2. *Dynamics of Correlation Functions*

For a Hamiltonian system we define the correlation function of two observables u at time t and v at time s to be the mean value of the product of the Heisenberg operators $u(t) = e^{(i/\hbar)Ht} u e^{-(i/\hbar)Ht}$ and $v(s)$ averaged with the density matrix ρ of the system at time $t_0 = 0$:

$$\langle u(t)\, v(s) \rangle^H = \operatorname{tr} u(t)\, v(s)\, \rho. \tag{2.25}$$

In general this correlation function is different from $\langle v(s)\, u(t) \rangle^H$ because of the noncommutativity of quantum observables. There even are many other functions

describing the mutual dependence of observables u and v at different times t and s, respectively, which all approach the same classical correlation function in the classical limit. Some are discussed in Ref. [43]. However, none of these quantum correlation functions can be interpreted as a correlation function of a classical process [43].

In contrast to a classical correlation function, (2.25) neither has an immediate physical interpretation nor is it a measurable quantity in general. For each particular experimental setup only an investigation of the mutual interactions of the system and the measuring apparatus can explain which kind of correlation function is measured [44]. For example, we mention idealized photon counters which measure normally or antinormally ordered products of creation and annihilation operators of the electromagnetic field at different space-time points, depending on whether the counter is operated by absorption or by stimulated emission [45, 46].

However, there are important theoretical quantities like, e.g., thermal Green's functions and response functions which are determined by correlation functions as defined in (2.25). Another reason for considering these correlation functions is the fact that they have simple properties by which they can be characterized. Some of these properties will be given in the sequel. A more complete discussion is given in Ref. [47].

A correlation function of observables of an open system S can in principle be calculated by taking into account the environment R of the system and by employing Eq. (2.25) with H being the Hamiltonian of the system plus environment, $S+R$, and ρ being the initial density matrix of $S+R$. In order to avoid such complicated calculations several authors postulated that if the density matrix obeys a Markovian master equation (2.15), correlation functions are mean values of products of Heisenberg operators of the open system as introduced at the end of the preceding section:

$$\langle u(t)\, v(s)\rangle = \operatorname{tr} v\rho(s)\, G^{\dagger}_{t-s} u \qquad \text{for} \quad t \geqslant s \tag{2.26a}$$

$$= \operatorname{tr} \rho(t)\, u G^{\dagger}_{s-t} v \qquad \text{for} \quad t \leqslant s. \tag{2.26b}$$

Here tr is the trace over the Hilbert space $\mathscr{H}_S$ of the systems, u, v are the operators representing the considered observables in $\mathscr{H}_S$, $\rho_s = G_s \rho(0)$ is the density matrix of S at time s, G_s is the propagator introduced in (2.16), and $G_s^{\dagger}$ is its adjoint. Because the dynamics of such a correlation function is solely determined by that of the mean values, namely, by the propagator G_t, this special form is based on an assumption analogous to the classical regression theorem and therefore we will call (2.26) the quantum regression hypothesis. As already mentioned and as will be shown explicitly for a Gaussian process in Section 3, this hypothesis entails the same regression of correlations and mean values. Further we note that in the classical limit (2.26) becomes a correlation function of a classical (2.6) Markov process.

If the observables of the considered open system obey Langevintype equations with δ-correlated fluctuating force the quantum regression hypothesis can be

proved to hold [34]. Therefore, it is often called a theorem [34]. By calling it a hypothesis we do not doubt these mathematical facts; rather we want to emphasize that it is an assumption to apply to a physical situation.

One can easily show that the following properties which hold for correlation functions of Hamiltonian systems and which consequently are exact properties of correlation functions even of open systems are indeed fulfilled by correlations of the form (2.26):

(i) Linearity in u and v:

$$\langle(\alpha u_1 + \beta u_2)(t)\, v(s)\rangle = \alpha\langle u_1(t)\, v(s)\rangle + \beta\langle u_2(t)\, v(s)\rangle, \tag{2.27a}$$

$$\langle u(t)(\alpha v_1 + \beta v_2)(s)\rangle = \alpha\langle u(t)\, v_1(s)\rangle + \beta\langle u(t)\, v_2(s)\rangle \tag{2.27b}$$

with complex numbers $\alpha_1 \beta$.

(ii) Compatibilities:

$$\langle u(t)\, v(t)\rangle = \langle (uv)(t)\rangle, \tag{2.28a}$$

$$\langle 1(t)\, v(s)\rangle = \langle v(s)\, 1(t)\rangle = \langle v(s)\rangle, \tag{2.28b}$$

where 1 is the unit operator in Hilbert space.

(iii) Hermiticity:

$$\langle u(t)\, v(s)\rangle^* = \langle v^+(s)\, u^+(t)\rangle.^3 \tag{2.29}$$

Correlation functions of more than two operators at different times cannot be determined by the regression hypothesis in general. However, for an important class of time orderings it yields a prescription compatible with the properties (i)–(iii) generalized to higher correlation functions [36]. In the following we will not consider higher than second-order correlation functions and so we do not enter this discussion.

3. Stationary Quantum Gauss Markov Processes

In this section we discuss the quantum analogue of a classical two-dimensional Ornstein Uhlenbeck process, in order both to illustrate the concepts introduced in the preceding section and to provide a whole class of processes on a purely phenomenological basis for further investigation.

[3] Because of the linearity (i) it is possible to consider arbitrary nonhermitian operators u, v.

3.1. *Gaussian Density Matrices*

Let p and q be the momentum and coordinate, respectively, of a spinless point-like particle obeying the well-known canonical commutation relation $[p, q] = \hbar/i$. The state of this particle is determined by the mean values of all powers $p^k q^l$ provided they exist. We will speak of a Gaussian state if mean values of higher powers factorize in sums of products of first and second moments according to either of the following rules:

$$\langle p^k q^l \rangle = (k-1)\langle p^2 \rangle \langle p^{k-2} q^l \rangle + l \langle pq \rangle \langle p^{k-1} q^{l-1} \rangle \tag{3.1a}$$

$$= k \langle pq \rangle \langle p^{k-1} q^{l-1} \rangle + (l-1)\langle q^2 \rangle \langle p^k q^{l-2} \rangle. \tag{3.1b}$$

Here we have assumed that the first moments vanish

$$\langle p \rangle = 0, \tag{3.2a}$$

$$\langle q \rangle = 0. \tag{3.2b}$$

Some comments are in order.

—Both rules of factorization yield the same result.

—The Gaussian factorization of an arbitrarily ordered product of p and q is compatible with the canonical commutation relations.

—Conversely, any pair of operators which is Gaussian distributed and the powers of which form a complete operator basis must have a commutator proportional to the unit operator.

From the general form of a mean value (2.14), the cyclic invariance of the trace, the canonical commutation relation, and from (3.1a, b) it follows that a Gaussian density matrix obeys two homogeneous equations

$$X_1 \rho_{\mathrm{st}} = 0, \tag{3.3a}$$

$$X_2 \rho_{\mathrm{st}} = 0, \tag{3.3b}$$

where

$$X_1 \rho = \rho p + \frac{i}{\hbar} \langle p^2 \rangle [\rho, q] + \frac{i}{\hbar} \langle pq \rangle [p, \rho], \tag{3.4a}$$

$$X_2 \rho = q\rho + \frac{i}{\hbar} \langle pq \rangle [\rho, q] + \frac{i}{\hbar} \langle q^2 \rangle [p, \rho]. \tag{3.4b}$$

These equations have a unique solution with unite trace:

$$\rho_{\mathrm{st}} = Z^{-1} e^{-h}, \tag{3.5}$$

where h is a quadratic form in the operators p and q,

$$h = \frac{\operatorname{arccth}\{(2/\hbar)(\langle p^2\rangle\langle q^2\rangle - 1/4\langle pq+qp\rangle^2)^{1/2}\}}{\hbar(\langle p^2\rangle\langle q^2\rangle - 1/4\langle pq+qp\rangle^2)^{1/2}} \times \{\langle q^2\rangle p^2 + \langle p^2\rangle q^2 - 1/2\langle pq+qp\rangle(pq+qp)\}, \tag{3.6}$$

and where $Z = \operatorname{tr} e^{-h}$ is the partition function given by

$$Z = \hbar^{-1}(\langle p^2\rangle\langle q^2\rangle - |\langle pq\rangle|^2)^{1/2}. \tag{3.7}$$

Note that h is hermitian and bounded from below and that consequently ρ is positive, provided that

$$\langle p^2\rangle\langle q^2\rangle > |\langle pq\rangle|^2. \tag{3.8}$$

Conversely, from the positivity of ρ and the Cauchy Schwarz inequality applied to the inner product $(u, v) = \langle uv\rangle$ for $u = p$, $v = q$, (3.8) follows including equality. In the latter case Eqs. (3.4) are solved by a pure state $|\psi)(\psi|$, where ψ is the gound state of the annihilation operator a defined by

$$a = \frac{1}{\hbar\langle p^2\rangle^{1/2}}(\langle p^2\rangle q - \langle pq\rangle p). \tag{3.9}$$

In summary we note that there is exactly one Gaussian density matrix for each choice of parameters $\langle p^2\rangle$, $\langle q^2\rangle$, $\langle pq\rangle$ within the physical region $\langle p^2\rangle\langle q^2\rangle \geqslant |\langle pq\rangle|^2$.

3.2. *The Dissipative Liouville Operator*

The Gaussian factorization rule and the particular form of Markovian correlation functions (2.26) uniquely determine the propagator of a time-homogeneous Gauss Markov process (see Appendix A):

$$\Gamma = Y_1 X_1 + Y_2 X_2, \tag{3.10}$$

where X_1 and X_2 are the superoperators defined in (3.4a, b) and Y_1 and Y_2 are given by

$$Y_1 = \frac{i}{\hbar}[r_1(L_p - R_p) + r_2(R_q - L_q)], \tag{3.11a}$$

$$Y_2 = \frac{i}{\hbar}[r_3(L_p - R_p) + r_4(R_q - L_q)]. \tag{3.11b}$$

Here L_u, R_u are left and right multiplication operators, respectively,

$$L_u x = ux, \qquad R_u x = xu, \tag{3.12}$$

and r_i, $i = 1,..., 4$, are real coefficients, which are determined by the time rate of change of the correlations $\langle q(t)\, q\rangle$, $\langle q(t)\, p\rangle$, $\langle p(t)\, q\rangle$, $\langle p(t)\, p\rangle$ at $t = 0$. For a precise definition see Appendix A.

Because Y_1 and Y_2 are linear combinations of commutators it follows from (3.10) that $\mathrm{tr}\, \Gamma\rho = 0$ for arbitrary ρ, and equivalently $\Gamma^\dagger 1 = 0$. Further, one finds from (3.14) and (3.3a, b) that

$$\Gamma \rho_{\mathrm{st}} = 0 \tag{3.13}$$

as should be. Hence, ρ_{st} is a right- and 1 a left-eigenvector of Γ belonging to the eigenvalue 0. We will come back to the spectral properties at the end of Section 3.3.

In conclusion we note that in a phase space representation Γ becomes a Fokker–Planck-type operator with a linear drift and a constant, but not necessarily positive diffusion matrix. For example, for the Wigner representation [49] we obtain

$$\begin{aligned}\Gamma_w = {} & \frac{\partial}{\partial q}(r_1 p + r_3 q) + \frac{\partial}{\partial p}(r_2 p + r_4 q) \\ & + (\tfrac{1}{2} r_1 \langle pq + qp\rangle + r_3 \langle q^2\rangle)\frac{\partial^2}{\partial q^2} \\ & + (r_1 \langle p^2\rangle + r_4 \langle q^2\rangle + \tfrac{1}{2}(r_2 + r_3)\langle pq + qp\rangle)\frac{\partial^2}{\partial p\, \partial q} \\ & + (r_2 \langle p^2\rangle + \tfrac{1}{2} r_4 \langle pq + qp\rangle)\frac{\partial^2}{\partial p^2}.\end{aligned} \tag{3.14}$$

Acting on a quasi-probability distribution Γ_w yields its time rate of change.

3.3. *Mean Relaxation and Stationary Correlation Functions*

Both the relaxation of mean values and the dynamics of stationary correlation functions are given by the Heisenberg operators

$$q(t) = G_t^\dagger q, \tag{3.15a}$$

$$p(t) = G_t^\dagger p. \tag{3.15b}$$

According to (2.17) their equations of motion read

$$\dot{q}(t) = G_t^\dagger \Gamma^\dagger q, \tag{3.16a}$$

$$\dot{p}(t) = G_t^\dagger \Gamma^\dagger p. \tag{3.16b}$$

Using (3.3), (3.10), and (3.11) we get

$$\Gamma^{\dagger} q = -r_3 q - r_1 p, \tag{3.17a}$$

$$\Gamma^{\dagger} p = -r_4 q - r_2 p, \tag{3.17b}$$

which yields with (3.15) and (3.16)

$$\dot{q}(t) = -r_3 q(t) - r_1 p(t), \tag{3.18a}$$

$$\dot{p}(t) = -r_4 q(t) - r_2 p(t). \tag{3.18b}$$

The initial conditions are

$$q(0) = q, \tag{3.19a}$$

$$p(0) = p. \tag{3.19b}$$

Using matrix notation the solution reads

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = e^{-\gamma t} \begin{pmatrix} q \\ p \end{pmatrix}, \tag{3.20}$$

where the relaxation matrix is given by

$$\gamma = \begin{pmatrix} r_3 & r_1 \\ r_4 & r_2 \end{pmatrix}. \tag{3.21}$$

The average of (3.20) over a nonstationary density matrix yields the relaxation of the mean values of the momentum and coordinate operator from initial non-equilibrium values $\langle q \rangle_0$, $\langle p \rangle_0$:

$$\begin{pmatrix} \langle q(t) \rangle_0 \\ \langle p(t) \rangle_0 \end{pmatrix} = e^{-\gamma t} \begin{pmatrix} \langle q \rangle_0 \\ \langle p \rangle_0 \end{pmatrix}. \tag{3.22}$$

Hence, we find exponential relaxation for the first moments which extends a well-known property of classical Gauss Markov processes [50].

The stationary correlation matrix is given by

$$C(t) = \begin{pmatrix} \langle q(t)\, q \rangle & \langle q(t)\, p \rangle \\ \langle p(t)\, q \rangle & \langle p(t)\, p \rangle \end{pmatrix}. \tag{3.23}$$

From (2.26) and (3.20) we find the same exponential behavior as for the relaxation of the moments

$$C(t) = e^{-\gamma t} C, \qquad t \geqslant 0, \tag{3.24a}$$

$$= C e^{\gamma^{+} t}, \qquad t \leqslant 0, \tag{3.24b}$$

where $C = C(0)$ is the matrix of stationary second moments and where γ^+ is the transposed of γ.

Again this is in accordance with the classical result [50]. In passing we remark that the expressions (A4) for r_i, $i = 1,..., 4$, can be obtained in a particularly simple way by computing the time derivative of (3.23) at $t = 0^+$. Equations (3.20) and (3.24) show that the mean relaxation from a nonstationary state and the time evolution of the stationary correlations obey the same law, which means that Onsager's regression hypothesis extends to the quantum case literally.

Analogously to a classical stationary Gauss Markov process we may introduce a matrix L of transport coefficients by

$$L = \gamma C. \tag{3.25}$$

The hermitian part of L is the diffusion matrix D

$$D = \tfrac{1}{2}(\gamma C + C\gamma^+) \tag{3.26}$$

which turns out to be positive even in the quantum case (see Appendix B). In contrast to the classical case C, L and D are complex matrices whose imaginary parts are fixed by the canonical commutation relations and the fact that γ must be a real matrix.

We emphasize that one must not mix up the diffusion as defined in Eq. (3.26) with an eventually indefinite "diffusion" matrix appearing in a c-number representation of Γ, e.g., (3.14). Moreover, a proper Fokker–Planck operator with positive diffusion matrix interpreted as a c-number representation need not necessarily define a proper dissipative Liouville operator. For an example see Appendix C.

As for a classical stationary Ornstein Uhlenbeck process the spectrum of Γ is determined by the eigenvalues

$$\lambda_\pm = \tfrac{1}{2}(r_2 + r_3) \pm [(r_2 - r_3)^2 + r_1 r_4]^{1/2} \tag{3.27}$$

of the relaxation matrix γ:

$$Sp(\Gamma) = \{ -n\lambda_+ - m\lambda_- \mid n, m = 0, 1, 2,... \}.$$

Generally these eigenvalues are not degenerate. Then one can show that Γ is a diagonable operator.

$$\Gamma = \sum_{n,m=0}^{\infty} (n\lambda_+ + m\lambda_-)\, P_{nm} \tag{3.28}$$

with one-dimensional projection operators

$$P_{nm} P_{kl} = \delta_{nk} \delta_{ml} P_{nm}, \tag{3.29}$$

which are a resolution of the identity

$$\sum_{n,m} P_{nm} = \mathbf{1}. \tag{3.30}$$

For the critically damped motion $\lambda_+ = \lambda_-$ all nonzero eigenvalues are degenerate and for Γ there exists a generalized spectral representation analogous to the Jordan normal form.

4. Detailed Balancing

Under the time reversal transformation momenta and spins reverse their sign, whereas coordinates remain unchanged. For a quantum system this transformation can be represented by an antiunitary operator θ. For a closed system with a time reversal invariant Hamiltonian an observable u at time t transforms as[4] [55]

$$\theta u(t)\,\theta^{-1} = \varepsilon_u u(-t), \tag{4.1}$$

where $\varepsilon_u = \pm 1$ is the parity of u under time reversal. A correlation function $\langle u(t)\, v\rangle$ in a stationary, time reversal invariant ensemble coincides with $\langle \theta u(t)\, v\theta^{-1}\rangle^*$ because of the time reversal invariance of the ensemble and because of the antiunitarity of θ. With (4.1) from the stationarity of the ensemble if follows

$$\langle u(t)\, v\rangle = \varepsilon_u \varepsilon_v \langle v^+(t)\, u^+\rangle. \tag{4.2}$$

This is true for any pair of operators with definite parity in an ensemble with the quoted properties. In particular, Eq. (4.2) holds for operators of a system which interacts with another system (a bath) if, e.g., the whole system is in thermal equilibrium described by a Gibbs state. Obviously (4.2) still holds in the thermodynamic limit when the bath becomes infinitely large. Hence, in thermal equilibrium the correlation functions of an open system must have the property (4.2) which is known as detailed balancing.

For a classical system detailed balancing may be expressed in terms of the joint probability

$$W^{(2)}(x_1, t; x_2) = W^{(2)}(\tilde{x}_1; \tilde{x}_2, t), \tag{4.3}$$

where $\tilde{x}_i$ is the time-reversed point x_i. For a classical Markov process detailed balancing implies particular forms of propagators and generators for which the stationary solutions are easily obtained [56–59].

The corresponding conditions for a dissipative Liouville operator of a quantum Markov process were derived in Ref. [60] and are reviewed in Section 4.1.

[4] We do not consider external magnetic fields, etc., because it is clear how to account for them.

The presence of detailed balancing leads for a stationary quantum Gauss Markov process to the same properties of the stationary second moments and the transport matrix as for a classical stationary Gauss Markov process (Section 4.2). We show that all stationary quantum Gauss Markov processes with detailed balancing are unitarily equivalent to a model of Weidlich and Haake for the damped motion of a single mode of the electromagnetic field. This, however, implies that there is no quantum Brownian oscillator obeying detailed balancing.

4.1. *Detailed Balancing for General Quantum Markov Processes*

Using the special form (2.26) of the correlation functions of a quantum Markov process and the symmetries (4.2) for all pairs of operators u, v of the open system, one finds for the propagator G_t

$$T^{-1}G_t L_\rho T = L_\rho G_t^\dagger, \tag{4.4}$$

where T is an antilinear superoperator multiplying with θ and θ^{-1} from the left and the right, respectively,

$$T = L_\theta R_{\theta^{-1}}, \tag{4.5}$$

and where L_ρ is a linear superoperator multiplying with the density matrix ρ from the left.

For $t=0$ it follows from (4.4) with (2.18) and (4.5) that ρ is time reversal invariant

$$\theta^{-1}\rho\theta = \rho. \tag{4.6}$$

Acting with (4.4) on the identity map in the Hilbert space it follows from (4.6) that ρ is a stationary state of G_t

$$G_t\rho = \rho. \tag{4.7}$$

Finally, the time derivative of (4.4) at $t=0^\dagger$ yields

$$T^{-1}\Gamma T L_\rho = L_\rho \Gamma^\dagger. \tag{4.8}$$

One easily shows that (4.6) and (4.8) are equivalent to (4.4). These conditions are completely analogous to those for propagators and generators of classical Markov processes with detailed balancing [61].

4.2. *Detailed Balancing for Stationary Quantum Gauss Markov Processes*

In order to determine the class of Gauss Markov processes with detailed balancing one could apply (4.8) to the general dissipative Liouville operator (3.14).

However, it is much simpler to employ the symmetry (4.2) to the stationary correlation functions of p and q yielding

$$C_{ij}(t) = \varepsilon_i \varepsilon_j C_{ji}(t), \tag{4.9}$$

where the $C_{ij}(t)$ are the elements of the correlation matrix $C(t)$ (3.23) and where $\varepsilon_q = 1$ and $\varepsilon_p = -1$, of course. For a Gauss process (4.9) implies the symmetries of detailed balancing for all correlation functions. Moreover for a Markov process it is sufficient to consider (4.9) and its time derivative at $t = 0^+$. Using (3.24) one finds

$$C_{ij} = \varepsilon_i \varepsilon_j C_{ji}, \tag{4.10}$$

$$L_{ij} = \varepsilon_i \varepsilon_j L_{ji}, \tag{4.11}$$

where $C_{ij} = C_{ij}(0)$, and L_{ij} are the elements of the transport matrix L (3.25).

Equations (4.10) and (4.11) are exactly the same conditions for detailed balancing as for a classical stationary Gauss Markov process [62]. However, because of the nonvanishing imaginary parts of C and L which are caused by the commutation relations of p and q for a quantum process the conditions (4.10) and (4.11) are much more restrictive than they are classically.

From (4.10) and $[p, q] = \hbar/i$ it follows

$$C = \begin{pmatrix} \langle q^2 \rangle & i\frac{\hbar}{2} \\ -i\frac{\hbar}{2} & \langle p^2 \rangle \end{pmatrix} \tag{4.12}$$

and from (4.11) with (3.21), (3.25), and (4.12) we find

$$\langle p^2 \rangle r_1 + \langle q^2 \rangle r_4 = 0, \tag{4.13}$$

$$\frac{\hbar}{2}(r_2 - r_3) = 0. \tag{4.14}$$

In the classical case (4.14) is fulfilled independently of which values are taken by r_2 and r_3 whereas in the quantum case r_2 and r_3 must coincide:

$$r_2 = r_3 = \kappa. \tag{4.15}$$

Because of (B5) κ is positive. Without loss of generality we may put

$$\frac{\langle p^2 \rangle}{\langle q^2 \rangle} = m^2\omega^2, \tag{4.16}$$

$$r_1 r_4 = -\omega^2. \tag{4.17}$$

Then γ reads

$$\gamma = \begin{pmatrix} \kappa & -m^{-1} \\ \omega^2 m & \kappa \end{pmatrix}. \tag{4.18}$$

This dissipative Liouville operator for the quantum Gauss Markov process with stationary correlation matrix C (4.14) and relaxation matrix γ (4.18) follows from (3.4), (3.10), (3.11), and (3.21):

$$\begin{aligned} \Gamma_{WH}\rho = &-i\omega[a^+a, \rho] + \gamma_\downarrow([a, \rho a^+] + [a\rho, a^+]) \\ &+ \gamma_\uparrow([a^+, \rho a] + [a^+\rho, a]), \end{aligned} \tag{4.19}$$

where a and a^+ are annihilation and creation operators, respectively,

$$a = (2\hbar m\omega)^{-1/2}(m\omega q + ip), \tag{4.20}$$

and where

$$\gamma_\uparrow = \left(\frac{m\omega}{\hbar}\langle q^2\rangle - \frac{1}{2}\right)\kappa, \tag{4.21a}$$

$$\gamma_\downarrow = \left(\frac{m\omega}{\hbar}\langle q^2\rangle + \frac{1}{2}\right)\kappa. \tag{4.21b}$$

The subscript WH stands for Weidlich and Haake, who have derived this generator from a microscopic model for the damped motion of a single mode of the electromagnetic field in a cavity [63].

It is well known that the process defined by Γ_{WH} obeys the symmetry of detailed balancing [60]. Moreover, we have shown now that, up to unitary transformations which map the annihilation operator a on $a\,\mathrm{ch}\,\varphi + a^+\,\mathrm{sh}\,\varphi$ with real φ, Γ_{WH} generates the only quantum Gauss Markov process with detailed balancing.

According to Ehrenfest's theorem one expects that the mean values of a quantum mechanical damped oscillator should obey the classical equations of motion

$$\langle \dot{q}\rangle = m^{-1}\langle p\rangle, \tag{4.22a}$$

$$\langle \dot{p}\rangle = -m\omega^2\langle q\rangle - \gamma_0\langle p\rangle. \tag{4.22b}$$

However, this is not in accordance with the equations for the mean values of a quantum damped oscillator with detailed balancing following from (3.21) and (4.18):

$$\langle \dot{q}\rangle = -\kappa\langle q\rangle + m^{-1}\langle p\rangle, \tag{4.23a}$$

$$\langle \dot{p}\rangle = -m\omega^2\langle q\rangle - \kappa\langle p\rangle. \tag{4.23b}$$

This raises the question of which of the assumptions leading to (4.23) is contrary to the equations of motion (4.22). The assumptions in question are:

1. the Gaussian assumption
2. detailed balancing
3. the Markov assumption.

ad. 1. In order to justify this assumption one may assume that the equations of motion of the total system are linear and that the density matrix is Gaussian at some initial time t_0. Hence, the Gaussian assumption is admissible. It is not in conflict with any basic physical principle.

ad. 2. As we have seen above, every system in thermal equilibrium shows detailed balancing and so must a damped harmonic oscillator.

ad. 3. It has been shown that for a system weakly coupled to a heat bath the long time dynamics of the reduced density matrix can be approximated by a Markovian master equation [37]. However, it has not been shown that the correlation functions can correctly be determined by the master equation. In order that the regression hypothesis could be derived from a microscopic model correlations of the system and the bath should be negligible for all times [64]. This repeated random-phase approximation is not implied by the Markovian assumption for the dynamics of the density matrix, although this has been claimed occasionally [17, 31, 65]. The derivation of the quantum regression hypothesis from Langevin equations for the coordinate and momentum with operator-valued, δ-correlated forces, as is done in Ref. [34], is merely another formulation of the Markovian assumption. For a further discussion see Section 7.

In concluding we find that the quantum regression hypothesis leads to the conflict of the principle of detailed balancing with Ehrenfest's theorem.

5. KMS Condition

Because the time evolution operator $e^{-(i/\hbar)Ht}$ and the Gibbs state $Z^{-1}e^{-\beta H}$ are essentially related by a Wick rotation, the correlation functions of arbitrary bounded operators u and v in a Gibbs state show particular analytical properties: $\langle u(t)\, v\rangle_\beta = \operatorname{tr} e^{(i/\hbar)Ht} u e^{-(i/\hbar)Ht} v Z^{-1} e^{-\beta H}$ can be continued to an analytical function in the interior of the strip $S_1 = \{z \mid z = t + iy,\ -\infty < t < \infty,\ -\hbar\beta \leqslant y \leqslant 0\}$, being continuous and bounded on the boundary of S_1; for $\langle vu(t)\rangle_\beta$ the same properties hold in $S_2 = \{z \mid z = t + iy,\ -\infty < t < \infty,\ 0 \leqslant y \leqslant \hbar\beta\}$ [66], and the two functions are connected by the KMS condition[5] [67]:

$$\langle u(z)\, v\rangle_\beta = \langle vu(z + i\hbar\beta)\rangle_\beta. \tag{5.1}$$

[5] Named after Kubo [72] and Martin and Schwinger [73].

For the significance and the wide-reaching consequences of the KMS conditions in statistical mechanics we refere to the literature [27, 68–71]. In the following sections we will draw conclusions from the analyticity and KMS conditions for Markov processes.

5.1. *KMS Condition for Markov Processes*

In order that the correlation functions of a quantum Markov process are analytical as described above, one finds as a necessary condition for the generator Γ of the process and the density matrix ρ_β from which the correlations are calulated

$$\text{(i)} \qquad \Gamma R_{\rho_\beta} = -R_{\rho_\beta}\Gamma^\dagger, \tag{5.2}$$

where R_{ρ_β} is the operator multiplying with ρ_β from the right. Equation (5.2) is proved by choosing a point $z \in S_1$ with $\operatorname{Re} z > 0$. Then $\langle u(z)\, v\rangle_\beta$ and $\langle u(-z^*)\, v\rangle_\beta$ are given by the analytical continuations of (2.26a) and (2.26b), respectively. In the limit $\operatorname{Re} z \to 0^+$ these expressions should coincide for all (bounded) operators u and v. Differentiating with respect to $\operatorname{Im} z$ in the limit $\operatorname{Im} z \to 0$ yields the desired result (5.2). If (5.2) acts on the identical Hilbert space operator we find with $\Gamma^\dagger 1 = 0$ (differentiate (2.22) with respect to t at 0^+) that ρ_β is stationary

$$\text{(ii)} \qquad \Gamma \rho_\beta = 0. \tag{5.3}$$

The KMS condition together with the quantum regression hypothesis implies

$$\text{(iii)} \qquad L_{\rho_\beta} G_z^\dagger = R_{\rho_\beta} G_{z+i\hbar\beta}^\dagger, \qquad \text{for all } z \in S_1 \text{ with } \operatorname{Re} z > 0, \tag{5.4}$$

and

$$\text{(iv)} \qquad \rho_\beta \text{ has an inverse.}$$

Corresponding conditions like (iii) exist for $z \in S_1$ and $\operatorname{Re} z < 0$, but since they do not contain anything new we do not give them here.

Choosing $z \in S_1$, $\operatorname{Re} z \geqslant 0$ the left- and the right-hand sides of (5.1) are given by the anaytical continuation of (2.26a), (2.26b), respectively. Using the fact that (5.1) holds for all bounded operators u and v immmediately yields (iii).

Conversely, the KMS condition (5.1) follows from (iii), if (iii) acts on u and if the result is multiplied by v and, finally, the trace is calculated.

Part (iv) is proved by assuming that ρ_β does not have an inverse. Then there are $\varphi, \psi \in \mathscr{H}$ for which $\rho_\beta \varphi = 0$ and $\rho_\beta \psi = \lambda\psi$ with $\lambda \neq 0$. Choosing $u = |\psi)(\varphi|$ and $v = |\varphi)(\psi|$ for $z = 0$ it follows from the left-hand side of (5.1)

$$\langle uv\rangle_\beta = \lambda(\varphi, \varphi)(\psi, \psi) \neq 0,$$

and for the right-hand side of (5.1)

$$\begin{aligned}\langle vu(i\hbar\beta)\rangle_\beta &= \operatorname{tr} v(G^\dagger_{i\hbar\beta}u)\,\rho_\beta \\ &= \operatorname{tr}(G^\dagger_{i\hbar\beta}u)\,\rho_\beta|\varphi)(\psi| = 0,\end{aligned}$$

where we have used the quantum regression hypothesis. Hence, the assumption that ρ_β is not invertible leads to a contradiction and consequently (iv) is proved.

Because of $\rho_\beta > 0$ and (iv) ρ_β can be used to define a scalar product of observables

$$(u, v)_\beta = \langle u^+ v\rangle_\beta. \tag{5.5}$$

From (iii) it follows that $\Gamma^\dagger$ is an antihermitian operator with respect to this scalar product

$$(u, \Gamma^\dagger v)_\beta = -(\Gamma^\dagger u, v)_\beta. \tag{5.6}$$

Hence, the spectrum of $\Gamma^\dagger$ is a part of the imaginary axis and because $\Gamma^\dagger$ is a "real" operator (i.e., $(\Gamma^\dagger u)^+ = \Gamma^\dagger u^+$), its spectrum is symmetric to the real axis. This resembles the spectrum of a Hamiltonian rather than a dissipative system, which one expects to lie in the complex left half plane. Actually, (i), (iii), and the quantum regression hypothesis only hold for Hamiltonian systems. This was first shown for systems in a finite-dimensional Hilbert space [47]. For the proof see Appendix C. For a general system in an infinite-dimensional Hilbert space a proof is given in Ref. [74].

As the main reason for this fact one will look upon the analyticity, because, e.g., the typical cusp of a Markovian autocorrelation function leads to a branch cut along the imaginary axis if time is continued to complex values. We can allow for these singularities by demanding analyticity in the half stripes $S_i^+ = S_i \cap \{z \mid \operatorname{Re} z > 0\}$ and $S_i^- = S_i \cap \{z \mid \operatorname{Re} z < 0\}$, $i = 1, 2$, separately. If, for the sake of simplicity, we consider systems with finite-dimensional Hilbert spaces the analyticity of Markovian correlation functions in $S_i^\pm$ already follows from the continuity of mean values. However, even in this case, the dissipative Liouville operator Γ is strongly restricted by the KMS condition (iv) [47]. In Appendix D we show that it is of the form

$$\Gamma\cdot = -\frac{i}{\hbar}[H, \cdot] - \sum_{k=1}^{N} \frac{2\pi n_k}{\beta\hbar} Q_k \cdot. \tag{5.7}$$

Here H is a hermitian operator defined by $H = -\ln \rho_\beta$ and n_k are positive integers; Q_k, $k = 1,..., N$, is a family of projection (super-) operators partitioning the unity, which commute with the Liouville operator defined by H:

$$\sum_{k=1}^{N} Q_k = \mathbf{1}, \tag{5.8}$$

$$Q_k Q_l = \delta_{kl} Q_l, \qquad \text{for all } k, l = 1, 2, \ldots, N, \tag{5.9}$$

$$[L_H - R_H, Q_k] = 0, \qquad \text{for all } k, l = 1, 2, \ldots, N. \tag{5.10}$$

The dissipative Liouville operator consists of a reversible Hamiltonian part $-(i/\hbar)[H, \cdot]$ and of an irreversible part $-\sum_{k=1}^{N} (2\pi n_k/\beta\hbar)\, Q_k$ which is a diagonable operator because of (5.8), (5.9). Of course, the first part is diagonable, too, and due to (5.10) even Γ. The spectrum of Γ consists in points $-(i/\hbar)(\varepsilon_i - \varepsilon_j) - (2\pi n_u/\beta\hbar)$, where ε_i, ε_j are the eigenvalues of H. Only if one of the n_k's is nonzero is Γ actually a dissipative Liouville operator. Then the damping constants are given by $\kappa = 2\pi/\hbar\beta$ or integer multiples of κ. For several reasons this is rather strange:

— The numerical value of κ for temperatures $T \geqslant 10^{-1}\mathrm{K}$ is too large: $\kappa/T \approx 10^{12}\,\mathrm{s}^{-1}\mathrm{K}^{-1}$. In contrast, e.g., atomic relaxation times vary from 10^{-10} s to 10^{-4}s.

— A linear temperature dependence of the damping constant is not observed experimentally.

— A damping constant measures the effective strength of the interaction of the considered system and its surroundings. For κ this is not the case, because κ is exclusively determined by the temperature and by Planck's and Boltzmann's constants of nature.

Hence, those Liouville operators (5.7), which are actually dissipative, are unphysical and merely mathematical artefacts. Therefore weakening the analyticity did not lead to the desired success.

In concluding we find that the quantum regression hypothesis and the KMS condition are compatible for Hamiltonian systems only. The results given so far are for systems with finite-dimensional Hilbert space. However, for systems with an infinite-dimensional Hilbert space at finite temperatures the dynamics can be approximated by disregarding states with an energy much larger than the thermal energy $\varepsilon \gg kT$. In many cases the remaining states span a finite Hilbert space. Moreover, in the next section we will draw the same conclusions as above for a system with an infinite-dimensional Hilbert space.

5.2. *KMS Condition for Stationary Quantum Gauss Markov Processes*

For Gauss processes it is sufficient to demand the analyticity and the KMS condition for the elements of the correlation matrix C (3.23), because then these properties hold for higher-order correlation functions automatically. From the analyticity it follows that $C(z)$ is an analytical function on the strip S_1. However, in general for a Gauss Markov process $C(z)$ has a branch cut for $\mathrm{Re}\, z = 0$ and a branching point at $z = 0$. The branch cut does not exist only if $C(t)$ is continuously

differentiable at $t=0$. With (3.28) it follows that this is the case exactly if the diffusion matrix D vanishes

$$D=\tfrac{1}{2}(\gamma C+C\gamma^{+})=0. \tag{5.11}$$

As one finds from (3.4), (3.10), and (3.11) this is the case only if Γ is a purely reversible, Hamiltonian Liouville operator

$$\Gamma\cdot=-\frac{i}{\hbar}[H,\cdot], \tag{5.12}$$

where

$$H=(2m)^{-1}p^2+\tfrac{1}{2}m\omega^2q^2+\tfrac{1}{2}r(pq+qp), \tag{5.12a}$$

m and ω being positive and r real with $|r|<\omega$. Hence, the Markov property and the analyticity are in conflict in general. Because this is the case for classical Markov processes, too, where analytical properties of correlation functions are violated at equal times (violation of higher sum rules [69]), this is not a severe objection against the quantum regression hypothesis. It merely displays the approximative nature of a Markovian description of a physical process at short times. Therefore we weaken the analyticity, by demanding it only in the half stripes S_1^+ and S_1^-, separately, as we already did in the preceding section. However, as a consequence of (3.24), this is fulfilled for any stationary Gauss Markov process. The KMS condition (5.2) for the correlation functions of a stationary Gauss process reads

$$C(z)=C(z^*-i\hbar\beta)^*. \tag{5.13}$$

Because of (3.24) this implies for a Markovian Gauss process

$$C=e^{i\hbar\beta\gamma}C^*. \tag{5.14}$$

From property (iv) of the preceding section and (3.8) it follows that C is invertible.[6] Therefore from (5.14) if follows

$$CC^{*-1}=e^{i\hbar\beta\gamma}. \tag{5.15}$$

One finds by inspection that CC^{*-1} is hermitian and even positive definite with respect to the scalar product

$$(x,y)=\sum_{i,j}x_iC_{ij}^{-1}y_j, \tag{5.16}$$

[6] Property (iii) implies that the state in which C is determined is a mixture because for a pure state ρ_β would not be invertible. For a mixture the inequality (3.8) holds. Consequently the determinant of C does not vanish.

where C^{-1} is used as a metric:

$$(x, CC^{*-1}y) = (CC^{*-1}x, y), \tag{5.17}$$

$$(x, CC^{*-1}x) \geqslant 0. \tag{5.18}$$

In this metric CC^{*-1} can be diagonalized and, consequently, γ too.[7] The eigenvectors of γ and CC^{*-1} coincide and for the eigenvalues $\lambda_{1,2}$ of γ it follows

$$\mu_{1,2} = e^{i\hbar\beta\lambda_{1,2}}, \tag{5.19}$$

where $\mu_{1,2}$ are the eigenvalues of CC^{*-1} which are positive because of (5.18). The product of μ_1 and μ_2 is unity because of $\det CC^{*-1} = 1$. Therefore we may put

$$\mu_{1,2} = e^{\mp \beta\hbar\omega}, \tag{5.20}$$

yielding

$$\lambda_{1,2} = \pm i\omega - \frac{2\pi n_{1,2}}{\hbar\beta}, \tag{5.21}$$

where $n_{1,2}$ are integer numbers, which must be positive because of the stationarity of the process.

The eigenvalues of the relaxation matrix determine the spectrum of the dissipative Liouville operator (3.28). Hence, we have the same results as in the finite-dimensional case. Again, the damping constants are linear functions of the temperature, independent of any parameter characterizing the coupling strength of the system and its environment. For the order of magnitude of the damping constant the same applies as in the finite-dimensional case: e.g., an electromagnetic field mode in a resonator may have a lifetime of 10^{-8}s or even longer.

In contrast to a system with finite-dimensional Hamiltonian for a Gauss process there should exist a classical limit which formally can be performed by sending $\hbar \to 0$. From (5.21) we obtain in this limit the damping constant being either diverging or zero. In the remainder of this section we will discuss the classical limit of the KMS condition. It implies that a classical Markov process is purely Hamiltonian provided that the correlation functions can be differentiated with respect to time. The latter condition excludes the case of a diverging damping, of course.

First we give the classical limit of the KMS condition. The differentiability with respect to t implies for small $\hbar$

$$\langle u(t)\, v\rangle_\beta = \langle vu(t)\rangle_\beta + i\hbar\beta \frac{d}{dt} \langle vu(t)\rangle_\beta + O(\hbar^2),$$

[7] Assume γ could be transformed to the Jordan normal form $\gamma = \lambda\mathbf{1} + N$, $N \neq 0$, $N^2 = 0$, only. Then (5.15) implies that $CC^{*-1} = e^{i\hbar\beta\lambda}(1 + N)$ cannot be diagonalized in contradiction to (5.17).

and consequently

$$\frac{i}{\hbar}\langle[u(t), v]\rangle_\beta = -\beta\frac{d}{dt}\langle vu(t)\rangle_\beta + O(\hbar). \tag{5.22}$$

In the limit $\hbar \to 0$ the observables u and v become phase space functions[8] and the commutator multiplied by $i/\hbar$ becomes the Poisson bracket

$$\lim_{\hbar\to 0}\frac{i}{\hbar}[u, v] = \{u, v\}, \tag{5.23}$$

where

$$\{u, v\} = \frac{\partial u}{\partial p}\frac{\partial v}{\partial q} - \frac{\partial u}{\partial q}\frac{\partial v}{\partial p}. \tag{5.23a}$$

Combining (5.22) and (5.23) yields the classical limit of the KMS condition [72, 75]:

$$\langle\{u(t), v\}\rangle_\beta = -\beta\frac{d}{dt}\langle u(t)\, v\rangle_\beta. \tag{5.24}$$

Now we may put

$$\rho = Z^{-1}e^{-\beta H}, \tag{5.25}$$

where

$$Z = \int dp\, dq\, e^{-\beta H}. \tag{5.26}$$

Then for the mean value of the Poisson bracket it follows

$$\langle\{u(t), v\}\rangle_\beta = \beta\langle v\{u(t), H\}\rangle_\beta. \tag{5.27}$$

For a classical Markov process the time derivative of a correlation function is given by (2.6), (2.11):

$$\frac{d}{dt}\langle vu(t)\rangle = \langle v\Gamma^\dagger u(t)\rangle, \tag{5.28}$$

where $\Gamma^\dagger$ is the generator of the Markov process. Because (5.24) should hold for all differentiable phase space functions v we find with (5.27), (5.28)

$$\Gamma^\dagger u = \{H, u\} \tag{5.29}$$

[8] For a more precise formulation of the classical limit see Ref. [76].

for all differentiable phase space functions u. Hence, the dynamics is Hamiltonian. This implies that the Poisson brackets of observables at different times cannot be described correctly in the Markovian approximation.

However, this is not a serious drawback because for a classical stochastic process the Poisson brackets have no special significance. This is rather different in the quantum case: here the KMS condition links different time orderings of correlation functions and represents an important symmetry of these correlation functions which, however, is violated by the quantum regression hypothesis.

6. Linear Response and FDT

For a Hamiltonian system which is initially prepared in a thermal equilibrium state and which is disturbed by small external forces $F_i(t)$ acting via the Hamiltonian $-\sum_i F_i(t)\, u_i$, the mean values of the observables u_i deviate from their equilibrium values by

$$\delta\langle u_i(t)\rangle = \sum_j \int_{-\infty}^{\infty} ds\, \chi_{ij}(t-s)\, F_j(s), \tag{6.1}$$

where the response function $\chi_{ij}(t)$ is given by the equilibrium expectation value of a commutator [72]

$$\chi_{ij}(t) = \theta(t)\langle [\delta u_i(t), \delta u_j]\rangle_\beta. \tag{6.2}$$

Here $\theta(t)$ is the unit step function and δu denotes the deviation of the operator u from its equilibrium mean value.

As is well known, the KMS condition relates the Fourier transform of the dissipative part of the response function

$$\chi''_{ij}(t) = \frac{1}{2i}(\chi_{ij}(t) - \chi_{ji}(-t)), \tag{6.3}$$

with the Fourier transform of the symmetrized correlation function

$$S_{ij}(t) = \tfrac{1}{2}\langle \delta u_i(t)\, \delta u_j + \delta u_j\, \delta u_i(t)\rangle_\beta \tag{6.4}$$

by the fluctuation dissipation theorem (FDT) [68, 72]:

$$\chi''_{ij}(\omega) = \frac{1}{\hbar} \operatorname{tgh} \frac{\hbar\omega\beta}{2} S_{ij}(\omega). \tag{6.5}$$

The classical limit of the FDT reads

$$\chi''_{ij}(\omega) = \frac{\omega\beta}{2} S_{ij}(\omega) \tag{6.6}$$

yielding in the time regime

$$\chi''_{ij}(t) = -\beta\theta(t)\frac{d}{dt}S_{ij}(t). \tag{6.7}$$

As for the KMS condition, the FDT still holds in the thermodynamic limit. Hence, for an open system being in thermal equilibrium with its surroundings the linear response to external forces acting on operators of the system is still determined by (6.1) and the FDT is valid in its present form (6.5).

For a classical process in thermal equilibrium the description by a continuous Markov process (i.e., by a Fokker–Planck equation) is compatible with the classical FDT [77]. This is not obvious because the classical KMS condition on which the proof of the classical FDT may be based is violated by any classical, non-Hamiltonian Markov process, as we have shown at the end of the preceding section. In deriving the FDT it is crucial to couple the external forces in the Fokker–Planck equation appropriately [23, 78]. Because the change of the transport coefficients due to the external forces turns out to be immaterial for the linear response, the stationary distribution function in the presence of constant external forces already determines the Fokker–Planck equation in the form of a transport equation [20–22] as far as it is needed in order to determine the linear response. In the remainder of Section 6 we will transfer these ideas to the quantum case and will determine the linear response of a quantum Gauss Markov process.

6.1. *The Linear Response for a Stationary Quantum Gauss Markov Process*

From microscopic considerations it is known that external forces acting on a classical open system alter both the stationary distribution of the system and the transport coefficients [78]. The same is true for quantum systems and in the case of a stationary quantum Gauss Markov process we must allow for changes both of the operators X_i determining the statics and of the operators Y_i determining the mean relaxations:

$$X_i^f = X_i + \delta X_i^f, \tag{6.8a}$$

$$Y_i^f = Y_i + \delta Y_i^f. \tag{6.8b}$$

We recall that X_i, Y_i, $i=1, 2$, defined by (3.4), (3.11), determine the dissipative Liouville operator $\Gamma = Y_1X_1 + Y_2X_2$ [3.10] in the absence of external forces. The deviations δX_i^f and δY_i^f are zero for vanishing external forces and they are nonlinear functionals of these forces in general. For the linear response the linear approximation in the forces is sufficient, of course. In the following we will denote the linear deviations by the same symbols as the exact ones, since there may be no confusion.

Before switching on the external forces the system is supposed to stay in the unperturbed stationary state

$$\rho(0) = \rho_{\mathrm{st}}, \tag{6.9}$$

where

$$\Gamma \rho_{\mathrm{st}} = 0. \tag{6.10}$$

Using (6.8a, b) in linear approximation in the external forces it follows from (2.15), (3.10) for the time rate of change of the deviation $\delta\rho(t) = \rho(t) - \rho_{\mathrm{st}}$:

$$\delta\dot{\rho}(t) = \Gamma\delta\rho(t) + (Y_1 \delta X_1^f + Y_2 \delta X_2^f)\, \rho_{\mathrm{st}}. \tag{6.11}$$

We note that the δY_i^f's do not contribute to the linear response. Hence, it is sufficient to know δX_i^f, which turn out to be already determined by the stationary density matrix in the presence of constant external forces.

6.1.1. *Stationary Density Matrix with External Forces*

Constant external forces acting on the coordinate and momentum operator of a Gaussian oscillator influence the stationary mean values of these operators but leave their variances unchanged. Hence, the stationary density matrix in the presence of external forces reads

$$\rho^f = Z^{-1} e^{-\beta(H - H^{\mathrm{ext}})}. \tag{6.12}$$

H is a quadratic form in q and p, which according to (3.6) is determined by the variances of q and p. Note that in contrast to (3.6) a factor β is extracted from the exponent, nevertheless H will be a function of β in general. H^{ext} is linear as well in q and p as in the external forces f_q, f_p:

$$H^{\mathrm{ext}} = -f_q q - f_p p. \tag{6.13}$$

f_q and f_p do not exactly coincide with the forces of the underlying microscopic model, rather they are renormalized by the system–bath interaction. We will determine the response to the forces appearing in (6.13). It is related to the response to the bare forces by a linear time-independent transformation which has to be determined from the microscopic model.

The mean values of coordinate and momentum with respect to ρ^f are linear in the external forces:

$$\begin{pmatrix} \langle q \rangle_f \\ \langle p \rangle_f \end{pmatrix} = \beta N^{-1} (\mathrm{arccth}\, N)^{-1} \frac{1}{2} (C + C^*) \begin{pmatrix} f_q \\ f_p \end{pmatrix}, \tag{6.14}$$

where

$$N = \frac{2}{\hbar} (\langle p^2 \rangle \langle q^2 \rangle - \frac{1}{4} \langle pq + qp \rangle^2)^{1/2}, \tag{6.15}$$

and where C are the stationary second moments in absence of the forces. Clearly ρ^f and ρ_{st} are connected by the unitary tranformation U, which shifts the mean values of coordinate and momentum by $-\langle q\rangle_f$ and $-\langle p\rangle_f$, respectively:

$$UqU^+ = q - \langle q\rangle_f, \tag{6.16}$$

$$UpU^+ = p - \langle p\rangle_f, \tag{6.17}$$

$$U\rho_{st}U^+ = \rho^f. \tag{6.18}$$

Replacing p and q in X_i by its shifted values (6.16), (6.17) yields the desired operators X_i^f:

$$X_1^f = X_1 - \langle p\rangle_f, \tag{6.19a}$$

$$X_2^f = X_2 - \langle q\rangle_f. \tag{6.19b}$$

By construction we have

$$X_i^f \rho^f = 0. \tag{6.20}$$

For the deviations it follows from (6.19)

$$\delta X_1^f = -\langle p\rangle_f, \tag{6.21a}$$

$$\delta X_2^f = -\langle q\rangle_f. \tag{6.21b}$$

Using (3.11), (6.21) the inhomogeneity in the equation of motion of the perturbed density matrix (6.11) can be written as the commutator with a hermitian operator H^f:

$$Y_1 \delta X_1^f + Y_2 \delta X_2^f = -\frac{i}{\hbar}[H^f, \cdot], \tag{6.22}$$

where

$$H^f = (r_1\langle q\rangle_f + r_3\langle p\rangle_f)\, p - (r_2\langle q\rangle_f + r_4\langle p\rangle_f)\, q. \tag{6.23}$$

H^f is linear in both q and p and the external forces f_q and f_p. H^f and H^{ext} do not coincide in general. Hence, one cannot couple the external forces by merely adding $-(i/\hbar)[H^{ext}, \cdot]$ to the dissipative Liouville operator.

6.1.2. *The Linear Response*

The functional dependence of X_i^f on the external forces is independent whether the forces are constant or time dependent. Using (6.21), (6.11) may be integrated with the initial condition (6.9) to yield

$$\delta\rho(t) = -\int_0^t ds\, e^{-\Gamma(t-s)}(\langle p\rangle_{f(s)}\, Y_1 + \langle q\rangle_{f(s)}\, Y_2)\, \rho_{st}. \tag{6.24}$$

Using the commutation relations of X_i and the symmetrized multiplications with q and p

$$[X_1, L_q + R_q] = \langle pq \rangle + \langle qp \rangle, \tag{6.25a}$$

$$[X_2, L_q + R_q] = 2\langle q^2 \rangle, \tag{6.25b}$$

$$[X_1, L_p + R_p] = 2\langle p^2 \rangle, \tag{6.25c}$$

$$[X_2, L_p + R_p] = \langle pq + qp \rangle \tag{6.25d}$$

yields

$$\begin{aligned} \Gamma(L_q + R_q)\,\rho_{\mathrm{st}} &= Y_1[X_1, L_q + R_q]\,\rho_{\mathrm{st}} + Y_2[X_2, L_q + R_q]\,\rho_{\mathrm{st}} \\ &= \langle pq + qp \rangle\, Y_1 \rho_{\mathrm{st}} + 2\langle q^2 \rangle\, Y_2 \rho_{\mathrm{st}}, \end{aligned} \tag{6.26}$$

and a similar equation for $\Gamma(L_p + R_p)\,\rho_{\mathrm{st}}$; these equations may be solved for $Y_i \rho_{\mathrm{st}}$:

$$\begin{pmatrix} Y_2 \rho_{\mathrm{st}} \\ Y_1 \rho_{\mathrm{st}} \end{pmatrix} = (C + C^*)^{-1} \begin{pmatrix} \Gamma(q\rho_{\mathrm{st}} + \rho_{\mathrm{st}} q) \\ \Gamma(p\rho_{\mathrm{st}} + \rho_{\mathrm{st}} p) \end{pmatrix}. \tag{6.27}$$

Combining (6.14) and (6.27) yields

$$\begin{aligned} \langle p \rangle_{f(s)}\, Y_1 + \langle q \rangle_{f(s)}\, Y_2 &= \tfrac{1}{2}\beta N^{-1}(\operatorname{arccth} N)^{-1} \\ &\quad \times \Gamma\{(q\rho_{\mathrm{st}} + \rho_{\mathrm{st}} q) f_q(s) + (p\rho_{\mathrm{st}} + \rho_{\mathrm{st}} p) f_p(s)\}. \end{aligned} \tag{6.28}$$

Now the linear response follows from (6.24), (6.28), and (6.26),

$$\begin{pmatrix} \delta\langle q(t) \rangle \\ \delta\langle p(t) \rangle \end{pmatrix} = \int_0^t ds\, \chi(t-s) \begin{pmatrix} f_q(s) \\ f_p(s) \end{pmatrix}, \tag{6.29}$$

where the response function is given by

$$\chi(t) = -\beta N^{-1}(\operatorname{arccth} N)^{-1}\, \theta(t) \frac{d}{dt} \frac{1}{2} (C(t) + C^*(t)). \tag{6.30}$$

Consequently, the Fourier transform of the dissipative response function (6.3) reads

$$\chi''(\omega) = \frac{\beta}{2} (N \operatorname{arccth} N)^{-1}\, \omega S(\omega), \tag{6.31}$$

where $S(\omega)$ is the Fourier transform of the symmetrized correlation matrix $\frac{1}{2}(C(t) + C^*(t))$.

In the classical limit, $\hbar \to 0$, the factor $N \operatorname{arccth} N$ becomes unity and the classical FDT (6.6) is recovered. For a Hamiltonian oscillator with frequency ω_0 the symmetrized correlation matrix $S(\omega)$ consists of two δ-functions at $\pm\omega_0$.

$$S(\omega) = S^+ \delta(\omega - \omega_0) + S^- \delta(\omega + \omega_0), \tag{6.32}$$

and N follows from (6.15)

$$N = \coth \frac{\beta\hbar\omega_0}{2}. \tag{6.33}$$

Because of the δ-functions in $S(\omega)$, ω_0 can be replaced by ω in the factor $(N \operatorname{arccth} N)^{-1}$, yielding the correct quantum FDT (6.5). For an irreversible quantum process the damping leads to a broadening and shift of the δ-functions in $S(\omega)$ and consequently (6.31) no longer represents the correct FDT. Because $S(\omega)$ is at least of second order in the damping constant, (6.31) still gives the correct result in the weak coupling limit, although the changes in the response due to environmental influences are not accounted for correctly.

7. Comparison with Different Approaches and Conclusions

In the present paper we investigated the description of open quantum systems by the quantum regression hypothesis. This hypothesis states that the dynamics of correlation functions is already known from that of mean values. In this sense it provides a generalization of the classical notion of a Markovian process to the quantum case. By comparing corresponding classical and quantum expressions for the time evolution of both mean values and correlation functions we showed the Markovian nature of a quantum process obeying the regression hypothesis more explicitly.

We only mention that an even deeper correspondence of classical and quantum processes than shown here can be established by introducing multitime density matrices which have similar properties as the joint multitime probabilities of a classical stochastic process [34, 35, 47]. For a system with observables commuting at all times these multitime density matrices become classical joint probabilities. Hence the multitime density matrices yield a key to a unified description of quantum and classical processes. Within this framework a Markovian process is defined as a process for which multitime density matrices at times $t_i,\ldots, t_n$ and $t_1,\ldots, t_n, t_{n+1}$ with $t_{n+1} \geqslant t_n \geqslant t_1, t_2,\ldots$ depend linearly on each other[9] [35, 47].

As a simple example we investigated the stationary Gauss Markov processes of an oscillator. As in the classical case the quantum Gauss Markov processes are completely determined by a transport matrix L with a positive hermitian part D and a positive correlation matrix C. Because of the commutation relation of coordinate and momentum L and C must be complex matrices in contrast to the classical case. Moreover, they are not independent of each other, because the relaxation matrix $\gamma = LC^{-1}$ must be real. Neither can γ and C be chosen independently because then D would not be positive in general. Therefore, there is less

[9] Classically this defines a Markov process as a whole class of processes having the same propagator but with arbitrary initial distributions, instead of a single process having the Markov property. In the latter case the generator may depend on the starting point or on the initial distribution [79, 80].

freedom in inventing quantum models than classical ones. A further complication arises for two interacting oscillators, or, more generally, for composed open systems with internal interactions. Then the interaction part of the Liouville operator does not only consist in a Hamiltonian part but it must contain a dissipative part in order that in the weak coupling limit (for the system with its environment) the stationary density matrix is given by the Gibbs state $Z^{-1}e^{-\beta H}$, where H is the Hamiltonian of the internally interacting system decoupled from its environment. No phenomenological means are known to determine the dissipative part of the interaction. In particular cases it was determined from microscopic models [81, 82].

So far the theory of quantum Markov processes appears to be somewhat more unwieldy than the classical one. However, applied to open systems in thermal equilibrium, quantum Markov processes violate basic symmetries of correlation functions which are proved to hold in the considered case. Such symmetries are

— the KMS condition

— the fluctuation dissipation theorem

— detailed balance (under certain conditions).

The violation of these basic physical principles does not necessarily imply that in certain limiting cases the predictions of the quantum regression hypothesis might not be in good quantitative agreement with the true behavior of the considered system. After a short discussion of other ways to describe open quantum systems we will come back to this important question.

First, we mention quantum Langevin equations, i.e., equations of motion for observables. According to these equations the time rate of change of an observable consists in a Hamiltonian part, a dissipative part, and a fluctuating force operator. In the presence of dissipation the latter is necessary in order to maintain commutation relations in the course of time [4, 28]. Hence, the fluctuating forces cause a unitary time evolution in spite of the damping forces. Because this unitary motion cannot take place in the system's Hilbert space, the fluctuating force operators are acting on a larger Hilbert space which in physical terms can be interpreted as the Hilbert space of the environment. Therefore, in the Langevin description the dynamics of the observables of the system evolves in a product space as it does microscopically. Mathematical aspects of this so-called stochastic dilation have been investigated recently [83]. For systems with an Euclidean state space the fluctuating forces are usually assumed to be Gaussian. As we have mentioned already, the assumption of δ-correlated fluctuating forces leads to the quantum regression hypothesis.

Most easily this can be seen for an oscillator. Then the following Langevin equations define a quantum Gauss Markov process

$$\dot{q}(t) = -r_3 q(t) - r_1 p(t) + F_q(t), \tag{7.1a}$$

$$\dot{p}(t) = -r_4 q(t) - r_2 p(t) + F_p(t), \tag{7.1b}$$

where r_i, $i = 1,..., 4$, are the elements of the relaxation matrix γ (3.21), and where the diffusion matrix D (3.26) is connected with the correlations of the fluctuating forces in the same way as classically

$$\begin{pmatrix} \langle F_q(t) F_q(s)\rangle & \langle F_q(t) F_p(s)\rangle \\ \langle F_p(t) F_q(s)\rangle & \langle F_p(t) F_p(s)\rangle \end{pmatrix} = 2D\,\delta(t-s). \tag{7.2}$$

The mean values of the fluctuating forces vanish

$$\langle F_q(t)\rangle = \langle F_p(t)\rangle = 0. \tag{7.3}$$

They constitute themselves a stationary quantum process which, however, is not in thermal equilibrium because the correlation functions of the fluctuating forces do not fulfill the KMS condition [84]. Consequently, the oscillator driven by these forces does not approach thermal equilibrium in general.

A Langevin equation for a Brownian particle of mass m moving in an external potential $V(q)$ and driven by a thermal equilibrium process was derived from a microscopic model in Ref. [29]:

$$m\ddot{q}(t) = -f\dot{q}(t) - \frac{\partial V}{\partial q} + E(t), \tag{7.4}$$

where f is the damping constant and $E(t)$ a Gaussian random force operator, independent of the initial values $q(0)$ and $\dot{q}(0)$, with vanishing mean value. Its second moments follow from

$$[E(t), E(s)] = 2i\hbar f \frac{\hat{o}}{\hat{o}t}\,\delta(t-s), \tag{7.5}$$

and

$$\tfrac{1}{2}\langle E(t)\,E(s) + E(s)\,E(t)\rangle = \frac{f}{\pi}\int_0^\infty d\omega\,\hbar\omega\,\coth\frac{\hbar\omega}{2kT}\cos\omega(t-s). \tag{7.6}$$

Note that the symmetrized mean (7.6) already follows from the commutator (7.5) by the KMS condition. Note further that in the limit $\hbar \to 0$ $E(t)$ becomes a classical white random force and (7.4) goes over to the classical Langevin equation.

Except for the case of a harmonic potential there is as yet nearly nothing known of how to gain information from the Langevin equations (7.4)–(7.6) [30, 85]. In particular the master equation corresponding to the Langevin equation is not known.

Some general properties of the master equations are known from microscopic considerations [23, 86]. For example, the master equation describing the relaxation of the reduced density matrix towards thermal equilibrium governs the dynamics of

the canonical equilibrium correlations, which for a Hamiltonian system are defined by

$$C_{uv}(t) = \beta^{-1} Z^{-1} \int_0^\beta d\alpha \, \mathrm{tr}\, e^{(i/\hbar)Ht} u e^{-(i/\hbar)Ht} e^{-\alpha H} v e^{-(\beta-\alpha)H}, \tag{7.7}$$

where u and v are observables, and where H is the Hamiltonian of the system. $Z = \mathrm{tr}\, e^{-\beta H}$ is the partition function. The time-ordered correlation function which we have dealt with as yet are connected with the canonical ones by the KMS condition:

$$\langle u(\omega)\, v \rangle = \frac{\hbar\omega\, \beta}{1 - e^{\hbar\omega\, \beta}} C_{uv}(\omega), \tag{7.8}$$

where $\langle u(\omega)\, v \rangle$, $C_{uv}(\omega)$ are the Fourier transforms of $\langle u(t)\, v \rangle$, $C_{uv}(t)$, respectively. These correlation functions obey the symmetry of detailed balancing as well as the fluctuation dissipation theorem (86–89). Hence, the canonical correlations are connected with the dynamics of the mean values by a regression theorem rather than the time-ordered correlations.

The path integral formulation of quantum mechanics provides yet another tool to deal with open quantum systems [32, 33]. For a Brownian particle moving in a harmonic potential the path integral treatment [90] and the Langevin equation (7.4) yield the same results both for relaxations of mean values from non-equilibrium states and for equilibrium correlations [91]. For the understanding of the influence of dissipation and of fluctuations on the decay rate of a metastable quantum state [7, 92, 93] and on the quantum coherence of a particle in a double well [94, 95] the path integral formulation has shown to be indispensable.

In the case of a harmonic oscillator its stationary behavior can be determined by a purely phenomenological consideration [96, 97]. It is based on the following assumptions:

(i) The mean values obey the classical equations of motion according to Ehrenfest's theorem.

(ii) The equilibrium correlation functions and the response functions are related by the FDT.

(iii) The process is a stationary Gauss process.

The first two assumptions are of general nature and the third one is based on the linearity of the considered problem. From the equations of motions of the mean values, given by assumption (i), the response function can easily be determined. With assumption (ii) this yields the matrix $C(t)$ of equilibrium correlation functions. By assumption (iii) the correlations $C(t)$ determine the process completely. The such defined process fulfills the KMS condition, it has the symmetry of detailed balancing, and by construction it obeys the Ehrenfest theorem and the

FDT. Starting from the equations of motion of mean values which follow from the Langevin equation (7.4) with a quadratic potential, and proceeding in the just described way, one gets the same stationary process as from this Langevin equation and the same one as from the path integral method. Thus for this particular simple case there are three equivalent phenomenological approaches. Moreover, in the succession of [29, 98] there are various microscopic investigations confirming these approaches [99–101].

Finally, we come back to the question of whether the quantum regression hypothesis could yield good quantitative predictions. We have already mentioned (see Section 4.2) that from a microscopic point of view the regression hypothesis can only hold if for all times the total density matrix factorizes in the reduced one and in that of the environment. Therefore the interaction of the open system with its environment must be small and consequently the damping constants of the reduced dynamics must be much smaller than the frequencies of the free time evolution

$$\gamma \ll \omega.$$

To be explicit, we consider the stationary Gaussian process with the classical mean value equations of a damped harmonic oscillator

$$\langle \dot{q} \rangle = m^{-1} \langle p \rangle, \tag{7.9a}$$

$$\langle \dot{p} \rangle = -m\omega_0^2 \langle q \rangle - \gamma \langle p \rangle. \tag{7.9b}$$

For weak damping the symmetrized correlation functions read [96]

$$\tfrac{1}{2}\langle q(t)\, q + qq(t) \rangle = \frac{\hbar}{2m\omega_0} e^{-(\gamma/2)t} \left\{ \coth \frac{\hbar\beta\,\omega_0}{2} \cos \omega_0 t + \frac{\beta\hbar\gamma}{4\mathrm{sh}^2(\hbar\beta\,\omega_0/2)} \sin \omega_0 t \right\} + \Delta_{qq}(t), \tag{7.10a}$$

$$\tfrac{1}{2}\langle p(t)\, q + qp(t) \rangle = -\frac{\hbar}{2} e^{-(\gamma/2)t} \left\{ \coth \frac{\hbar\beta\,\omega_0}{2} \sin \omega_0 t + \frac{\gamma}{2\omega_0} \left(\coth \frac{\hbar\beta\,\omega_0}{2} - \frac{\beta\hbar\omega_0}{2\mathrm{sh}^2(\hbar\beta\,\omega_0/2)} \right) \cos \omega_0 t \right\} + \Delta_{pq}(t), \tag{7.10b}$$

$$\tfrac{1}{2}\langle p(t)\, p + pp(t) \rangle = \frac{\hbar m\omega_0}{2} e^{-(\gamma/2)t} \left\{ \coth \frac{\hbar\beta\,\omega_0}{2} \cos \omega_0 t - \frac{\gamma}{2\omega_0} \left(2 \coth \frac{\hbar\beta\,\omega_0}{2} - \frac{\beta\hbar\omega_0}{2\mathrm{sh}^2(\hbar\beta\,\omega_0/2)} \right) \sin \omega_0 t \right\} + \Delta_{pp}(t), \tag{7.10c}$$

where $t \geqslant 0$ and where the functions $\Delta_{qq}(t)$, $\Delta_{pq}(t)$, $\Delta_{pp}(t)$ are defined by

$$\Delta_{qq}(t) = \frac{2\gamma}{m\beta} \sum_{n=1}^{\infty} \frac{\nu_n e^{-\nu_n t}}{(\nu_n^2 - (\gamma/2 + i\omega_0)^2)(\nu_n^2 - (\gamma/2 - i\omega_0)^2)}, \tag{7.11a}$$

$$\Delta_{pq}(t) = \frac{2\gamma}{\beta} \sum_{n=1}^{\infty} \frac{\nu_n^2 e^{-\nu_n t}}{(\nu_n^2 - (\gamma/2 + i\omega_0)^2)(\nu_n^2 - (\gamma/2 - i\omega_0)^2)}, \tag{7.11b}$$

$$\Delta_{pp}(t) = \frac{2\gamma m}{\beta} \sum_{n=1}^{\infty} \frac{\nu_n^3 e^{-\nu_n t}}{(\nu_n^2 - (\gamma/2 + i\omega_0)^2)(\nu_n^2 - (\gamma/2 - i\omega_0)^2)}. \tag{7.11c}$$

Here $\nu_n = 2\pi n/\hbar\beta$ are the Matsubara frequencies. Note that $\Delta_{pp}(t)$ and, hence, $\frac{1}{2}\langle p(t)\, p + p\, p(t)\rangle$ diverges at $t = 0$ [75]. If one allows for a damping coefficient which vanishes at a cutoff frequency $\omega_D \gg \omega_0$, $\Delta_{pp}(0)$ becomes finite. At very high temperatures one finds [96] asymptotically for $\hbar\beta\, \omega_D \ll 1$

$$\Delta_{pp}(0) \approx \tfrac{1}{12}(\hbar\beta)^2\, \gamma\, \omega_D\, \langle p^2\rangle_{\mathrm{cl}}. \tag{7.12}$$

Hence, $\Delta_{pp}(0)$ is very small compared with the classical value $\langle p^2\rangle_{\mathrm{cl}} = m/\beta$ which is assumed by the first part of (7.10c) at $t = 0$. At finite times $\Delta_{pp}(t)$ decreases faster than the first contribution of (7.10c). The same considerations apply for $\Delta_{pq}(t)$ and $\Delta_{qq}(t)$ and, hence, in the high-temperature limit the correlation functions of a classical Brownian oscillator are recovered. For lower temperatures, where $\beta\hbar\omega_c \gg 1$, $\Delta_{pp}(0)$ diverges logarithmically in the cutoff frequency

$$\Delta_{pp}(0) \approx \frac{\hbar\gamma M}{\pi} \ln(\beta\hbar\omega_D). \tag{7.13}$$

At very low temperatures where $\hbar\beta\, \gamma \gg 1$, $\Delta_{pp}(0)$ becomes

$$\Delta_{pp}(0) \approx 2\frac{\gamma}{\omega_0} \langle p^2\rangle_0 \ln\frac{\omega_D}{\omega_0}, \tag{7.14}$$

where $\langle p^2\rangle_0 = \frac{1}{2} m\hbar\omega_0$ is the momentum dispersion of an unperturbed oscillator in the ground state. In the latter case the Matsubara frequency ν_1 is much smaller than the damping constant γ and, according to (7.10), (7.11), the long time dynamics is governed by ν_1.[10]

The quantum regression hypothesis allows for a decay of correlations at the rate γ only, and, in view of the preceding remark, its validity is at least restricted to temperatures for which

$$\gamma \ll \nu_1, \tag{7.15a}$$

[10] At $T = 0$ all Matsubara frequencies contribute and add up to an algebraic decay, e.g., $\langle q(t)\, q + q\, q(t)\rangle \sim t^{-2}$ [96]. Similarly, the second moments of q and p relax algebraically form non-equilibrium initial states to their equilibrium values [102].

or equivalently

$$\hbar\beta\gamma \ll 1 \tag{7.15b}$$

is fulfilled. For these temperatures $\Delta_{qq}(t)$, $\Delta_{pq}(t)$, $\Delta_{pp}(t)$ assume values of the order ω_0/γ at time $t=0$ and decrease rapidly to zero on the time scale $\hbar\beta$. Such initial slips are well known for certain non-Markovian processes [103, 104], but they cannot be accounted for by the quantum regression hypothesis.

In the weak coupling limit, i.e., for $\gamma \to 0$, $t \to \infty$ and γt held finite, the correlation functions become

$$\langle q(t)\, q\rangle = \frac{\hbar}{2m\omega_0} e^{-(\gamma/2)t} \left\{ \coth\frac{\hbar\beta\omega_0}{2} \cos\omega_0 t - i \sin\omega_0 t \right\}, \tag{7.16a}$$

$$\langle p(t)\, q\rangle = -\frac{i\hbar}{2} e^{-(\gamma/2)t} \left\{ \cos\omega_0 t - i \coth\frac{\hbar\beta\omega_0}{2} \sin\omega_0 t \right\}, \tag{7.16b}$$

$$\langle p(t)\, p\rangle = \frac{\hbar m\omega_0}{2} e^{-(\gamma/2)t} \left\{ \coth\frac{\hbar\beta\omega_0}{2} \cos\omega_0 t - i \sin\omega_0 t \right\}, \tag{7.16c}$$

where we have used (7.10) and the fact that the expectation value of the commutator follows with the FDT immediately from the equations of motion of the mean values:

$$\langle [q(t), q]\rangle = \frac{\hbar}{i}\chi_{qq}^{(t)} = -\frac{i\hbar}{m\omega_0} e^{-(\gamma/2)t} \sin\omega_0 t. \tag{7.17}$$

Equations (7.16) are of the form of Markovian correlation functions. By use of (3.4), (3.10), (3.11) we recover the dissipative Liouville operator of Weidlich and Haake. A discussion of the stationary process of a damped quantum oscillator in the whole range of damping and temperature is found in Ref. [105].

In concluding we remark that the quantum regression hypothesis can only give correct results in zeroeth order in the damping constant according to the weak coupling limit. This is quite different from the classical case where large damping does not exclude a Markovian modelling.

A. The Dissipative Liouville Operator (3.10)

For a more detailed derivation of the dissipative Liouville operator see Refs. [47, 48].

For a Gauss process we may restrict ourselves to correlation functions of two operators at different times because more complicated multitime expectations can be determined by means of the Gaussian property.

First we formulate the Gaussian property for a process described by p and q. The

momentum and coordinate form a Gaussian process if the correlation functions of two arbitrary products $p^k q^l$ at different times $t_1 = t + \tau$, $t_2 = t$, factorize into a sum of products of $\langle p(t_i)\, p(t_j)\rangle$, $\langle p(t_i)\, q(t_j)\rangle$, $\langle q(t_i)\, p(t_j)\rangle$, $\langle q(t_i)\, q(t_j)\rangle$, with $i, j = 1, 2$ according to one of the following recursion relations:

$$\begin{aligned}\langle (p^k q^l)(\tau)\, p^m q^n\rangle &= (k-1)\langle p^2\rangle \langle (p^{k-2} q^l)(\tau)\, p^m q^n\rangle \\ &\quad + l\langle pq\rangle \langle (p^{k-1} q^{l-1})(\tau)\, p^m q^n\rangle \\ &\quad + m\langle p(\tau)\, p\rangle \langle (p^{k-1} q^l)(\tau)\, p^{m-1} q^n\rangle \\ &\quad + n\langle p(\tau)\, q\rangle \langle (p^{k-1} q^l)(\tau)\, p^m q^{n-1}\rangle \qquad \text{(A.1a)} \\ &= k\langle pq\rangle \langle (p^{k-1} q^{l-1})(\tau)\, p^m q^n\rangle \\ &\quad + (l-1)\langle q^2\rangle \langle (p^k q^{l-2})(\tau)\, p^m q^n\rangle \\ &\quad + m\langle q(\tau)\, p\rangle \langle (p^k q^{l-1})(\tau)\, p^{m-1} q^n\rangle \\ &\quad + n\langle q(\tau)\, q\rangle \langle (p^k q^{l-1})(\tau)\, p^m q^{n-1}\rangle. \qquad \text{(A.1b)}\end{aligned}$$

In (A.1a) we have factorized with respect to one of the p's in the product $(p^k q^l)(\tau)$ and in (A.1b) with respect to one of the q's in the same product $(p^k q^l)(\tau)$. The corresponding factorizations with respect to a p or q in the product $p^m q^n$ are also possible because they lead to the same result. Gaussian correlation functions of operators with more than two times can be found by analogous factorization procedures, but we will not give them here because their form is obvious.

For $\tau = 0$ (A.1a, b) can be obtained directly from (3.1a, b) so that (A.1a, b) lead to the same stationary density matrix, of course. Further we remark that the above definition of a quantum mechanical Gauss process is not restricted to the Markovian case. In order to get a Gauss Markov process, the correlation functions must have the special form (2.26). Because the propagator $G_t^\dagger$ is uniquely determined by the generator $\Gamma^\dagger$ (see (2.17)), it is sufficient to look at the time rates of change of the correlation functions at $\tau = 0$. Therefore, we differentiate (A.1a, b) with respect to $\tau > 0$ and put $\tau = 0$ afterwards. Using (2.26), the cyclic invariance of the trace, and the canonical commutation relations we get from the fact that $p^k q^l$ are linearly independent operators for $k, l = 0, 1, 2, \ldots$:

$$\begin{aligned}&-\frac{\hbar}{i}[L_p, \Gamma^\dagger] + \langle pq\rangle [L_p - R_p, \Gamma^\dagger] + \langle p^2\rangle [R_q - L_q, \Gamma^\dagger] \\ &\quad = \frac{\langle \dot{p}p\rangle(\langle p^2\rangle\langle q^2\rangle - \langle pq\rangle^2) + (\hbar/i)\langle \dot{p}q\rangle\langle p^2\rangle}{\langle p^2\rangle\langle q^2\rangle - |\langle pq\rangle|^2} L_q - \langle \dot{p}p\rangle R_q \\ &\quad\quad - \frac{\langle \dot{p}q\rangle(\langle p^2\rangle\langle q^2\rangle - \langle qp\rangle^2) - (\hbar/i)\langle \dot{p}p\rangle\langle q^2\rangle}{\langle p^2\rangle\langle q^2\rangle - |\langle pq\rangle|^2} L_p + \langle \dot{p}q\rangle R_p \\ &\quad\quad -\frac{\hbar}{i}[R_q, \Gamma^\dagger] + \langle pq\rangle [R_q - L_q, \Gamma^\dagger] + \langle q^2\rangle [L_p - R_p, \Gamma^\dagger] \qquad \text{(A.2a)}\end{aligned}$$

$$= \frac{\langle \dot{q}p \rangle (\langle p^2 \rangle \langle q^2 \rangle - \langle pq \rangle^2) + (\hbar/i) \langle \dot{q}q \rangle \langle p^2 \rangle}{\langle p^2 \rangle \langle q^2 \rangle - |\langle pq \rangle|^2} L_q - \langle \dot{q}p \rangle R_q$$

$$- \frac{\langle \dot{q}q \rangle (\langle p^2 \rangle \langle q^2 \rangle - \langle qp \rangle^2) - (\hbar/i) \langle \dot{q}p \rangle \langle q^2 \rangle}{\langle p^2 \rangle \langle q^2 \rangle - |\langle pq \rangle|^2} L_p - \langle \dot{q}q \rangle R_p, \quad \text{(A.2b)}$$

where L_u and R_u are left and right multiplication operators, respectively, defined in (3.12), and where $\langle \dot{q}q \rangle$, $\langle \dot{q}p \rangle$, $\langle \dot{p}p \rangle$ are derivatives of the respective correlation functions at $\tau = 0^+$, e.g.,

$$\langle \dot{q}q \rangle = \lim_{\tau \to 0^+} \frac{d}{d\tau} \langle q(\tau)\, q \rangle. \quad \text{(A.3)}$$

Equations (A.2a, b) are linear inhomogeneous equations for the generator Γ which have (3.10) as a unique solution, satisfying $\Gamma^\dagger 1 = 0$.

The constants r_i, $i = 1$–4, appearing in (3.10) are determined by the stationary second moments and the time derivatives of correlation functions $\tau = 0$:

$$r_1 = -\frac{\langle \dot{q}q \rangle \langle qp \rangle - \langle \dot{q}p \rangle \langle q^2 \rangle}{\langle p^2 \rangle \langle q^2 \rangle - |\langle pq \rangle|^2}, \quad \text{(A.4a)}$$

$$r_2 = \frac{\langle \dot{p}p \rangle \langle q^2 \rangle - \langle \dot{p}q \rangle \langle qp \rangle}{\langle p^2 \rangle \langle q^2 \rangle - |\langle pq \rangle|^2}, \quad \text{(A.4b)}$$

$$r_3 = \frac{\langle \dot{q}q \rangle \langle p^2 \rangle - \langle \dot{q}p \rangle \langle pq \rangle}{\langle p^2 \rangle \langle q^2 \rangle - |\langle pq \rangle|^2}, \quad \text{(A.4c)}$$

$$r_4 = -\frac{\langle \dot{p}p \rangle \langle pq \rangle - \langle \dot{p}q \rangle \langle p^2 \rangle}{\langle p^2 \rangle \langle q^2 \rangle - |\langle pq \rangle|^2}. \quad \text{(A.4d)}$$

B. Positivity of the Dissipative Liouville Operator (3.10)

We consider the relaxation of the second moments $\langle q^2(t) \rangle_0$, $\langle (pq)(t) \rangle_0$, $\langle p^2(t) \rangle_0$ which form a positive semidefinite matrix $N(t)$ for $t \geqslant 0$:

$$N(t) = \begin{pmatrix} \langle q^2(t) \rangle_0 & \langle (qp)(t) \rangle_0 \\ \langle (pq)(t) \rangle_0 & \langle p^2(t) \rangle_0 \end{pmatrix}. \quad \text{(B.1)}$$

The positivity is a consequence of $\langle q^2(t) \rangle_0 > 0$ and

$$\det N(t) = \langle q^2(t) \rangle_0 \langle p^2(t) \rangle_0 - |\langle (pq)(t) \rangle_0|^2 \geqslant 0 \quad \text{(B.2)}$$

as follows by the same kind of argument explained after (3.8). As a special case of (B.1) we note

$$C > 0. \quad \text{(B.3)}$$

The equations of motion of the matrix elements of $N(t)$ follow from those of the corresponding Heisenberg operators $p^2(t) = G_t^\dagger p^2$, etc. after averaging over an initial nonequilibrium density matrix. In matrix notation they read

$$\dot{N}(t) = -\gamma N(t) - N(t)\,\gamma^+ + 2D \tag{B.4}$$

where the diffusion matrix D is defined in (3.26). Again, this is in accordance with the classical result. Starting from any nonequilibrium value $N(0)$, for a stationary process $N(t)$ relaxes to C. Hence, the real part of the eigenvalues of γ must be positive. A necessary condition for this to hold is

$$r_2 + r_3 \geqslant 0. \tag{B.5}$$

The general solution of (B.4) is simply

$$N(t) = e^{-\gamma t} N(0)\, e^{-\gamma^+ t} + 2\int_0^t ds\, e^{-\gamma s} D e^{-\gamma^+ s}. \tag{B.6}$$

Hence, D being semipositive definite is sufficient for $N(t)$ to stay positive semidefinite for all $t \geqslant 0$ provided $N(0) > 0$. We now show that it is even necessary for D to be positive semidefinite in order to have a positive $N(t)$. For this purpose we consider a particular $N(0)$, which implies just equality in (B.2):

$$N(0) = \begin{pmatrix} \langle q^2\rangle_0 & \sigma\sqrt{\langle p^2\rangle_0 \langle q^2\rangle_0 - \left(\frac{\hbar}{2}\right)^2} + \frac{i\hbar}{2} \\ \sigma\sqrt{\langle p^2\rangle_0 \langle q^2\rangle_0 - \left(\frac{\hbar}{2}\right)^2} - \frac{i\hbar}{2} & \langle p^2\rangle_0 \end{pmatrix}, \tag{B.7}$$

where $\sigma = \pm 1$; $\langle p^2\rangle_0$, $\langle q^2\rangle_0$ may have arbitrary positive values in the physical range $\langle p^2\rangle_0 \langle q^2\rangle_0 \geqslant (\hbar/2)^2$. Then there is a vector $\mathbf{x}_0$

$$\mathbf{x}_0 = \begin{pmatrix} \sigma\sqrt{\langle p^2\rangle_0 \langle q^2\rangle_0 - \left(\frac{\hbar}{2}\right)^2} + \frac{i\hbar}{2} \\ -\langle q^2\rangle_0 \end{pmatrix}, \tag{B.8}$$

which is annihilated by $N(0)$:

$$N(0)\,\mathbf{x}_0 = 0. \tag{B.9}$$

By the scalar multiplication of $N(t)\,\mathbf{x}_0$ with $\mathbf{x}_0$ we find for sufficiently small times from the positivity of $N(t) = N(0) + \dot{N}(0)\,t + O(t^2)$

$$(\mathbf{x}_0, D\mathbf{x}_0) \geqslant 0, \tag{B.10}$$

where we used (B.4) and (B.9). Because $\mathbf{x}_0$ is not an arbitrary vector the positivity of D does not follow immediately from (B.10). From (B.8) and (B.10) it follows

$$D_{11}x^2 - 2(\sigma\sqrt{1-y^2}\,\mathrm{Re}\,D_{12} + y\,\mathrm{Im}\,D_{12})\,x + D_{22} \geqslant 0, \tag{B.11}$$

where D_{ij} are the elements of the matrix D and where

$$x = \sqrt{\frac{\langle p^2\rangle_0}{\langle q^2\rangle_0}}, \tag{B.12a}$$

$$y = \frac{\hbar}{2\sqrt{\langle p^2\rangle_0\langle q^2\rangle_0}}. \tag{B.12b}$$

x is an arbitrary positive number, and, hence, D_{11} and D_{22} must not be negative. From (3.26) and (B.5) it follows $\mathrm{Im}\,D_{12} \geqslant 0$. Now we can choose $\sigma = \pm 1$ and $y \in (0, 1]$ such that

$$\sigma\sqrt{1-y^2}\,\mathrm{Re}\,D_{12} + y\,\mathrm{Im}\,D_{12} = |D_{12}|. \tag{B.13}$$

Then (B.11) becomes

$$D_{11}x^2 - 2|D_{12}|x + D_{22} \geqslant 0 \qquad \text{for all } x > 0, \tag{B.14}$$

and consequently

$$D_{11}D_{22} \geqslant |D_{12}|^2. \tag{B.15}$$

Hence, as in the classical case D must be positive semidefinite. It is worth noting that a dissipative Liouville operator of the form given in Section 3.2 with positive semidefinite D is even completely positive [51]. The ordinary positivity which guarantees that mean values of positive observables stay positive for all times is generally a weaker condition. However, in the present case of a stationary Gauss Markov process, already the positivity of the second moments is sufficient for the complete positivity to hold.

C. Counterexample of a Positive Dissipative Liouville Operator

Let us consider the Fokker–Planck operator of a Brownian oscillator

$$\Gamma_{\mathrm{BO}} = -\frac{\partial}{\partial q}\frac{p}{m} + \frac{\partial}{\partial p}(m\omega^2 q + \gamma_0 p) + \gamma_0\langle p^2\rangle\frac{\partial^2}{\partial p^2} \tag{C.1}$$

as the Wigner representation of a dissipative Liouville operator, which according to (3.14) reads

$$\Gamma\rho = -\frac{i}{\hbar}[H, \rho] - \frac{i}{\hbar}\frac{\gamma_0}{2}[q, p\rho + \rho p] - \frac{\langle p^2\rangle}{\hbar^2}\gamma_0[q, [q, \rho]], \tag{C.2}$$

where

$$H=\frac{1}{2m}p^2+\frac{1}{2}m\omega^2q^2. \tag{C.3}$$

This form has repeatedly been postulated in the literature [52–54].

From (C.2), (C.3) we find $r_1=-1/m$, $r_2=\gamma_0$, $r_3=0$, $r_4=m\omega^2$, and $\langle p^2\rangle = m^2\omega^2\langle q^2\rangle$. However, this yields the diffusion matrix

$$D=\gamma_0\begin{pmatrix} 0 & \frac{i\hbar}{4} \\ -\frac{i\hbar}{4} & \langle p^2\rangle \end{pmatrix} \tag{C.4}$$

which is not positive semidefinite.

In order to demonstrate the unphysical nature of the dissipative Liouville operator (C.2) we consider as initial state a pure state $|\psi)(\psi|$ where ψ is the normalized ground state of the annihilation operator b:

$$b=\frac{\sigma}{\hbar}\left(q+i\frac{\hbar}{2\sigma^2}p\right), \qquad \sigma>0, \tag{C.5}$$

$$b\psi=0. \tag{C.6}$$

In this state we find

$$\langle q\rangle_0=\langle p\rangle_0=0, \tag{C.7}$$

$$\langle q^2\rangle_0=\left(\frac{\hbar}{2\sigma}\right)^2, \tag{C.8}$$

$$\langle p^2\rangle_0=\sigma^2, \tag{C.9}$$

$$\langle pq\rangle_0=\frac{\hbar}{2i}. \tag{C.10}$$

Hence, ψ is a squeezed state in general. By construction, the expectation value of the observable b^+b in this state vanishes. Hence, for short times it follows

$$\begin{aligned}\langle (b^+b)(t)\rangle_0 &= t\ \mathrm{tr}\ b^+b\Gamma\rho_0 \\ &= -t\frac{\gamma_0}{2\sigma^2}(\sigma^2-\langle p^2\rangle),\end{aligned} \tag{C.11}$$

where we have used (C.2). Choosing σ^2 larger than the stationary dispersion $\langle p^2\rangle$ we find a negative expectation value of the positive observable b^+b.

D. The Dissipative Liouville Operator (5.7)

First we will prove the form (5.7) of a dissipative Liouville operator of a system in a finite-dimensional Hilbert space, the correlation functions of which satisfy the KMS condition. Finally, we will draw the consequences following from the condition of analyticity (5.2).

It is well known that every continuous one-parameter semigroup of linear operators G_t, $t \geqslant 0$, on a finite-dimensional vector space can be continued to an analytical group on the complex plane,

$$G_{z_1} G_{z_2} = G_{z_1 + z_2} \qquad \forall z_1, z_2 \in \mathbb{C}, \tag{D.1}$$

consequently

$$[G_{z_1}, G_{z_2}] = 0 \qquad \forall z_1, z_2 \in \mathbb{C}. \tag{D.2}$$

We recall the KMS condition (5.4)

$$L_{\rho_\beta} G^\dagger = R_{\rho_\beta} G^\dagger_{z + i\hbar\beta}, \tag{D.3}$$

where ρ_β can be written as (see property (iv) in Section 5.1)

$$\rho_\beta = Z^{-1} e^{-\beta H}. \tag{D.4}$$

$Z = \operatorname{tr} e^{-\beta H}$ is the partition function and H is a hermitian operator depending on β in general.

Equations (D.3) and (D.4) imply with $G_0^\dagger = \mathbf{1}$

$$G^\dagger_{i\hbar\beta} = e^{i\hbar\beta L^\dagger}, \tag{D.5}$$

where $L^\dagger$ is the Liouville operator defined by H

$$L^\dagger = \frac{\hbar}{i}(L_H - R_H). \tag{D.6}$$

Here we have made use of some trivial properties of multiplication operators: R_x and L_x are invertible if and only if x is invertible, and one has

$$R_x^{-1} = R_{x^{-1}}, \tag{D.7a}$$

$$L_x^{-1} = L_{x^{-1}}. \tag{D.7b}$$

Left and right multiplication operators commute

$$R_x L_y = L_y R_x \qquad \text{for all operators, } x \text{ and } y. \tag{D.8}$$

If one operator is a function of another the same functional dependence applies for the corresponding multiplication operators

$$L_{f(x)} = f(L_x), \tag{D.9a}$$

$$R_{f(x)} = f(R_x). \tag{D.9b}$$

From (D.2) and (D.5) we find

$$[G_z^\dagger, e^{i\hbar\beta L^\dagger}] = 0 \tag{D.10}$$

and by differentiating with respect to z at $z = 0$

$$[\Gamma^\dagger, e^{i\hbar\beta L^\dagger}] = 0, \tag{D.11}$$

where $\Gamma^\dagger$ is the generator of the semigroup $G_t^\dagger$. As a commutator with a hermitian operator, $L^\dagger$ is diagonable and has purely imaginary eigenvalues. Therefore (D.11) implies that $\Gamma^\dagger$ and $L^\dagger$ commute:

$$[\Gamma^\dagger, L^\dagger] = 0. \tag{D.12}$$

Hence, (D.5) implies

$$e^{i\hbar\beta(\Gamma^\dagger - L^\dagger)} = \mathbf{1}. \tag{D.13}$$

With the logarithm of the identity [108] we find from (D.12), (D.13) the desired representation (5.7)–(5.10).

We recall that because of the analyticity $\Gamma^\dagger$ is antihermitian (see (5.6)) with respect to the scalar product (5.5). It is easy to show that the same is true for $L^\dagger$. Consequently the exponent of the left-hand side of (D.13) is hermitian and we find as the unique solution of (D.13)

$$\Gamma^\dagger = L^\dagger = \frac{\hbar}{i}[H, \cdot] \tag{D.14}$$

as we have claimed in Section 5.1.

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References

1. V. Weisskopf and E. P. Wigner, *Z. Phys.* **63** (1930), 54.
2. G. S. Agarwal, "Quantum Statistical Theories of Spontaneous Emission and Their Relation to Other Approaches," Springer Tracts in Modern Physics, Vol. 70, Springer–Verlag, Berlin, 1974.

3. C. P. SLICHTER, "Principles of Magnetic Resonance," Harper, New York, 1963.
4. H. HAKEN, "Handbuch für Physik," Bd. XXV/2c, Springer–Verlag, Berlin, 1970.
5. V. M. KENKRE AND P. REINEKER, "Exciton Dynamics in Molecular Crystals and Aggregates," Springer Tracts in Modern Physics, Vol. 94, Springer–Verlag, Berlin, 1982.
6. V. NARAYANAMURTI AND R. O. POHL, *Rev. Modern Phys.* **42** (1970), 201.
7. A. O. CALDEIRA AND A. J. LEGGETT, *Ann. Phys. (N. Y.)* **149** (1983), 374.
8. P. RING AND P. SCHUCK, "The Nuclear Many-Body Problem," Springer–Verlag, Berlin, 1980.
9. E. SCHRÖDINGER, *Naturwissenschaften* **23** (1935), 807.
10. A. EINSTEIN, *Ann. Physik* **17** (1905), 549; **19** (1906), 371.
11. N. WAX, "Selected Papers on Noise and Stochastic Processes," Dover, New York, 1954.
12. R. GRAHAM, "Statistical Theory of Instabilities in Stationary Nonequilibrium Systems with Applications to Lasers and Nonlinear Optics," Springer Tracts in Modern Physics, Vol. 66, Springer–Verlag, Berlin, 1973.
13. H. HAKEN, *Rev. Modern Phys.* **47** (1975), 67.
14. P. C. HOHENBERG AND B. I. HALPERIN, *Rev. Modern Phys.* **49** (1977), 435.
15. N. G. VAN KAMPEN, "Stochastic Processes in Physics and Chemistry," North–Holland, Amsterdam, 1981.
16. P. HÄNGGI AND H. THOMAS, *Phys. Rep.* **88** (1982), 207.
17. C. W. GARDINER, "Handbook of Stochastic Methods," Springer–Verlag, Berlin, 1983.
18. H. RISKEN, "The Fokker Planck Equation," Springer–Verlag, Berlin, 1983.
19. L. ONSAGER, *Phys. Rev.* **37** (1931), 405; **38** (1931), 2265.
20. M. S. GREEN, *J. Chem. Phys.* **20** (1952), 1281.
21. H. GRABERT AND M. S. GREEN, *Phys. Rev. A* **19** (1979), 1747.
22. H. GRABERT, R. GRAHAM, AND M. S. GREEN, *Phys. Rev. A* **21** (1980), 2136.
23. H. GRABERT, "Projection Operator Techniques in Nonequilibrium Statistical Mechanics," Springer Tracts in Modern Physics, Vol. 95, Springer–Verlag, Berlin, 1982.
24. R. W. HASSE, *J. Math. Phys.* **16** (1975), 2005.
25. R. W. HASSE, *Rep. Progr. Phys.* **41** (1978), 1027.
26. F. BLOCH, *Phys. Z.* **29** (1928), 58.
27. A. L. FETTER AND J. D. WALECKA, "Quantum Theory of Many Particle Systems," McGraw–Hill, New York, 1971.
28. I. R. SENITZKY, *Phys. Rev.* **119** (1960), 670; *Phys. Rev.* **124** (1961), 642.
29. G. W. FORD, M. KAC, AND P. MAZUR, *J. Math. Phys.* **6** (1965), 504.
30. R. BENGURIA AND M. KAC, *Phys. Rev. Lett.* **46** (1981), 1.
31. F. HAAKE, *in* "Springer Tracts in Modern Physics," Vol. 66, p. 98, Springer–Verlag, Berlin, 1973.
32. R. P. FEYNMAN AND A. R. HIBBS, "Quantum Mechanics and Path Integrals," McGraw–Hill, New York, 1965.
33. R. P. FEYNMAN AND F. L. VERNON, *Ann. Phys. (N. Y.)* **24** (1963), 118; siehe auch [32], Kapitel 12.
34. M. LAX, *Phys. Rev.* **172** (1968), 350.
35. R. BAUSCH AND A. STAHL, *Z. Phys.* **194** (1966), 436; **204** (1967), 32.
36. H. HAKEN AND W. WEIDLICH, *Z. Phys.* **205** (1967), 96.
37. H. SPOHN, *Rev. Modern Phys.* **52** (1980), 569.
38. H. DEKKER, *Phys. Rep.* **80** (1981), 1.
39. K. YOSIDA, "Functional Analysis," Springer–Verlag, Berlin, 1971.
40. J. VON NEUMANN, "Mathematische Grundlagen der Quantenmechanik," Springer–Verlag, Berlin, 1968.
41. E. B. DAVIES, "Quantum Theory of Open Systems," Academic Press, New York/London, 1976.
42. V. GORINI, A. FRIGERIO, M. VERRI, A. KOSSAKOWSKI, AND E. C. G. SUDARSHAN, *Rep. Math. Phys.* **13** (1978), 149.
43. H. GRABERT, P. HÄNGGI, AND P. TALKNER, *Phys. Rev. A* **19** (1979), 2440.
44. F. HAAKE AND W. WEIDLICH, *Z. Phys.* **213** (1968), 451.
45. L. MANDEL, *Phys. Rev.* **152** (1966), 438.

46. R. J. GLAUBER, *in* "Les Houches 1964, Quantum Optics and Electronics" (C. DeWitt, A. Blandin, and C. Cohen–Tannoudji, Eds.), Gordon & Breach, New York, 1965.
47. P. TALKNER, "Untersuchungen irreversibler Prozesse in quantenmechanischen Systemen," Dissertation, Stuttgart, 1979.
48. P. TALKNER, *Z. Phys. B* **41** (1981), 365.
49. E. P. WIGNER, *Phys. Rev.* **40** (1932), 749.
50. M. CH. WANG AND G. E. UHLENBECK, *Rev. Modern Phys.* **17** (1945), 323.
51. G. LINDBLAD, *Rep. Math. Phys.* **10** (1976), 393.
52. G. S. AGARWAL, *Phys. Rev. A* **4** (1971), 739.
53. S. CARUSOTTO, *Phys. Rev. A* **11** (1975), 1397.
54. V. K. FEDYANIN, G. M. GAVRILENKO, AND D. MIHALACHE, *Physica A* **109** (1981), 305.
55. A. MESSIAH, "Quantum Mechanics," Wiley, New York, 1962.
56. H. HAKEN, *Phys. Lett. A* **46** (1974), 443.
57. N. G. VAN KAMPEN, *Physica* **23** (1957), 707, 816.
58. U. UHLHORN, *Ark. Fys.* **17** (1960), 361.
59. R. GRAHAM AND H. HAKEN, *Z. Phys.* **243** (1971), 289.
60. G. S. AGARWAL, *Z. Phys.* **258** (1973), 409.
61. H. RISKEN, *Z. Phys.* **251** (1972), 231.
62. S. R. DE GROOT AND P. MAZUR, "Nonequilibrium Thermodynamics," North–Holland, Amsterdam, 1962.
63. W. WEIDLICH AND F. HAAKE, *Z. Phys.* **185** (1965), 30.
64. B. SWAIN, *J. Phys. A: Math. Gen.* **14** (1981), 2577.
65. B. R. MOLLOW, *Phys. Rev. A* **12** (1975), 1919.
66. R. HAAG, N. M. HUGENHOLTZ, AND M. WINNINK, *Comm. Math. Phys.* **5** (1967), 215.
67. H. B. CALLEN AND T. A. WELTON, *Phys. Rev.* **83** (1951), 34.
68. R. KUBO, *Rep. Progr. Phys.* **29** (1966), 225.
69. D. FORSTER, "Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions," Benjamin, Reading, Mass., 1975.
70. N. M. HUGENHOLTZ, *in* "Mathematics of Contemporary Physics" (R. F. Streater, Ed.), Academic Press, London/New York, 1972.
71. H. SPOHN AND J. L. LEBOWITZ, *in* "Advances in Chemical Physcis" (S. A. Rice, Ed.), Vol. 38, p. 109, Wiley, New York, 1978.
72. R. KUBO, *J. Phys. Soc. Japan* **12** (1957), 570.
73. P. C. MARTIN AND J. SCHWINGER, *Phys. Rev.* **115** (1959), 1342.
74. G. LINDBLAD, "Non-equilibrium Entropy and Irreversibility," p. 143 *ff.*, Reidel, Dordrecht, 1983.
75. G. GALLAVOTTI AND E. VERBOVEN, *Nuovo Cimento B* **28** (1975), 274.
76. L. G. YAFFE, *Rev. Modern Phys.* **54** (1982), 407.
77. R. GRAHAM, *Z. Phys. B* **26** (1977), 397.
78. H. GRABERT, P. HÄNGGI, AND P. TALKNER, *Phys. Lett. A* **66** (1978), 255.
79. P. HÄNGGI, H. THOMAS, G. GRABERT, AND P. TALKNER, *J. Statist. Phys.* **18** (1978), 155.
80. E. B. DYNKIN, "Markov Processes I," Springer–Verlag, Berlin, 1965.
81. H. J. CARMICHAEL AND D. F. WALLS, *J. Phys. A* **6** (1973), 1552.
82. F. SHIBATA AND N. HASHITSUME, *Z. Phys. B* **34** (1979), 197.
83. R. L. HUDSON AND R. F. STREATER, *Phys. Lett. A* **85** (1981), 64.
84. R. KUBO, *J. Phys. Soc. Japan* **26**, Suppl. 1 (1969).
85. H. MAASSEN, *J. Statist. Phys.* **34** (1984), 239.
86. H. GRABERT, *Z. Phys. B* **49** (1982), 161.
87. H. GRABERT AND P. TALKNER, *Helv. Phys. Acta* **56** (1983), 797.
88. H. GRABERT AND P. TALKNER, *in* "Noise in Physical Systems and $1/f$ Noise" (M. Savelli, G. Lecoy, and J. P. Nougier, Eds.), p. 27, Elsevier, Amsterdam/New York, 1983.
89. H. GRABERT AND P. TALKNER, *Phys. Rev. Lett.* **50** (1983), 1335.
90. A. O. CALDEIRA AND A. J. LEGGETT, *Physica A* **121** (1983), 587.

91. H. P. HAFFNER, "Das Feynmannsche Funktionalintegral angewandt auf das harmonisch gebundene Brownsche Teilchen," Diplomarbeit, Basel, 1983.
92. H. GRABERT, U. WEISS, AND P. HÄNGGI, *Phys. Rev. Lett.* **52** (1984), 2193.
93. H. GRABERT AND U. WEISS, *Phys. Rev. Lett.* **53** (1984), 1787.
94. A. J. BRAY AND M. A. MOORE, *Phys. Rev. Lett.* **49** (1982), 1546.
95. S. CHAKRAVARTY AND A. J. LEGGETT, *Phys. Rev. Lett.* **52** (1984), 5.
96. H. GRABERT, U. WEISS, AND P. TALKNER, *Z. Phys. B* **55** (1984), 87.
97. L. D. LANDAU AND E. M. LIFSHITZ, "Statistical Physics," Pergamon, London, 1959.
98. P. ULLERSMA, *Physica* **32** (1966), 27, 56, 74, 90.
99. K. LINDENBERG AND B. J. WEST, *Phys. Rev. A* **30** (1984), 568.
100. P. S. RISEBOROUGH, P. HÄNGGI, AND U. WEISS, *Phys. Rev. A* **31** (1985), 471.
101. F. HAAKE AND R. REIBOLD, *Phys. Rev. A* **32** (1985), 2462.
102. F. HAAKE AND R. REIBOLD, *Acta Phys. Austriaca* **56** (1984), 37.
103. V. GEIGENMÜLLER, U. M. TITULAER, AND B. V. FELDERHOF, *Physica A* **119** (1983), 41.
104. F. HAAKE AND M. LEWENSTEIN, *Phys. Rev. A* **28** (1983), 3606.
105. G. INGOLD, "Beschreibung von Dissipation bei quantenmechanischen Gaussprozessen," Diplomarbeit, Stuttgart, 1985.
106. W. WEIDLICH, *Z. Phys.* **241** (1971), 325.
107. T. KATO, "Perturbation Theory for Linear Operators," Springer–Verlag, Berlin, 1966.
108. F. R. GANTMACHER, "Matrizenrechnung I," p. 222, Deut. Verlag Wissenschaften, Berlin, 1958.