ELSEVIER

Can quantum Brownian motion be Markovian?

Hermann Grabert *

Physikalisches Institut, Albert-Ludwigs-Universität, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany

Abstract

The question whether a dissipative quantum system can approximately be described by a Markov process is reexamined using Brownian motion in a field of force as an example. The exactly solvable model of a damped harmonic oscillator allows for a precise identification of the range of validity of Markovian evolution equations. Such equations are valid both in the limits of weak and strong damping if the temperature is not too low. From these findings the parameter domain within which the weak coupling quantum master equation and the strong coupling quantum Smoluchowski equation can be employed to describe nonlinear quantum systems is outlined.
© 2005 Elsevier B.V. All rights reserved.

Keywords: Dissipative quantum systems; Quantum Markov process; Quantum master equation; Quantum Smoluchowski equation

1. Introduction to quantum Brownian motion and the quantum master equation

With the centennial of Einstein's explanation of classical Brownian motion as an effect of fluctuations that are intrinsic to molecular kinetics, the concepts of quantum Brownian motion have also found renewed attention. While for quantum dissipative systems there is an amazingly large body of work that starts from ad hoc postulates or assumptions, such as quantization "rules" for dissipative systems, one can hope that the large majority of physicists adheres to the idea that a dissipative quantum system is a system $\mathscr{S}$ in interaction with a reservoir $\mathscr{R}$. Then $\mathscr{S} + \mathscr{R}$ evolves in time according to the standard rules of quantum mechanics, meaning that the density matrix $\rho_{SR}(t)$ of $\mathscr{S} + \mathscr{R}$ at time t can in principle be calculated from the density matrix $\rho_{SR}(0)$ at some initial time $t = 0$ as $\rho_{SR}(t) = U(t)\rho_{SR}(0)U^\dagger(t)$ with the unitary time evolution operator $U(t)$ of $\mathscr{S} + \mathscr{R}$. Dissipative dynamics then emerges for the reduced density matrix $\rho(t) = \text{tr}_R \rho_{SR}(t)$ of the subsystem $\mathscr{S}$ of $\mathscr{S} + \mathscr{R}$ whenever the reservoir $\mathscr{R}$,

which is traced out in the trace tr_R over a complete set of reservoir states, has certain general properties. Essentially, the reservoir must be a large system with a quasi-continuous, sufficiently smooth energy spectrum, which interacts with $\mathscr{S}$ is such a way that each transition between two eigenstates of $\mathscr{S}$ is coupled to a huge number of transitions in $\mathscr{R}$ with coupling functions that depend again sufficiently smoothly on the reservoir energies.

This system + reservoir concept is also a widely accepted basis of the statistical mechanical description of classical dissipative systems, and it has been employed to derive the generalized Fokker–Planck equation describing the time evolution of the phase space distribution function $f(t)$ of a system $\mathscr{S}$ in contact with a thermal bath. $f(t)$ is the classical analogue of the reduced density matrix $\rho(t)$ which approaches $f(t)$ in the classical limit. Let us discuss in the sequel specifically the problem of Brownian motion in one dimension. This allows us to keep things simple, be more concrete, and give some explicit results, while the model is at the same time exemplary, since similar conclusions can be drawn for other dissipative systems. For a particle of mass M moving in a potential field $V(q)$ while interacting with a heat bath, the classical Fokker–Planck equation (FPE) reads [1]

* Tel.: +49 761 203 5882; fax: +49 761 203 5881.
 E-mail address: grabert@physik.uni-freiburg.de.

$$\frac{\partial}{\partial t} f(p, q, t) = \left\{ -\frac{\partial}{\partial q} \frac{p}{M} + \frac{\partial}{\partial p} \frac{dV}{dq} \right\} f(p, q, t)$$
$$+ \frac{\partial}{\partial p} \gamma \left\{ p + Mk_B T \frac{\partial}{\partial p} \right\} f(p, q, t),$$

where p, q are the phase space variables momentum and position of the Brownian particle. The first line of the FPE describes the reversible classical dynamics of an ensemble of particles with distribution $f(t)$ in a potential field, while the second line adds the effects of the heat bath environment at absolute temperature T. The influence of the reservoir, which is characterized by the damping constant γ, gives rise to a frictional force $-\gamma p$ and a diffusive broadening of the distribution function $f(t)$ caused by the term $D_p(\partial^2 f / \partial p^2)$ with the diffusion constant (in momentum space) $D_p = Mk_B T \gamma$.

The generalized FPE derived from a microscopic system + reservoir model differs from the conventional FPE in the second line, which now reads [2]

$$\int_0^t ds \frac{\partial}{\partial p} \gamma(t - s) \left\{ p + Mk_B T \frac{\partial}{\partial p} \right\} f(p, q, s)$$

with the damping kernel $\gamma(s)$. This simple form holds for linear coupling when the Hamiltonian of the model is translationally invariant in the absence of the potential $V(q)$. There are further generalizations of the FPE allowing, e.g., for a position dependence of the damping kernel. Here, we will focus on the most important feature, as far as basic concepts are concerned, arising within a microscopic model, namely the retardation effects described by $\gamma(s)$. The statistical mechanical derivation relates the damping kernel with the time correlation function of the fluctuations $\delta F(t)$ of the force exerted by the heat bath on the Brownian particle

$$\langle \delta F(t) \delta F(s) \rangle = Mk_B T \gamma(|t - s|).$$

Usually, this correlation function decays within a characteristic memory time $1/\omega_R$, where ω_R characterizes the bandwidth of reservoir modes coupled to the Brownian particle. Within classical statistical mechanics it is entirely consistent to consider the limit of vanishing memory time, i.e., $\omega_R \to \infty$. In this limit of "Ohmic" dissipation the force $\delta F(t)$ becomes δ-correlated in time, that is the frequency spectrum turns white, and one has

$$\gamma(|t|) = 2\gamma\delta(t),$$

so that the generalized FPE reduces to the ordinary one.

The powerful concept of Fokker–Planck equations, or of statistically equivalent Langevin equations, for classical dissipative systems has been exemplary for the construction of evolution equations for the reduced density matrix $\rho(t)$ of a quantum system $\mathscr{S}$ in contact with a heat bath $\mathscr{R}$. It seems natural to aim at an equation of motion in the form of a quantum master equation (QME)

$$\frac{\partial}{\partial t} \rho(t) = \mathbf{L}_{\text{diss}} \rho(t),$$

where the dissipative Liouville operator

$$\mathbf{L}_{\text{diss}} = \frac{i}{\hbar} [H_S,] + \mathbf{\Lambda}$$

contains the commutator with the Hamiltonian H_S governing the reversible dynamics of $\mathscr{S}$ [3] and a term $\mathbf{\Lambda}$ describing the influence of the reservoir. The study of dissipative quantum dynamics by means of QMEs has started systematically about 50 years ago [4], and this approach was very successful, in particular in quantum optics.

A prototype for further developments was the QME for a damped harmonic oscillator derived by Weidlich and Haake [5], for which a spectral decomposition of the dissipative Liouville operator in terms of a bi-orthogonal set of basis operators can be explicitly constructed (similar to the bi-orthogonal left and right eigenfunctions of a Fokker–Planck operator [1]). This has allowed to demonstrate explicitly that the QME propagates any positive initial reduced density matrix $\rho(0)$ through a sequence of positive density matrices $\rho(t)$ to a unique equilibrium state ρ^{eq}. The mathematical analysis of the underlying structure has led to the concept of a completely positive semigroup of time evolution operators for dissipative quantum systems and to the identification of the generators of these semigroups as Liouville operators of Lindblad form [6]

$$\mathbf{L}_{\text{diss}} \rho = \frac{i}{\hbar} [H_S, \rho] + \frac{1}{2\hbar} \sum_i \left\{ [L_i \rho, L_i^\dagger] + [L_i, \rho L_i^\dagger] \right\},$$

where the L_i are arbitrary operators of $\mathscr{S}$. In view of the apparent evidence and considerable mathematical beauty of the theory [7], many physicists in the field of quantum statistics consider a Liouville operator of Lindblad form as *the* quantum mechanical generalization of a Fokker–Planck operator.

Like the FPE, the QME should be put on a statistical mechanical basis by starting from the unitary time evolution $\rho_{\text{SR}}(t) = U(t) \rho_{\text{SR}}(0) U^\dagger(t)$ of the entire system $\mathscr{S} + \mathscr{R}$. To obtain the time evolution of the reduced density matrix $\rho(t) = \text{tr}_R \rho_{\text{SR}}(t)$ of the subsystem $\mathscr{S}$, the reservoir needs to be traced out. This can be achieved with the help of projection operator techniques [4,8] that lead to a formally exact evolution equation for $\rho(t)$ of the form

$$\frac{\partial}{\partial t} \rho(t) = \frac{i}{\hbar} [H_S, \rho(t)] + \int_0^t ds \mathbf{\Lambda}(\mathbf{t} - \mathbf{s}) \rho(s).$$

In this generalized QME the influence of $\mathscr{R}$ is described in terms of a memory kernel $\mathbf{\Lambda}(\mathbf{s})$. An ordinary QME is then obtained in the so-called *Markov approximation* where memory effects are disregarded. However, for the QME the limitations of such a "derivation" are substantially more serious than those arising in the derivation of the FPE from the generalized FPE, as we shall discuss now.

First, a closed evolution equation for $\rho(t)$ (or likewise for $f(t)$ in the classical limit) can only be obtained for a specific class of initial states. Consider again our example of a Brownian particle. In the classical case one usually assumes that an initial state of the particle with momentum p_0 and