Dynamics of Dissipative Quantum Systems—from Path Integrals to Master Equations[*]

Joachim Ankerhold[†]

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

The path integral approach offers not only an exact expression for the nonequilibrium dynamics of dissipative quantum systems, but is also a convenient starting point for perturbative treatments. An alternative way to explore the influence of friction in the quantum realm is based on master equations which require, however, in one or the other aspect approximations. Here it is discussed under which conditions and limitations Markovian master equations can be derived from exact path integrals thus providing a firm basis for their applicability.

I. INTRODUCTION

Quantum systems coupled to a heat bath environment can be found almost everywhere in physics and chemistry. Recently, challenging problems e.g. in realizing quantum computers, in manipulating Bose-Einstein condensates, or in understanding low temperature dynamics in molecular systems have triggered a substantial amount of research.

The description of quantum dissipative processes reaches back to the late 1960s [1], when it was mainly concerned with weakly damped quantum optical systems. The conventional framework relied on quantum Langevin or quantum master equations. A breakthrough beyond the limitations of the weak coupling approach was made in the early 1980s [2]. Path integral techniques were shown to be powerful means to formulate the reduced dynamics of dissipative quantum systems for all damping strengths, temperatures and bath memory times. While applications, particular in condensed phase systems, have proven the advantage of this approach, e.g. the non-exponential decay of low temperature correlation functions, it has rarely been used to put the known master equations on a firm basis and to derive new master equations for strong damping/low temperatures. In fact, it turned out that the quantum stochastic process is strongly non-Markovian and intimately depends on the initial correlations between system and bath [3]. As a consequence, "simple" master equations do in general not exist and the known results can be derived only in an approximate way [4]. What has been essentially unexplored so far, namely the range of strong friction, has been analyzed recently in detail [5, 6]. It has been shown that in this limit quantum noise is squeezed and that the Wigner transform of the reduced density obeys a quantum Fokker Planck equation [7]. In the low temperature quantum domain the latter one can be reduced to a generalization of the classical Smoluchowski equation [6]. Since the path integral formulation is exact in the system-bath coupling and includes also correlated initial states, it is basically the only way to derive these findings consistently.

Thus, we are now in a position to give a more or less comprehensive account about the validity and limitations of Markovian master equations. The following study is a brief attempt in this direction. It is not intended, however, to include all developments and to consider the most general case. Instead, to keep things as transparent as possible I restrict myself to (i) a single one-dimensional continuous system with a well defined ground state coupled to a single heat bath where (ii) the bath cut-off frequency is assumed to be the largest frequency scale. Further, I look only for Markovian master equations with (iii) time evolution generators independent of time and initial preparation. It turns out that already within this frame the analysis is rather subtle and reveals most of the complexity we encounter in describing dissipative dynamics.

In Sections II and IV I briefly introduce the path integral approach for dissipative quantum systems. Based on this in Sec. IV some general conditions for the existence of Markovian master equations are derived which are then specified in Sec. V for weak and in Sec. VI for strong damping, respectively.

II. PATH INTEGRALS FOR DISSIPATIVE QUANTUM SYSTEMS

The description of classical Brownian motion in terms of generalized Langevin equations or, equivalently, in terms of Fokker-Planck equations for phase space distributions has a long tradition [8]. In contrast, the inclusion of dissipation

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[†] ankerhold@physik.uni-freiburg.de

within quantum mechanics in a non-perturbative way has been established only since the early 80s [2]. In the standard formulation one starts with a system+heat bath formulation

$$H = H_{\mathrm{S}} + H_{\mathrm{R}} + H_{\mathrm{I}} \tag{1}$$

where the total Hamiltonian contains a system, a reservoir (heat bath), and a system-bath interaction part, respectively. The dynamics of the total density matrix starting at $t = 0$ from a general initial state $W(0)$ evolves according to

$$W(t) = \exp(-iHt/\hbar) \, W(0) \, \exp(iHt/\hbar). \tag{2}$$

The crucial point is now, that dissipation is *not a priori* inherent in the system, but arises only if one looks on the effective impact of the bath degrees of freedom within a reduced picture $\varrho(t) = \mathrm{tr}_{\mathrm{R}}\{W(t)\}$. The Gaussian statistics of the heat bath is modeled by a quasi-continuum of harmonic oscillators bilinearly coupled with the relevant system degree of freedom. Although the interaction between each bath degree of freedom and the system is supposed to be weak, the overall impact of the reservoir may cause also strong friction. Along this reasoning two steps need to be done: an appropriate formulation to arrive at a reduced description has to be found and the initial state has to be defined.

The only non-perturbative way to deal with the elimination of the bath degrees of freedom is to apply the path integral approach. Denoting the degrees of freedom in coordinate space by $\vec{x}$ for the bath and q for the system, the coordinate representation of (2) follows as

$$
\begin{aligned}
\langle q_f, \vec{x}_f | W(t) | q_f', \vec{x}_f' \rangle \;=\; & \int \mathrm{d}q_i \mathrm{d}q_i' \, \mathrm{d}\vec{x}_i \mathrm{d}\vec{x}_i' \, G(q_f, \vec{x}_f, t, q_i, \vec{x}_i) \\
& \langle q_i, \vec{x}_i | W(0) | q_i', \vec{x}_i' \rangle \, G(q_f', \vec{x}_f', t, q_i', \vec{x}_i')^*
\end{aligned}
\tag{3}
$$

where the $*$ means complex conjugation. The transition amplitudes on the rhs are expressed as path integrals, e.g.,

$$G(q_f, \vec{x}_f, t, q_i, \vec{x}_i) = \int \mathcal{D}[q] \, \mathcal{D}[\vec{x}] \, \mathrm{e}^{iS[q,\vec{x}]/\hbar} \tag{4}$$

with the total action $S = S_{\mathrm{S}} + S_{\mathrm{R}} + S_{\mathrm{I}}$ according to the three parts of the Hamiltonian (2). The sum goes over all paths running in time t from $q(0) = q_i, \vec{x}(0) = \vec{x}_i$ to $q(t) = q_f, \vec{x}(t) = \vec{x}_f$. Switching to a reduced description is achieved by taking the trace over the bath degrees of freedom

$$\varrho(q_f, q_f', t) = \int d\vec{x}_f \, \langle q_f, \vec{x}_f | W(t) | q_f', \vec{x}_f \rangle. \tag{5}$$

To carry out all integrations over the bath degrees of freedom in (4) explicitly, the initial state must be specified.

III. INITIAL STATE AND INFLUENCE FUNCTIONAL

In the ordinary Feynman Vernon theory [2] the initial state is assumed to be a factorizing state $W(0) = \varrho_{\mathrm{S}}(0) \, Z_{\mathrm{R}}^{-1} \exp(-\beta H_{\mathrm{R}})$ (Z_{R} is the partition function of the bath) so that each one, system and equilibrated bath, lives in splendid isolation at $t = 0$. While this assumption may be justified in the weak friction/high temperature range, it definitely fails for moderate to strong dissipation or lower temperature. Even the Langevin equation is not regained in the classical limit, but differs by initial boundary terms that may persist up to long times. A realistic initial state reflecting the experimental situation is thus a correlated one described by [3]

$$W(0) = Z_\beta^{-1} \sum_i O_{\mathrm{S}}^i \, \mathrm{e}^{-\beta H} \, \tilde{O}_{\mathrm{S}}^i \tag{6}$$

where Z_β is the partition function of the total system and the operators $O_{\mathrm{S}}^i, \tilde{O}_{\mathrm{S}}^i$ act onto the system degree of freedom only and prepare a nonequilibrium state. In the sequel I focus on the case where the preparation operators depend exclusively on coordinate and refer to [3] for the generalization. As an example think about a position measurement with a Gaussian slit, in which case the preparation operators are Gaussian weighted projection operators onto position. Representing the statistical operator in (6) as path integrals in imaginary time we have

$$\langle q_i, \vec{x}_i | W(0) | q_i', \vec{x}_i' \rangle = Z_\beta^{-1} \, \lambda(q_i, q_i') \int \mathcal{D}[\bar{q}] \mathcal{D}[\vec{\bar{x}}] \, \mathrm{e}^{-\bar{S}[\bar{q}, \vec{\bar{x}}]/\hbar} \tag{7}$$

with the preparation function $\lambda(\cdot)$ being the coordinate representation of the preparation operators in (6) and the total Euclidian action $\bar{S} = \bar{S}_S + \bar{S}_R + \bar{S}_I$. Paths contributing to (7) run in imaginary time in the interval $\hbar\beta$ from $\bar{q}(0) = q_i, \vec{\bar{x}}(0) = \vec{x}_i$ to $\bar{q}(\hbar\beta) = q_i', \vec{\bar{x}}(\hbar\beta) = \vec{x}_i'$.

The integrations over the bath degrees of freedom in (3) can now together with (7) be performed exactly due to the harmonic nature of the bath. After some tedious algebra one ends up with the coordinate representation of the reduced density matrix

$$\varrho(q_f, q_f', t) = \int dq_i \, dq_i' \; J(q_f, q_f', t, q_i, q_i') \; \lambda(q_i, q_i'). \tag{8}$$

The propagating function $J(\cdot)$ is a threefold path integral over the system degree of freedom only

$$J(q_f, q_f', t, q_i, q_i') = Z^{-1} \int \mathcal{D}[q] \, \mathcal{D}[q'] \, \mathcal{D}[\bar{q}] \; e^{i\Sigma[q,q',\bar{q}]/\hbar} \tag{9}$$

with $Z = Z_\beta / Z_R$. The two real time paths $q(s)$ and $q'(s)$ connect in time t the initial points q_i and q_i' with the fixed end points q_f and q_f', while the imaginary time path $\bar{q}(\sigma)$ runs from q_i to q_i' in the interval $\hbar\beta$. The contribution of each path is weighted with an effective action $\Sigma[q, q', \bar{q}] = S_S[q] - S_S[q'] + i\bar{S}_S[\bar{q}] + i\phi[q, q', \bar{q}]$. It consists of the actions of the bare system in real and imaginary time, respectively, and additional interaction contributions (influence functional)

$$
\begin{aligned}
\phi[q, q', \bar{q}] = & -i \int_0^{\hbar\beta} d\tau \int_0^\sigma d\sigma \, \bar{q}(\tau) \, K(-i\tau + i\sigma) \, \bar{q}(\sigma) + i \int_0^{\hbar\beta} d\tau \frac{\mu}{2} \, \bar{q}(\tau)^2 \\
& + \int_0^{\hbar\beta} d\tau \int_0^t ds \, K^*(s - i\tau) \, \bar{q}(\tau) \, x(s) - M r_i \, \gamma(s) \, x(s) \\
& - \int_0^t ds \, x(s) \left[M \int_0^s du \, \gamma(s - u) \, \dot{r}(u) - \frac{i}{2} \int_0^t du \, K'(s - u) \, x(u) \right].
\end{aligned}
\tag{10}
$$

Here, for convenience, we have introduced sum and difference real time paths, namely, $r(s) = [q(s) + q'(s)]/2$ and $x(s) = [q(s) - q'(s)]$. Further, the effective impact of the bath is controlled by the damping kernel

$$K(\theta) = \int_0^\infty \frac{d\omega}{\pi} \, I(\omega) \, \frac{\cosh[\omega(\hbar\beta/2 - i\theta)]}{\sinh(\omega\hbar\beta/2)} \tag{11}$$

where $\theta = s - i\tau$, $0 \leq s \leq t$, $0 \leq \tau \leq \hbar\beta$ and $I(\omega)$ is the spectral density of the heat bath. For an interaction term between system and bath of the form $H_I = q\xi_R(\theta)$ with $\xi_R(\theta) = \vec{c}\vec{x}$ (coupling constants $\vec{c}$) one shows that the damping kernel is basically the bath autocorrelation function, i.e. $K(\theta) = \langle \xi_R(\theta) \, \xi_R(0) \rangle_R / \hbar$. In real time $K(s) = K'(s) + iK''(s)$ is related to the macroscopic damping kernel

$$\gamma(s) = \frac{2}{M} \int_0^\infty \frac{d\omega}{\pi} \frac{I(\omega)}{\omega} \, \cos(\omega s) \tag{12}$$

via $K''(s) = \frac{M}{2} d\gamma(s)/ds$ and $K'(s) \to M\gamma(s)/\hbar\beta$ in the classical limit $\omega_c \hbar\beta \to 0$ (M is the mass of the Brownian particle). The term with $\mu = \lim_{\hbar\beta \to 0} \hbar\beta K(0)$ in the first line in (10) gives a potential renormalization in the Euclidian action due to shifts of the minima of the bath oscillators by the coupling to the system. The corresponding renormalization in the real-time part of the action has already been incorporated in the form it is written in (10).

Apparently, $\phi[q, q', \bar{q}]$ contains the bath induced non-local interactions between the various system paths. Particularly, it turns out that the last term (with K') acting as a Gaussian weighting factor for the quantum fluctuations $x(s)$ suppresses coherences and gives rise to relaxation, while the second last term depending on $K''(s)$ leads to dephasing during the dynamics. The influence of initial correlations between system and bath is contained in the term with K^* coupling real and imaginary time motion.

While in (8) the imaginary time paths describe the initial state, the two real time paths govern the dynamics of the reduced system. Accordingly, the distribution of end-points of the former and starting points of the latter q_i, q_i' are weighted in (8) also by the preparation function $\lambda(\cdot)$. In the limit $t \to 0$ one has $J(q_f, q_f', t, q_i, q_i') \to \varrho_\beta(q_i, q_i') \, \delta(q_f - q_i) \, \delta(q_f' - q_i')$ so that

$$\varrho(q_f, q_f', 0) = \varrho_\beta(q_i, q_i') \, \lambda(q_i, q_i') \tag{13}$$

with the reduced equilibrium density matrix $\varrho_\beta(q, q') = Z_\beta^{-1} \langle q | tr_R \exp(-\beta H) | q' \rangle$. In fact, this formulation reproduces in the classical limit the generalized Langevin equation.

The nonequilibrium time evolution of a dissipative quantum system is governed by (8) together with (13). The good news is that this path integral expression is exact, also in the system-bath coupling. The bad news is that its evaluation is even numerically feasible only for specific systems and certain ranges in parameter space. Since the propagating function is highly oscillatory, numerical algorithms inevitably become unstable for sufficiently long times. In this situation "simple" time evolution equations are of great practical importance and the path integral formulation provides a very convenient basis for deriving them. The severe problem, however, is the non-locality, in time, of the influence functional; the reduced time evolution in the time interval $s \in [t', t] \subset [0, t]$ is affected by the history of the dynamics for $0 < s < t'$ and particularly by the initial correlations between system and bath at $s = 0$. Even worse, it has been shown that *different* initial densities $W(0)$ of the full compound may lead to *identical* reduced initial densities $\rho(0)$, but give rise to quite different quantum stochastic processes due to *different initial correlations* [3]. Hence, in general a time evolution equation $\dot{\varrho} = \mathcal{L} \varrho$ of the reduced density with a generator $\mathcal{L}$ independent of time and independent of the initial preparation does not exist.

I mention here that an alternative procedure to eliminate the bath degrees of freedom has been developed by invoking projection operator techniques [2, 9]. This way generalized equations of motion in form of integro-differential equations for the reduced density have been derived. It turns out, however, that this approach is convenient only in the weak damping/high temperature range. In contrast, the path integral formulation offers an elegant starting point for perturbative treatments, e.g. semiclassical approximations, perturbation theory à la Feynman etc., for all temperatures and spectral bath densities. Moreover, its close relation to the formulation of classical statistical mechanics has allowed to adopt and extend numerical techniques like e.g. Monte Carlo simulations to quantum dissipative systems.

IV. GENERAL CONDITIONS FOR MARKOVIAN MARKOVIAN MASTER EQUATIONS

As the time evolution of the reduced density matrix cannot be cast into the form $\dot{\varrho} = \mathcal{L} \varrho$ exactly, one may wonder under which conditions at least approximate time evolution operators $\mathcal{L}$, independent of time and the initial state, can be derived from the expression (8). Before I turn to specific cases, in this section, we first want to formulate some general conditions. Accordingly, we analyze the influence functional (10) with respect to its non-Markovian nature and with respect to the friction induced entanglement of the bare time evolution operators.

For this purpose let us consider the real-time part of the damping kernel (11) in the limit of $\omega_c \to \infty$. One has

$$K(t) = -\frac{\pi M \gamma}{(\hbar \beta)^2} \frac{1}{\sinh^2(\pi t / \hbar \beta)} + iM\gamma \dot{\delta}(t). \tag{14}$$

Hence, while $K''(t)$ is local in time, $K'(t)$ is not. In fact, for $\hbar \beta \to \infty$ it only decays algebraically $K'(t) \propto \gamma/t^2$ so that strong non-local quantum fluctuations in the influence functional (10) become important and lead e.g. to non-exponential long time tails for zero-temperature correlation functions [2].

One concludes that a time evolution operator, local in time, can only exist on a coarse grained time scale $s \gg \hbar \beta, 1/\omega_c$. In fact, a coarse graining procedure is only meaningful if the time scale on which the relevant dynamics takes place, e.g. the relaxation time scale t_r, obeys

$$t_r \gg \hbar \beta, 1/\omega_c. \tag{15}$$

Compared to the typical time scale of the bare system time evolution $1/\omega_0$ with ω_0 e.g. its ground state frequency, t_r can be very large. For $T \to 0$ the thermal time scale exceeds all other time scales and the above condition can never be fulfilled.

The immediate consequence of (15) is that the influence functional becomes local on the coarse grained time scale. This is fine, but it is not all we need. Namely, the bath mediated coupling between forward and backward time evolution and also between the time evolution and the initial state—accounted for by the x dependence of the influence functional (10)—is a genuine quantum effect, so that the x paths can be interpreted to describe quantum noise. For anharmonic potential fields $V(r - x/2)$ the effective action contains also anharmonic x dependent terms meaning that quantum noise is in general non-Gaussian. In the spirit of a classical Kramers-Moyal expansion [8] one would expect that a time evolution generator $\mathcal{L}$ of the reduced dynamics $\rho(x_f, r_f, t)$ must be represented as an infinite power series in x_f and $\partial/\partial r_f$ (leading in the Wigner transform to derivatives $\partial/\partial p$, $\partial/\partial q$) with an infinite number of diffusion coefficients—a hopeless situation. For further exploring this point it is useful to introduce the dimensionless quantity

$$\kappa = \left| \frac{1}{M \omega_0} \int_0^{t_r} ds \int_0^{t_r} du \, K'(s - u) \right| = \frac{2 \, t_r \, \gamma}{\omega_0 \, \hbar \beta} \,. \tag{16}$$

This parameter is obtained by considering the last term of (10), which acts as a Gaussian weight for the x-paths, for times of the order of t_r, putting $x(s) = const.$, exploiting (14), and performing the coarse graining. Accordingly, the typical size of $|x|/\sqrt{\hbar/M\omega_0}$ is approximated to be of the order $1/\sqrt{\kappa}$ and quantum noise tends to be small in domains of parameter space where $\kappa \gg 1$.

In the overdamped range $\gamma/\omega_0 \gg 1$ relaxation takes place on the scale $t_r = \gamma/\omega_0^2$ so that $\kappa = (\gamma/\omega_0)\,\gamma/\omega_0\hbar\beta$ is large under (15). For sufficiently strong damping the Gaussian weighting factor in the influence functional then causes quantum noise to be squeezed by friction. This allows for a semiclassical type of approximation with generators $\mathcal{L}$ containing at most second order diffusion coefficients (ranges I and II in Fig. 1). In the underdamped case $\gamma/\omega_0 < 1$ the dissipative system equilibrates on the time scale $t_r \sim 1/\gamma$ so that (15) reads $\gamma\hbar\beta \ll 1$ and $\kappa = 2/\omega_0\hbar\beta$ is large as well. We this way recover the well-known fact that in the high temperature range $\omega_0\hbar\beta \ll 1$ quantum fluctuations are small and quantum nonequilibrium dynamics happens to be close to classical nonequilibrium dynamics (range III in Fig. 1). The coarse graining condition in the underdamped regime $\gamma\hbar\beta \ll 1$ covers also the range IV in Fig. 1. There, quantum noise is non-Gaussian and not small at all but the entanglement due to friction can be treated perturbatively. To see this we estimate the contribution of kinetic terms in the bare real-time actions to be of order $M(x/\hbar\beta)^2\,(t_r/\hbar) = (x/\sqrt{\hbar/M\omega_0})^2\,1/[\gamma\omega_0(\hbar\beta)^2]$, while the x^2 term in the influence functional is $(x/\sqrt{\hbar/M\omega_0})^2\,\kappa = (x/\sqrt{\hbar/M\omega_0})^2 2/\omega_0\hbar\beta$. Thus in the domain where the condition (15) is obeyed for $\gamma/\omega_0 < 1$, i.e. $\gamma\hbar\beta \ll 1$, friction terms are supposed to be much smaller than bare kinetic contributions.

To summarize this discussion we can expect to derive from the exact path integral expression (8) approximate time evolution operators $\mathcal{L}$ on a coarse grained time scale only in the domains I–IV of Fig. 1. In the sectors I–III quantum noise is essentially Gaussian—either due to strong friction (I) or due to high temperature (II, III)— while in sector IV it is non-Gaussian, but the coupling it induces between the foward and backward time evolution of the bare system is weak. In the remaining parts of parameter space there is no reduction in a simple way possible and one has to work either with the full path integrals or master equations with complicated non-local integro-differential operators. In the sequel I will focus on the ranges III, IV for weak damping and I, II for strong friction in detail.

V. WEAK DAMPING REGIME

It is well-known that for sufficiently high temperatures and/or sufficiently weak friction time evolution equations for the reduced dynamics can be derived [1]. This has been done already in the late 60s motivated by the experimental progress for quantum optical devices. Here, I discuss how these results in the underdamped range can be regained from the exact path integral expression (8).

In case where fluctuations tend to be small $\omega_0\hbar\beta \ll 1$ (range III in Fig. 1) master equations have been explicitly derived for harmonic systems. From (8) an equation of motion for $\varrho(x_f, r_f, t)$ is obtained which, in operator representation, coincides with the well-known Agarwal equation [10]: $\dot{\varrho}(t) = \mathcal{L}_{\mathrm{Ag}}\,\varrho(t)$ with

$$\mathcal{L}_{\mathrm{Ag}}\,\varrho = -\frac{i}{\hbar}[H_0, \varrho] - \frac{i\gamma}{2\hbar}[q, \{p, \varrho\}] - \frac{\gamma M^2 \omega_0^2}{2\hbar^2}\,\langle q^2 \rangle_\beta\,[q, [q, \varrho]] \tag{17}$$

where $H_0 = p^2/2M + M\omega_0^2 q^2/2$ and $[\cdot, \cdot]$ ($\{\cdot, \cdot\}$) denotes the commutator (anticommutator). The equilibrium position variance is approximated to read

$$\langle q^2 \rangle_\beta \approx \frac{\hbar}{M\omega_0}\coth\left(\frac{\omega_0\hbar\beta}{2}\right). \tag{18}$$

Since for a harmonic system quantum noise is always Gaussian, the above finding can be generalized to the wider range $\gamma\hbar\beta \ll 1$ (ranges III and IV in Fig. 1). The result is an additional p-q diffusion term, i.e.

$$\mathcal{L}_{\mathrm{ext}}\,\varrho = \mathcal{L}_{\mathrm{Ag}}\,\varrho + \frac{D_{pq}}{\hbar}\,[p, [q, \varrho]]. \tag{19}$$

The form of this additional diffusion coefficient for the harmonic case has been first derived from the path integral approach in [4]

$$D_{pq} = \frac{1}{\hbar}\,\left(M\omega_0^2 \langle q^2 \rangle_\beta - \frac{\langle p^2 \rangle_\beta}{M}\right) \tag{20}$$

with $\langle p^2 \rangle_\beta$ the equilibrium momentum variance of a harmonic oscillator. For the parameter range considered here $\gamma\hbar\beta \ll 1$ ($\omega_0 \ll \omega_c$) one has

$$\langle p^2 \rangle_\beta \approx M^2 \omega_0^2\,\langle q^2 \rangle + \frac{\hbar\gamma M}{\pi}\,[\psi\,(1 + \omega_c\hbar\beta/2\pi) + C] \tag{21}$$
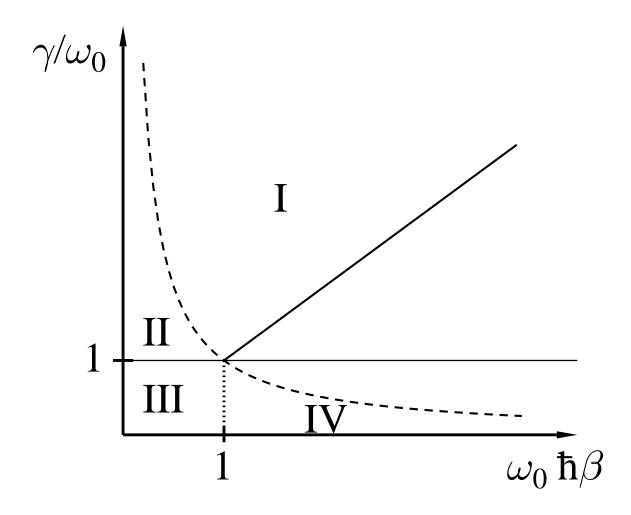
FIG. 1: Sectors in parameter space where for $\omega_c \gg \omega_0, \gamma$ various types of master equations can be derived I–IV. The thin horizontal line separates the overdamped from the underdamped range, the thick solid line defines the range $\gamma\hbar\beta \gg 1$ in the overdamped region, the dashed line defines $\gamma\hbar\beta \ll 1$, and the dotted vertical line specifies $\omega_0\hbar\beta \ll 1$ in the underdamped sector. See text for details.

where $\psi(x)$ is the psi function and $C \approx 0.577$ Euler's constant. Accordingly, we infer from (20) in ranges III/IV

$$D_{pq} \approx -\frac{\gamma}{\pi} \left[\psi \left(1 + \omega_c \hbar \beta / 2\pi \right) + C \right]. \tag{22}$$

This D_{pq} tends to its classical limit $D_{pq} = 0$ for $\omega_c \hbar \beta \to 0$ with fixed $\omega_c \gg \omega_0$. From the Wigner transform of $\mathcal{L}_{\text{ext}}$ we then regain the classical Fokker-Planck operator [8]. For finite but still small $\omega_0 \hbar \beta \ll 1$ the influence of D_{pq} is supposed to be small only, if additionally $\omega_c \hbar \beta \ll 1$, which gives us the precise validity of the Agarwal equation (17) in range III. For lower temperatures, sectors III (partially) and IV, the p-q diffusion becomes important and $\mathcal{L}_{\text{ext}}$ with D_{pq} as in (22) defines a master equation derived by Haake and Reibold [11]. Within the Nakajima-Zwanzig projection operator technique [9] an identical equation has been obtained within Redfield theory [12]. In the limit $\omega_c \hbar \beta \gg 1$ the expression (22) simplifies to leading order to $D_{pq} \approx (\gamma/\pi) \log(\omega_c \hbar \beta / 2\pi)$.

So far I have discussed only master equations for harmonic systems. In case of anharmonic systems and within the range $\omega_0 \hbar \beta \ll 1$ in principle a semiclassical type of approximation applies so that the potential field $V(r - x/2)$ can be expanded up to second order in x. This way, as mentioned above, it is shown that the $x-$paths describe effectively white Gaussian noise in the reduced system. Diffusion related terms thus appear in $\mathcal{L}$ at most in second order and the Wigner transform of $\mathcal{L}$ into phase space contains at most second order derivatives in the phase space variables leading to a generalized Fokker-Planck operator. However, according to the previous section, in the wider range III/IV a weak damping perturbation theory of the bath induced entanglement is feasible anyway. Exploiting this very fact, the nonequilibrium quantum dynamics can be cast, after an additional coarse graining $s \gg 1/\omega_0$, into the form of the famous Lindblad equation [13]

$$\dot{\varrho}(t) = -\frac{i}{\hbar}[H', \varrho(t)] + \frac{1}{2\hbar} \sum_l [L_l \varrho(t), L_l^\dagger] + L_l, \varrho(t)L_l^\dagger]. \tag{23}$$

Here, H' is a hermitian operator which must not necessarily coincide with the bare system Hamiltonian, and the L_l describe the effective influence of the specific heat bath. In case of a harmonic system and using creation and annihilation operators the resulting master equation is also known as the Haake-Weidlich equation [14].

Before I turn to the strong friction range two remarks are in order here. First, all time evolution operators $\mathcal{L}$ specified in (17) and (19) are not of Lindblad form (23) and thus do not respect complete positivity. This is not astonishing since they are derived based upon a coarse graining procedure. Their validity is restricted to a certain subspace where transient components have died out, while Lindblad theory itself requires a Markovian master equation for all times. The path integral approach reveals explicitly that from a physical point of view this requirement is not necessary (see also [15]) and even does not reflect the exact nonequilibrium dynamics. Second, master equations have also been derived starting with factorizing initial states (Feynman-Vernon theory), see Sec. II, e.g. the Caldeira-Leggett master equation [16]. The problem there is that the factorizing initial state itself makes only sense in the weak damping limit meaning that a weak friction perturbation theory within Feynman Vernon theory is somewhat inconsistent. Particularly even the known Fokker-Planck operator cannot be re-derived in the classical limit [17]. Hence, the Caldeira-Leggett or related master equations cannot be obtained from (8) [4].

VI. STRONG FRICTION RANGE

In classical physics the strong friction domain is well-known as the Smoluchowski limit. Its characteristic property is that one has a separation of time scales between fast equilibration of momentum and slow relaxation in position. This way the Fokker-Planck equation for the phase space distribution can be reduced to a Smoluchowski equation for the marginal distribution in position space. For quantum dissipative systems one would think that strong friction makes the reduced system to behave effectively more classically so that the complicated path integral expression (8) simplifies considerably. That this is indeed the case has been analyzed in detail only recently [6, 7] and I have given the general argument already in Sec. IV. In particular, strong dissipation has quite a different influence on position and momentum.

To see that in detail we define a typical damping strength as

$$\gamma \equiv \hat{\gamma}(0) = \lim_{\omega \to 0} \frac{I(\omega)}{M\omega} \tag{24}$$

with $\hat{\gamma}(\omega)$ the Laplace transform of the classical damping kernel $\gamma(t)$ (12). For instance, in the ohmic case $I(\omega) = M\bar{\gamma}\omega$ and also for the more realistic Drude model $I(\omega) = M\bar{\gamma}\omega\omega_c^2/(\omega^2 + \omega_c^2)$ one finds $\gamma = \bar{\gamma}$. Given a typical frequency ω_0 of the bare system, e.g. the ground state frequency, by strong damping we then mean

$$\frac{\gamma}{\omega_0^2} \gg \hbar\beta, \frac{1}{\omega_c}, \frac{1}{\gamma}. \tag{25}$$

In other words, we assume the time scale separation well-known from the classical overdamped regime [8] and extend it to the quantum range by incorporating the time scale for quantum fluctuations $\hbar\beta$. Correspondingly, according to the discussion in Sec. IV we consider the dynamics (8) on the coarse grained time scale $s \gg \hbar\beta, \frac{1}{\omega_c}, \frac{1}{\gamma}$ and $\sigma \gg \frac{1}{\omega_c}, \frac{1}{\gamma}$. The consequences are threefold: (a) the strong friction suppresses non-diagonal elements of the reduced density matrix during the time evolution; (b) the real-time part $K(s)$ of the damping kernel becomes local on the coarse grained time; (c) initial correlations as described by the first term in (10) survive for times of the order γ/ω_0^2 so that factorizing initial states cannot be used.

Following the above simplifications the path integral formulation now allows for a perturbative treatment in the *strong damping limit*. According to Sec. V the strategy is then to evaluate the path integrals in the sense of a semiclassical approximation by assuming self-consistently that non-diagonal elements, i.e. $\bar{x} = \bar{q}(\hbar\beta) - \bar{q}(0)$ and $x(s)$ dependent terms, remain small during the time evolution. Hence the effective action $\Sigma[r, x, \bar{q}]$ is expanded up to second order in $\bar{x}$ of the imaginary time paths and in the excursions $x(s)$ of the real-time path integrals. Doing so we take sufficiently smooth potentials for granted. It is worthwhile to note that we do not need to restrict the value of $\gamma\hbar\beta$ meaning that the strong damping analysis covers a broad temperature range from the classical ($\gamma\hbar\beta \ll 1$, range II in Fig. 1) to the deep quantum domain ($\gamma\hbar\beta \gg 1$, range I).

Before I turn to the dynamical case, it is instructive to consider the thermal equilibrium only. The corresponding imaginary time path integral can approximately be solved for an anharmonic potential and the result is

$$\varrho_\beta(\bar{x}, \bar{r}) = \frac{1}{Z} e^{-\beta V(\bar{r}) - \langle p^2 \rangle \bar{x}^2/2\hbar^2} e^{\Lambda\beta[\beta V'(\bar{r})^2/2 - 3V''(\bar{r})/2]} \tag{26}$$

where $\bar{r} = [\bar{q}(\hbar\beta) + \bar{q}(0)]/2$ and $Z = \int dq \varrho_\beta(0, q)$. Further,

$$\Lambda = \frac{2}{M\beta} \sum_{n=1}^{\infty} \frac{1}{\nu_n^2 + \nu_n \hat{\gamma}(\nu_n)} \quad , \quad \langle p^2 \rangle = \frac{M}{\beta} + \frac{2M}{\beta} \sum_{n=1}^{\infty} \frac{\hat{\gamma}(\nu_n)}{\nu_n + \hat{\gamma}(\nu_n)} . \tag{27}$$

Apparently, Λ measures the typical strength of quantum fluctuations in position space. In case of Drude damping with a high frequency cut-off ω_c both Λ and $\langle p^2 \rangle$ can be expressed in terms of Ψ functions. Then, for high temperatures $\gamma\hbar\beta \ll 1$ we find $\Lambda \approx \hbar^2\beta/12M$ and $\langle p^2 \rangle \approx M/\beta$. The friction dependence appears as a genuine quantum effect for lower temperatures and for $\gamma\hbar\beta \gg 1$ one has $\Lambda \approx (\hbar/M\gamma\pi) \log(\gamma\hbar\beta/2\pi)$ and $\langle p^2 \rangle \approx (M\hbar\gamma/\pi) \log(\omega_c/\gamma)$. With increasing γ the strong squeezing of quantum fluctuations in position induces enhanced quantum fluctuations in momentum, thus suppressing non-diagonal elements in the density matrix. Interestingly, the probability distribution is Gaussian in $\bar{x}$, i.e. its Wigner transform ($\bar{x}/\hbar \to p$) Gaussian in momentum, even at low temperatures. Anharmonic corrections in $\bar{x}$ to the exponent are at most of order $1/\gamma^2$. Hence, for strong friction the equilibrium density consists of a part which in phase space takes the form of a classical distribution, however, with an $\hbar$ dependent $\langle p^2 \rangle$ and a part with Λ dependent quantum corrections.

In a similar way the dynamics can be treated. In essence, since deviations from diagonality $x(s) = q(s) - q'(s)$ remain small during the time evolution, they run effectively at each instantaneous mean position $r(s) = [q(s) + q'(s)]/2$ in a harmonic force field $V''(r)x$. Exploiting also the sluggish motion of $r(s)$, this allows for an analytical solution which eventually leads to a time evolution equation for $\varrho(q_f, q_f', t)$. After switching to classical phase space $\{x_f, r_f\} \to \{p, q\}$, i.e. $\varrho(x_f, r_f, t) \to W(p, q, t)$, one arrives at [7]

$$\frac{\partial}{\partial t} W(p, q, t) = \left\{ \frac{\partial}{\partial p} \left[V'_{\text{eff}}(q) + \gamma p \right] - \frac{p}{M} \frac{\partial}{\partial q} + \gamma \langle p^2 \rangle \frac{\partial^2}{\partial p^2} \right.$$
$$\left. + \frac{\partial^2}{\partial q \partial p} \left[1/\beta + \Lambda V''(q) - \langle p^2 \rangle/M \right] \right\} W(p, q, t) . \tag{28}$$

Here, we have introduced an effective potential $V_{\text{eff}} = V + (\Lambda/2) V''$. The first line on the r.h.s coincides with a classical Fokker-Planck operator in an effective force field, the second line describes quantum mechanical coupled p-q diffusion, a necessary ingredient as already seen for the weak damping case in the previous section. In the high temperature limit $\gamma\hbar\beta \to 0$ the quantum Fokker-Planck equation (QFP) tends to the classical Kramers equation [8]. Small but finite $\gamma\hbar\beta \ll 1$ means in the overdamped region also $\omega_0\hbar\beta \ll 1$ so that in case of a *harmonic* potential the QFP becomes identical to the master equation gained by Haake and Reibold specified through (19) and (20). However, while this known master equation is restricted (for $\gamma/\omega_0 > 1$) to the range $\gamma\hbar\beta \ll 1$, the above QFP is valid for *all* $\gamma\hbar\beta$ and for anharmonic potentials as well. It is also not of Lindblad form due to the coarse graining procedure on which its derivation is based. Of course, the equilibrium solution to (28) is given by the Wigner transform of (26). Let us briefly touch the question about higher order diffusion terms to (28). For harmonic systems they do not occur so that the QFP is in this sense exact [18]. In case of anharmonic potentials they result from non-Gaussian quantum

TABLE I: Collection of approximate master equations that have been derived within the exact path integral approach in certain domains of parameter space.

Master equation	Validity[a]	harmonic	anharmonic	Remarks
Agarwal	III	yes	no	$\omega_c \hbar \beta \ll 1$
Haake-Reibold	II, III, IV	yes	no	derived also for $\omega_c > \omega_0$
Haake-Weidlich	III, IV	yes	no	coarse graining $t \gg 1/\omega_0$
Lindblad	III, IV	yes	yes	coarse graining $t \gg 1/\omega_0$
QFP	I, II	yes	yes	can be reduced to QSE

[a]Range of validity according to Fig. 1

fluctuations attributed to higher than second order derivatives in $V(q)$. A rough estimate shows that anharmonic terms in x_f (leading to higher than second order derivatives in p) in the crucial low temperature range $\gamma \hbar \beta \gg 1$ are of order $1/[\hbar \gamma^{3/2} \log(\omega_c/\gamma)]$ compared to the leading terms.

With the QFP at hand, we are now able to follow the reasoning of classical mechanics and reduce it to an equation in position space– the quantum Smoluchowski equation (QSE). For this purpose we employ the projection operator techniques invoked in [19]. Along these lines one introduces the operators $\mathcal{P} = f_\beta(p) \int dp$ and $\mathcal{Q} = 1 - \mathcal{P}$ where $f_\beta(p)$ is the normalized momentum distribution in equilibrium according to (26). The next steps are straightforward and not presented here in detail. After some algebra one arrives to order Λ/γ^3 at an equation for the position distribution $n(q,t) = f_\beta^{-1} \mathcal{P} W$ of the form

$$\frac{\partial}{\partial t} n(q,t) = \frac{1}{\gamma M} \frac{\partial}{\partial q} \left\{ 1 + \frac{1}{M\gamma^2} \left[V''_{\text{eff}} + \Lambda V''' \right] \right\} L_{\text{QSE}}\, n(q,t). \tag{29}$$

Here, to leading order the time evolution is determined by

$$L_{\text{QSE}} = V'_{\text{eff}} + \partial/\partial q [1/\beta + \Lambda V''] \tag{30}$$

derived first in [6]. Inertia corrections appear in curly brackets: A classical ($\Lambda = 0$) correction $\propto V''$ shows up, while quantum fluctuations enter through third and forth order derivatives of the potential. Overdamped quantum Brownian motion in position space thus becomes much more sensitive to the details of the potential profile at lower temperatures.

VII. CONCLUSIONS

Based on the exact path integral approach I have explored to what extent the nonequilibrium dynamics of a dissipative quantum system can be described by a time evoution operator independent of time and initial preparation. The main results of this study are summarized in Table 1 together with Fig. 1. The Agarwal equation, the Haake-Reibold, and the Haake-Weidlich master equations are restricted to harmonic systems, where only the Haake-Reibold result is also applicable for strong damping/high temperature. The Lindblad equation can be used in the weak damping domain for general potential fields but includes an additional coarse graining on the time scale of the bare system time evolution. For strong damping and high as well as low temperatures only the recently found quantum Fokker-Planck/Smoluchowski equation approximates the exact dynamics. Combining both, Lindblad's equation and the latter one, allows to conveniently treat dissipative quantum systems in a considerable range of parameter space. To obtain corresponding generators $\mathcal{L}$, a coarse graining procedure is required which renders either a semiclassical type of approximation due to squeezed Gaussian quantum noise or a perturbative treatment due to weak bath induced entanglement to be successful.

The area in Fig. 1 where no reduction to a simple time evolution equation is possible is a real challenge for further developments. One direction in which progress has been made uses Hubbard-Stratonovich transformations to disentangle forward and backward paths in the influence functional (10) at the expense of new auxiliary fields. Along these lines the reduced dynamics has been expressed in terms of stochastic, nonlinear Schrödinger equation with complex noise [20]. In the same spirit, the quantum stochastic process has been described to involve discontinuous jumps [23]. So far, however, the applicability of related methods is restricted to specific systems and/or certain regions

in parameter space. Efficient algorithms to solve the exact path integrals (8) have been successfully developed and applied, e.g. real-time Monte Carlo schemes [21] or the so-called QUAPI-method [22], but the broad range of long times, intermediate damping, low temperatures, and long bath memory times is still out of reach. Strong efforts to overcome this lack are being on the way.

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