1. Non-Markovian Quantum State Diffusion

1.1. The Microscopical Model

Although the first and foremost goal of our work is the description of the system's reduced dynamics, we focus on a full system-environment description at first. On one hand this serves the purpose to better understand the emergence of the typical phenomena when dealing with open quantum systems and their dependence on the bath. But more important, starting with a closed quantum system is the only strategy that enables a derivation from first principles, in our case the Schrödinger equation. A last argument in favor of the microscopic approach, PRODUCT STATES, ENTANGLEMENT, etc. —we will not dwell on the this any further.

As a starting point we consider an environment consisting of a finite number N of uncoupled harmonic oscillators. This model has been studied extensively for example in the book of Weiss [Wei99]. The generalization to an infinite number can be carried out formally along the same lines, replacing sums by infinite series or even integrals; a different approach within our framework is presented later. The dynamics of both the system and the environment are then described by a unitary time evolution governed by the Hamiltonian

$$H_{\text{tot}} = H \otimes \mathrm{I} + \mathrm{I} \otimes H_{\text{env}} + H_{\text{int}}, \tag{1.1}$$

where H and H_{env} are the free Hamiltonians of the system and the bath respectively.[1] The later is a sum over independent harmonic oscillators $H_{\text{env}} = \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda$ expressed in the ladder operators a_λ and $a_\lambda^\dagger$ of the λ-th mode with frequency ω_λ. Treating a

[1] For some models like the damped harmonic oscillator [CL83] an additional renormalization term arises from the interaction. Nevertheless such a contribution is best attributed to H since it only acts on the system's Hilbert space.

finite number of independent reservoirs poses no further difficulties and therefore is not elaborated in this section.

For the interaction between environment and system we confine ourselves to the case of linear coupling

$$H_{\text{int}} = \sum_{\lambda} g_{\lambda}^{*} L \otimes a_{\lambda}^{\dagger} + g_{\lambda} L^{\dagger} \otimes a_{\lambda}. \tag{1.2}$$

Here L denotes the coupling operator in the system's Hilbert space and $g_{\lambda} \in \mathbb{C}$ the coupling strength of the λ-th mode. Since in typical examples the coupling of an individual bath mode scales inversely with the environment size [Wei99] the linear coupling in (1.2) seems reasonable for macroscopic large environments. But our framework also incorporates small environments—even to the extreme of a single harmonic oscillator—with strong coupling as well. For such cases the linearity needs to be seen as a further assumption of the model.

Beside the Hamiltonian the choice of initial conditions influences the system's subdynamics as well. Throughout this work we only consider product initial conditions, where the bath is in the vacuum state with respect to all a_{λ}

$$|\Psi_0\rangle = |\psi_0\rangle \bigotimes_{\lambda} |0_{\lambda}\rangle. \tag{1.3}$$

These allow us to treat thermal bath states as we show in Sect. 1.5.

To absorb the free dynamics of the environment in time dependent creation and annihilation operators, we switch to the interaction picture with respect to H_{env}. Since the bath operators only obtain an additional phase $\mathrm{e}^{\pm \mathrm{i}\omega_{\lambda} t}$, the transformed Hamiltonian from Eq. (1.4) reads[2]

$$H_{\text{tot}}(t) = H \otimes \mathrm{I} + \sum_{\lambda} \left(g_{\lambda}^{*} \mathrm{e}^{\mathrm{i}\omega_{\lambda} t} L \otimes a_{\lambda}^{\dagger} + g_{\lambda} \mathrm{e}^{-\mathrm{i}\omega t} L^{\dagger} \otimes a_{\lambda} \right). \tag{1.4}$$

Our choice of unentangled initial conditions with a thermal bath state ensures that the reduced density operator remains unaffected under the change of time-evolution picture.

[2] We refrain from introducing another label to distinguish between time-evolution pictures—in what follows we always work in the interaction picture.

It is instructive to rewrite the last equation using the operator valued force

$$B(t) = \sum_\lambda g_\lambda a_\lambda \mathrm{e}^{-\mathrm{i}\omega_\lambda t}. \tag{1.5}$$

The total Hamiltonian then reads $H_{\mathrm{tot}}(t) = H\otimes\mathrm{I} + L\otimes B(t)^\dagger + L^\dagger\otimes B(t)$. Already from this equation it can be seen, that the complete action of the environment on the system is encoded in the operators $B(t)$. In Sect. 1.4.3 we introduce an explicit representation of these force operators and discuss their relation with the classical driving and friction forces. An important—and within our model the only—characteristic of them is the correlation function

$$\alpha(t-s) = \left\langle (B(t)+B(t)^\dagger)(B(s)+B(s)^\dagger)\right\rangle_\rho,$$

where $\langle\cdot\rangle_\rho$ stands for the quantum average over the bath state ρ. For a thermal state at temperature T, the correlation function can be calculated analytically [FHS10]

$$\alpha_\beta(t-s) = \sum_\lambda |g_\lambda|^2 \left(\coth\frac{\beta\omega_\lambda}{2}\,\cos\omega_\lambda(t-s) - \mathrm{i}\sin\omega_\lambda(t-s)\right). \tag{1.6}$$

In the limit of zero temperature and under the natural assumption that $\omega_\lambda > 0$, Equation (1.6) goes over to

1.2. Linear NMSSE

The first step toward a solution of the full equations of motion **??** for a realistic system is a reformulation first proposed by Diósi and Strunz [DS97]: Expressing the bath degrees of freedom in the Segal-Bargmann Hilbert space of analytic functions [Bar61, **?**] provides a representation that is well suited for a Monte-Carlo treatment. To this end we introduce the unnormalized coherent state $|z_\lambda\rangle = \exp(z_\lambda a_\lambda^\dagger)|0_\lambda\rangle$ for each mode. With the shorthand notation $|\boldsymbol{z}\rangle = \bigotimes_\lambda |z_\lambda\rangle$, the resolution of the identity for the environment reads

$$\mathrm{I} = \int \frac{\mathrm{e}^{-|\boldsymbol{z}|^2}}{\pi^N}\,|\boldsymbol{z}\rangle\langle\boldsymbol{z}|\,\mathrm{d}^{2N}z, \tag{1.7}$$

where the integration measure is given by $\mathrm{d}^{2N}z = \prod_\lambda \mathrm{d}\Re z_\lambda \, \mathrm{d}\Im z_\lambda$. Throughout this work we often use the shorthand notation $\mu(\mathrm{d}z) = \pi^{-N}\exp(-|\boldsymbol{z}|^2)\,\mathrm{d}^{2N}z$, which turns out to be meaningful even for an uncountable number of bath oscillators. Equation (1.7) allows us to express the full state in a time-independent environment basis

$$|\Psi_t\rangle = \int |\psi_t(\boldsymbol{z}^*)\rangle \otimes |\boldsymbol{z}\rangle \, \mu(\mathrm{d}z).$$

For the following derivation it is important to notice that the Segal-Bargmann transform $\boldsymbol{z} \mapsto \psi_t(\boldsymbol{z}^*)$ is an anti-holomorphic, $\mathcal{H}_{\mathrm{sys}}$ valued function. It is equivalent to any other representation of the full state $|\Psi_t\rangle$. Although the coherent states are not orthogonal, but rather satisfy $\langle \boldsymbol{w}|\boldsymbol{z}\rangle = \exp(\sum_\lambda w_\lambda^* z_\lambda)$, we can write for the reduced density matrix

$$\rho(t) = \mathrm{Tr}_{\mathrm{env}} |\Psi_t\rangle\langle\Psi_t| = \int |\psi_t(\boldsymbol{z}^*)\rangle\langle\psi_t(\boldsymbol{z}^*)| \, \mu(\mathrm{d}z). \tag{1.8}$$

After fixing the kinematic structure, the next step is to rewrite the dynamics: the representation of the ladder operators follow from the usual rules $\langle \boldsymbol{z}|a_\lambda^\dagger = z_\lambda^* \langle \boldsymbol{z}|$ and $\langle \boldsymbol{z}|a_\lambda = \partial_{z_\lambda^*}\langle \boldsymbol{z}|$ [?]. These expressions give us the complete Schrödinger equation ?? in the transformed space

$$\partial_t \psi_t(\boldsymbol{z}^*) = -\mathrm{i}H\psi_t(\boldsymbol{z}^*) - \mathrm{i}L\sum_\lambda g_\lambda^* \mathrm{e}^{-\mathrm{i}\omega_\lambda t} z_\lambda^* \, \psi_t(\boldsymbol{z}^*) - \mathrm{i}L^\dagger \sum_\lambda g_\lambda \mathrm{e}^{\mathrm{i}\omega_\lambda t} \frac{\partial \psi_t}{\partial z_\lambda}(\boldsymbol{z}^*). \tag{1.9}$$

Introducing an effective driving process similar to Eq. (1.5)

$$Z_t^*(\boldsymbol{z}^*) = -\mathrm{i}\sum_\lambda g_\lambda^* \mathrm{e}^{\mathrm{i}\omega_\lambda t} z_\lambda^* \tag{1.10}$$

allows us to combine the effect of the first bath-interaction term into a single operator. A similar conversion works for the second term as well with the help of the functional chain rule $\frac{\partial}{\partial z_\lambda^*} = \int \frac{\partial Z_s^*}{\partial z_\lambda^*} \frac{\delta}{\delta Z_s^*} \, \mathrm{d}s$. our new equation of motion for the Segal-Bargmann transform reads

$$\partial_t \psi_t = -\mathrm{i}H\psi_t + LZ_t^*\psi_t - L^\dagger \int_0^t \alpha(t-s)\frac{\delta \psi_t}{\delta Z_s^*} \, \mathrm{d}s. \tag{1.11}$$

As we shown in Sect. 1.4.2, the integral boundaries arise due to the vacuum initial conditions (1.3). These render ψ_0 independent from the driving process, such that causality can be used to confine the integral domain.

Up to now we have always referred to Eq. (1.11) as a transformed Schrödinger equation in the full Hilbert space of both system and bath. A different attitude is common as well: Equation (1.22) can be rewritten as $\rho_t = \mathbb{E}\,(|\psi_t\rangle\langle\psi_t|)$, where $\mathbb{E}\,\ldots$ denotes the average over $\mu(\mathrm{d}z) = \pi^{-N}\exp(-|\boldsymbol{z}|^2)\,\mathrm{d}^{2N}z$. Put differently the reduced density matrix ρ_t arises as average over the stochastic pure state projectors $|\psi_t(\boldsymbol{z})\rangle\langle\psi_t(\boldsymbol{z})|$. Hence we regard Eq. (1.11) as a stochastic differential equation for the realisation $\psi_t(\boldsymbol{z})$. We refer to the later either as system state relative to $|\boldsymbol{z}\rangle$ or, in the spirit of the stochastic Schrödinger equations emerging from continuous measurements [Car93], as quantum trajectory. In this approach the driving process Z_t^* is implemented as classical stochastic process. For now it is defined by its concrete version (1.10) and the underlying probability measure μ. Hence we see that it is a complex gaussian process with

$$\mathbb{E}\,Z_t = 0, \quad \mathbb{E}\,Z_t Z_s = 0, \quad \text{and} \quad \mathbb{E}\,Z_t Z_s^* = \alpha(t-s), \tag{1.12}$$

where α is the zero-temperature correlation function **??**. Later on we use these properties to generalize our framework to an environment of infinite size.

Except in the limit $\alpha(t) \sim \delta(t)$, which is elaborated in the next paragraph, the driving process Z_t^* shows correlation for different times. This non-Markovian behavior, which makes a complete understanding of the dynamics highly desirable for application but also considerably harder, shows up in the equation of motion (1.11) as well. The last term contains the functional derivative over the whole timespan and therefore takes the complete history of $\psi_t(Z^*)$ into account. In its own right the derivative is just as problematic: Since its computation requires not only the realisation Z_t^*, but in some sense all adjacent ones too, it even seems questionable to regard the NMSSE (1.11) as a genuine stochastic differential equation, not speaking of a numerical implementation.

1.2.1. Markov Limit

The application of stochastic differential equations in the field of open quantum systems (and quantum optics in particular) has a long tradition [?]. However most of this work is concerned with Markovian systems, which rely on two physical assumptions:

weak coupling of the system to the reservoir and

memoryless environment, that is the time evolution is completely time-local.

Although in the next section we introduce an equivalent convolutionless formulation, which disposes the time-nonlocal functional derivative, the NMSSE does not in general satisfy the latter condition due to the driving process. It is only in the standard Markovian limit $\alpha(t) = \gamma\delta(t)$ we can expect to obtain an equation of motion that describes a reduced time evolution without memory. A rescaling of the coupling operator L allows us to set $\gamma = 1$ without loss of generality.

As shown in **??** the vacuum initial conditions $\frac{\delta\psi_0}{\delta Z_s^*} = 0$ for all $s \in \mathbb{R}$ imply for an arbitrary bath correlation function

$$\frac{\delta\psi_t}{\delta Z_t^*} = L\psi_t \quad (t > 0). \tag{1.13}$$

Since we assumed $\alpha(t-s)$ to be heavily sharply peaked around $s = t$ this is the only contribution of the functional derivative. Using the convention $\int_0^t \delta(t-s)\,\mathrm{d}s = \frac{1}{2}$ Eq. (1.11) then reads

$$\partial_t\psi_t(Z^*) = -\mathrm{i}H\psi_t(Z^*) + LZ_t^*\psi_t(Z^*) - \frac{1}{2}L^\dagger L\psi_t(Z^*),$$

where the driving process is a complex White Noise with $\mathbb{E}Z_tZ_s^* = \delta(t-s)$. In a formally exact manner the equation above should be written as

$$\mathrm{d}\psi_t = (-\mathrm{i}H\psi_t - \frac{1}{2}L^\dagger L\psi_t)\,\mathrm{d}t + L\psi_t\,\mathrm{d}\xi_t^* \tag{1.14}$$

with a complex Brownian motion ξ_t. In order to define the solution ψ_t uniquely we need to specify an appropriate interpretation of the stochastic differential equation [Øks03, p. 36]: We imagine the Brownian motion as a limit of stochastic processes $\xi_t^{(n)} \to \xi_t$, which are continuously differentiable with respect to time, then

Eq. (1.14) transforms into a deterministic differential equation. The limit of corresponding solutions $\psi_t^{(n)}$ coincides with ψ_t only if we understand Eq. (1.14) it the Stratonovich sense. However, in our case the Itō- and the Stratonovich form agree since $\mathbb{E}Z_t Z_s = 0$ [G$^+$85, ???].

The Belavkin or simply stochastic Schrödinger equation (1.14) is a well known result in continuous measurement theory or quantum optics, where it appears as an unravelling of the Linblad master equation [BG09, ?]. Nevertheless our main ingredient in its derivation, namely the singular bath correlation function $\alpha(t) = \delta(t)$, shows how unphysical the Markov assumption is: As α is given by the Fourier transform of the spectral density J,

1.2.2. Convolutionless Formulation

As a cure for the last point Diósi, Gisin and Strunz [DGS98] proposed the powerful O-Operator substitution: It is based on the additional assumption, that one can replace the functional derivative by a system operator O, which may only depend on the realisation of Z^* itself

$$\frac{\delta\psi_t(Z^*)}{\delta Z_s^*} = O(t, s, Z^*)\psi_t(Z^*). \tag{1.15}$$

Besides getting rid of the derivative we use this substitution to derive a convolutionless form of ?? by rewritting it as

$$\partial_t\psi_t = -\mathrm{i}H\psi_t(Z^*) + LZ_t^*\psi_t(Z^*) - L^\dagger\bar{O}(t, Z^*)\psi_t(Z^*) \tag{1.16}$$

with the time-local operator

$$\bar{O}(t, Z^*) := \int_0^t \alpha(t-s)O(t, s, Z^*)\,\mathrm{d}s. \tag{1.17}$$

Finally Eq. (1.16) is a genuine stochastic differential equation for the trajectory $\psi_t(Z^*)$, but in the much smaller Hilbert space of the system. This makes it exceptionally well suited for dealing with infinite sized environments numerically, provided the $\bar{O}$ is known. Depending on the validity of the O-substitution the corresponding NMSSE (1.16) might be just as good as the original microscopic equation of motion ??.

For a few simple models—one is presented in ??—an exact analytic expression for

O is known. In these cases one proocedes as follows [DGS98]: From the consistency condition

$$\partial_t \frac{\delta \psi_t(Z^*)}{\delta Z_s^*} = \frac{\delta}{\delta Z_s^*} \partial_t \psi_t(Z^*) \tag{1.18}$$

and the initial condition familiar from **??**

$$O(s, s, Z^*) = L \tag{1.19}$$

we can derive an equation of motion for $O(t, s, Z^*)$. It still contains the functional derivative, but with an appropriate ansatz for the Z^*-dependence of O, this is transformed into a system of coupled equations independent of the noise. Nevertheless most treatments rely on approximation schemes, for example perturbation expansion for a small coupling parameter or nearly-Markovian environments [YDGS99].

1.2.3. Master Equation

In the last section we introduced the convolutionless formulation primarily to simplify the treatment of the non-Markovian stochastic Schrödinger equation (1.11). Now we use it to show the connection of our approach to the master equations commonly used in the theory of open quantum systems. The latter is formulated in terms of the reduced density operator, which is recovered from the trajectories $\psi_t(Z^*)$ by averaging over the pure states projectors $P_t = |\psi_t(Z^*)\rangle\langle\psi_t(Z^*)|$. In certain cases this can be done analytically in order to derive a master equation.

As a simple example we focus on models which yield a Z^* independent $\bar{O}$-operator, such as the Jaynes-Cummings model presented in **??**. We follow the lines of Yu et al. [YDGS99, YDGS00], who also treat the general case by a systematic expansion of O in the noise. The equation of motion for P_t

$$\partial_t P_t = -\mathrm{i}[H, P_t] + Z_t^* L P_t - L^\dagger \bar{O}(t) P_t + Z_t P_t L^\dagger - P_t \bar{O}(t)^\dagger L \tag{1.20}$$

yields a closed evolution equation for rho_t after averaging over the bath degrees of freedom only if we can restate the terms containing Z_t^* in noise-independent manner. This can be done with the help of Novikov's formula [Nov65]

$$\mathbb{E}\left(Z_t P_t\right) = \mathbb{E}\left(\int \mathrm{d}s \alpha(t-s) \frac{\delta}{\delta Z_s^*} P_t\right).$$

A formal proof is provided in **??** but the main idea is simple: Under a Gaussian integral $\int \mathrm{d}^2 z \exp(-|z|^2) \ldots$ the multiplication by z can be rewritten as a derivation ∂_{z^*}. By partial integration a similar result to the equation above is obtained.

The right hand side of Novikov's formula can be simplified further. Since ψ_t is holomorphic in Z^* we have

$$\frac{\delta}{\delta Z_s^*}\left(|\psi_t(Z^*)\rangle\langle\psi_t(Z^*)|\right) = \left(\frac{\delta}{\delta Z_s^*}|\psi_t(Z^*)\rangle\right)\langle\psi_t(\boldsymbol{z})| = O(t,s)|\psi_t(Z^*)\rangle\langle\psi_t(Z^*)|$$

with the O-operator substitution (1.15). Averaging over the equation of motion for the pure state projector (1.20) finally gives the master equation for the reduced density matrix ρ_t

$$\partial_t \rho_t = -\mathrm{i}[H, \rho_t] + [L, \rho_t \bar{O}(t)^\dagger] + [\bar{O}(t)\rho_t, L^\dagger]. \tag{1.21}$$

This expression already resembles the well known Lindblad master equation **??** for Markovian open quantum systems. Indeed, in the Markovian limit $\alpha(t) = \frac{\gamma}{2}\delta(t)$ the $\bar{O}$-operator is given by $\bar{O}(t) = \frac{\gamma}{2}L$ as shown in **??**. For some models the same holds true even for genuine non-Markovian environments except the coefficients may become time-dependent.

1.3. Nonlinear NMSSE

In the last section we emphasize that the non-Markovian stochastic Schrödinger equation (1.11) can be interpreted either as a system-environment Schrödinger equation or as a stochastic differential equation for the trajectories $\psi_t(Z^*)$. In the theory of Markovian systems the latter is often referred to as an unravelling of the corresponding master equation [**?**]. Either way in a numerical treatment the reduced density operator of the open system is determined by a Monte-Carlo evaluation of the partial trace (or stochastic average)

$$\rho_t = \mathbb{E}\left(|\psi_t\rangle\langle\psi_t|\right) = \int |\psi_t(\boldsymbol{z})\rangle\langle\psi_t(\boldsymbol{z})|\, \mu(\mathrm{d}z). \tag{1.22}$$

The fineness of such a scheme is drastically reduced if there are few highly peaked contributions [DS11]. As shown in a numerical investigation [**?**] the NMSSE shows exactly this behavior: for most trajectories the norm $\langle\psi_t(Z^*)|\psi_t(Z^*)\rangle$ goes to zero

due to growing entanglement with the environment. To recover the unitarity of the closed time evolution $\mathbb{E}\left(\langle\psi_t|\psi_t\rangle\right) = \langle\Psi_t|\Psi_t\rangle = 1$ the few trajectories with significant contribution have to be taken into consideration. As we further elaborate in **??** this requires an insurmountable sample size for certain system parameters.

Seen purely as a stochastic tool to determine the reduced density operator the unravelling in Eq. (1.22) is not unique: we can perform any transformation under the integral which keeps its value fixed and obtain equally well relative states with a different measure. As it improves the behavior of the Monte-Carlo evaluation noticeably we perform a change of measure such that the average can be taken over normalized states. Such a procedure is well known from the theory of Markovian stochastic Schrödinger equation [**?**] and results in a nonlinear equation of motion—the same is true for our non-Markovian approach. Since the general case is treated later we focus on the convolutionless formulation of Eq. (1.16).

Of course it is trivial to rewrite Eq. (1.22) as an average over normalized states

$$\rho_t = \int \frac{\mathrm{d}^{2N}z}{\pi^N}\,\mathrm{e}^{-|\boldsymbol{z}|^2}\langle\psi_t(\boldsymbol{z}^*)|\psi_t(\boldsymbol{z}^*)\rangle\,\frac{|\psi_t(\boldsymbol{z}^*)\rangle\langle\psi_t(\boldsymbol{z}^*)|}{\langle\psi_t(\boldsymbol{z}^*)|\psi_t(\boldsymbol{z}^*)\rangle},$$

now expressed with a time dependent density function. To highlight the physical significance of the norm we notice that the latter is just the Q- or Husimi-function[3] of the bath given by [Sch11]

$$Q_t(\boldsymbol{z},\boldsymbol{z}^*) = \frac{\mathrm{e}^{-|\boldsymbol{z}|^2}}{\pi^N}\,\langle\boldsymbol{z}|\,\mathrm{Tr}_{\mathrm{sys}}\left(|\Psi_t\rangle\langle\Psi_t|\right)|\boldsymbol{z}\rangle = \frac{\mathrm{e}^{-|\boldsymbol{z}|^2}}{\pi^N}\,\langle\psi_t(\boldsymbol{z}^*)|\psi_t(\boldsymbol{z}^*)\rangle. \tag{1.23}$$

Expressed in terms of Q_t the reduced density operator reads

$$\rho_t = \int Q_t(\boldsymbol{z},\boldsymbol{z}^*)\,\frac{|\psi_t(\boldsymbol{z}^*)\rangle\langle\psi_t(\boldsymbol{z}^*)|}{\langle\psi_t(\boldsymbol{z}^*)|\psi_t(\boldsymbol{z}^*)\rangle}\mathrm{d}^{2N}z. \tag{1.24}$$

Due to being non-negative and normalized to unity $\int Q(\boldsymbol{z},\boldsymbol{z}^*)\,\mathrm{d}z = 1$ the Husimi-function can be regarded as the (quasi)-probability distribution on phase space of the bath degrees of freedom: Since a coherent state $|z\rangle$ resembles a wave packet localized around $z = (q + \mathrm{i}\,p)/\sqrt{2}$, there is a well defined correspondence between coherent state labels z and the canonical variables (q, p). Hence the norm of $\psi_t(\boldsymbol{z}^*)$

[3] We point out that the Husimi function is usually defined in terms of normalized coherent states. Hence the additional factor $\exp(-|z|^2)$ for each oscillator in our notation.

simply determines the probability to find the bath oscillators in the coherent state $|\boldsymbol{z}\rangle$.

We can now incorporate the dynamics of the environment in a comoving coherent state basis for our trajectories $\psi_t(\boldsymbol{z}^*)$. Making use of the microscopic Hamiltonian (1.9) and the analyticity $\partial_{z_\lambda}|\psi_t(\boldsymbol{z}^*)\rangle$ gives the time evolution of the Husimi-function

$$\partial_t Q_z(\boldsymbol{z},\boldsymbol{z}^*) = -\sum_\lambda \partial_{z_\lambda^*}\big(\mathrm{i}g_\lambda \mathrm{e}^{-\mathrm{i}\omega_\lambda t}\,\langle L^\dagger\rangle_t\, Q_t(\boldsymbol{z},\boldsymbol{z}^*)\big) - \text{c.c.} \tag{1.25}$$

It is obvious that the equation of motion above contains the full back-reaction of the system due to the quantum average[4]

$$\langle L^\dagger\rangle_t = \frac{\langle\psi_t(\boldsymbol{z}^*)|L^\dagger|\psi_t(\boldsymbol{z}^*)\rangle}{\langle\psi_t(\boldsymbol{z}^*)|\psi_t(\boldsymbol{z}^*)\rangle}.$$

Remarkably Eq. (1.25) can be solved with the method of characteristics since it has exactly the form of a (complex) Liouville equation. The corresponding characteristic curves are are described by

$$\dot{z}_\lambda^*(t) = \mathrm{i}g_\lambda \mathrm{e}^{-\mathrm{i}\omega_\lambda t}\langle L^\dagger\rangle_t. \tag{1.26}$$

We denote the corresponding flow by $\boldsymbol{\phi}_t$; hence by the usual abuse of notation $z_\lambda^*(t) = \phi_{\lambda,t}^*(z_\lambda^*)$ with initial conditions $z_\lambda^*(0) = \phi_{\lambda,0}^*(z_\lambda^*) = z_\lambda^*$. Equation (1.26) tells us that if the full state at time t is $|\psi_t(\boldsymbol{z}^*)\rangle\otimes|\boldsymbol{z}\rangle$ and therefore the Husimi-function is localised around $\boldsymbol{z} = (\boldsymbol{q}+\mathrm{i}\,\boldsymbol{p})/\sqrt{2}$ then the dominant contribution at $t+\Delta t$ comes from the coherent state $|\boldsymbol{z}+\dot{\boldsymbol{z}}\Delta t\rangle$. For this reason we should use system states relative to $|\boldsymbol{z}(t)\rangle$ instead in order to avoid vanishing contributions of single trajectories to ρ_t.

By construction the flow $\boldsymbol{\phi}_t$ also gives as a solution to Eq. (1.25) for the Husimi-function

$$Q_t(\boldsymbol{z},\boldsymbol{z}^*) = \int Q_0(\boldsymbol{z}_0,\boldsymbol{z}_0^*)\,\delta(\boldsymbol{z}-\boldsymbol{\phi}_t(\boldsymbol{z}_0))\,\mathrm{d}^{2N}z_0$$

where $\delta(\boldsymbol{z}-\boldsymbol{z}') = \prod_\lambda \delta(\Re(z_\lambda - z'_\lambda))\delta(\Im(z_\lambda - z'_\lambda))$. Since at the beginning our total state is given by the product $|\Psi_t\rangle = |\psi_0\rangle\otimes|\boldsymbol{z}\rangle$ the initial condition for the Husimi-function reads $Q_0(\boldsymbol{z},\boldsymbol{z}^*) = \pi^{-N}\mathrm{e}^{-|\boldsymbol{z}|^2}$ as seen from Eq. (1.23). With $\psi'_t = \psi_t\circ\boldsymbol{\phi}_t$ we

[4] We do not indicate its (non-holomorphic) dependence on $\boldsymbol{z}^*$ explicitly because our main goal is not the solution of ??. Instead Q_t is only used to derive normalized versions of our NMSSE-trajectories.

can rewrite Eq. (1.22) for the reduced density matrix as[5]

$$\rho_t = \int \frac{\mathrm{d}^{2N} z}{\pi^N} \, \mathrm{e}^{-|\boldsymbol{z}|^2} \, \frac{|\psi_t(\boldsymbol{\phi}_t^*(\boldsymbol{z}^*))\rangle\langle\psi_t(\boldsymbol{\phi}_t^*(\boldsymbol{z}^*))|}{\langle\psi_t(\boldsymbol{\phi}_t^*(\boldsymbol{z}^*))|\psi_t(\boldsymbol{\phi}_t^*(\boldsymbol{z}^*))\rangle} = \mathbb{E}\left(\frac{|\tilde{\psi}_t\rangle\langle\tilde{\psi}_t|}{\langle\tilde{\psi}_t|\tilde{\psi}_t\rangle}\right). \tag{1.27}$$

By its definition $\tilde{\psi}_t(\boldsymbol{z}^*)$ is just the relative state of $|\Psi_t\rangle$ belonging to the coherent state $|\boldsymbol{\phi}_t(\boldsymbol{z}^*)\rangle$. Put differently these are exactly tho expansion coefficients of the full system-bath pure state in the comoving environmental basis. It is quite remarkable that a closed equation of motion for the $\tilde{\psi}_t$ can be derived starting with

$$\partial_t(\psi_t \circ \boldsymbol{\phi}_t^*) = \partial_t\psi_t \circ \boldsymbol{\phi}_t^* + \sum_\lambda (\partial_{z_\lambda^*}\psi_t \circ \boldsymbol{\phi}_t^*) \cdot (\partial_t \phi_{t,\lambda}^*). \tag{1.28}$$

For the first term we can use the evolution equation (1.16) of the fixed-basis relative states ψ_t with the O-operator substitution in place. Replacing the coherent state labels by their comoving counterparts leads us to a shifted process: The integral form of Eq. (1.26)

$$\phi_{t,\lambda}^*(z_\lambda^*) = z_\lambda^* + \mathrm{i}g_\lambda \int_0^t \exp(-\mathrm{i}\omega_\lambda s)\langle L^\dagger\rangle_s \, \mathrm{d}s$$

plugged into the microscopic version of the process (1.10) yields the shifted stochastic driving as

$$\tilde{Z}_t^*(\boldsymbol{z}^*) := Z_t^*(\boldsymbol{\phi}_t^*(\boldsymbol{z}^*)) = Z_t^*(\boldsymbol{z}^*) + \int_0^t \alpha(t-s)^*\langle L^\dagger\rangle_s \, \mathrm{d}s. \tag{1.29}$$

Since the O-operator substitution ensures that the equations of motion for ψ_t are local with respect to Z^*, the comoving dynamics just amount to replacing Z_t^* by $\tilde{Z}_t^*$ in the first addend of (1.28).

The second addend, due to the intrinsic time dependence of the shifted coherent states, is treated on the same footing: It is just the well-known functional derivative

[5] Instead of directly introducing the normalized states $\tilde{\psi}_t$ as done by Strunz [Str01] we explicitly define the interim state ψ_t' to compare with the corresponding result for the hierarchy in ??.

term from the NMSSE as Eq. (1.26) reveals:

$$\begin{aligned}\sum_\lambda \frac{\partial \phi^*_{t,\lambda}}{\partial t}(z^*_\lambda)\cdot\frac{\partial \psi_t}{\partial z^*_\lambda}(\boldsymbol{\phi}^*_t(\boldsymbol{z}^*)) &= \mathrm{i}\sum_\lambda g_\lambda \mathrm{e}^{-\mathrm{i}\omega_\lambda t}\langle L^\dagger\rangle_t \frac{\partial \psi_t}{\partial z^*_\lambda}(\boldsymbol{\phi}^*_t(\boldsymbol{z}^*))\\ &= \langle L^\dagger\rangle_t \int_0^t \alpha(t-s)\frac{\delta \psi_t}{\delta Z^*_s}(\boldsymbol{\phi}^*_t(\boldsymbol{z}^*))\,\mathrm{d}s\\ &= \langle L^\dagger\rangle_t \bar{O}(t,\tilde{Z}^*)\tilde{\psi}_t(\tilde{Z}^*),\end{aligned}$$

where the last line reflects the definition of the $\bar{O}$-operator in Eqs. (1.15) and (1.17). Both terms of (1.28) combined yield the desired closed equation for $\tilde{\psi}_t$

$$\partial_t\tilde{\psi}_t = -\mathrm{i}H\tilde{\psi}_t + L\tilde{Z}^*_t\tilde{\psi}_t - (L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,\tilde{Z}^*)\tilde{\psi}_t. \tag{1.30}$$

We want to recall that $\tilde{\psi}_t$ was introduced to allow averaging over normalized states in Eq. (1.27). It does not imply $\tilde{\psi}_t(\tilde{Z}^*)$ being normalized for all times, which would be favourable for interpreting the NMSSE as an stochastic equation for genuine pure system states. It is quite remarkable that an extended version of Eq. (1.30) exists that even preserves normalization of single realizations: By considering the trajectories $|\psi'_t\rangle = |\tilde{\psi}_t\rangle/\sqrt{\langle\tilde{\psi}_t|\tilde{\psi}_t\rangle}$ it is straightforward to derive the corresponding equation of motion [**?**]

$$\begin{aligned}\partial_t\psi'_t = &-\mathrm{i}H\psi'_t + (L-\langle L\rangle_t)\,\tilde{Z}^*_t\psi'_t\\ &-\Big((L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,\tilde{Z}^*) - \langle(L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,\tilde{Z}^*)\rangle\Big)\,\psi'_t\end{aligned} \tag{1.31}$$

As mentioned in the motivation the nonlinear equations should be given precedence over the linear version when it comes to Monte-Carlo simulation. They allow us to compute the density matrix as an average over realizations with same order of magnitude while restoring the reference measure (in the microscopic model) to the well known, time-independent Gaussian weight (1.7). Therefore generating realizations of the shifted processes $\tilde{Z}^*_t$ is within the scope of general methods, as long as the expectation value $\langle L^\dagger\rangle_s$ for all times $0 \le s \le t$ is known. This is the only contribution to the nonlinear NMSSE which is explicitly time-nonlocal; but since it involves only the average value there is no storage problem for numerical application. Of course these comments neglect the question how to obtain the $\bar{O}$-operator, which contains

all non-Markovian feedback of the environment. For to application to any realistic physical system—except a few exactly solvable ones—this is actually the critical part in the implementation.

1.4. Interpretation of NMSSE

1.4.1. NMSSE as Continous Measurement

1.4.2. Linear NMSSE as Schrödinger Equation

1.4.3. A Time-Nonlocal Picture

1.5. Finite Temperature Theory

Until now we were only concerned with the temperature zero theory, which was defined by an initial product state with the environment in the vacuum state $|\Psi_0\rangle = |\psi_0\rangle \otimes |\mathbf{0}\rangle$. It translates into our NMSSE-framework as the demand of vanishing functional derivatives at the time $t = 0$

$$\frac{\delta\psi_0}{\delta Z_s^*} = 0 \quad (s \in \mathbb{R}).$$

This allows us to restrict the integral domain for the derivatives in Eq. (1.11) and is therefore crucial for the O-operator substitution. Without the upper limit t for the integral the hierarchical equations of motion presented in **??** fail as well. In order to treat non-zero temperature systems with the non-Markovian stochastic Schrödinger equation we devise two methods that map to the vacuum initial conditions of the zero-temperature case.

To start off we assume a product initial state, but this time with a Gibbs state $\rho(\beta) = \frac{\mathrm{e}^{-\beta H_{\mathrm{env}}}}{Z}$ on the environment's side

$$\rho_0 = |\psi_0\rangle\langle\psi_0| \otimes \rho(\beta) \tag{1.32}$$

with the bath partition function $Z = \mathrm{Tr}_{\mathrm{exp}}[-\beta H_{\mathrm{env}}]$ at inverse temperature $\beta = 1/k_B T$. This choice amounts to the following experimental setting: At $t_{\mathrm{init}} \to -\infty$ the environment is brought into contact with an even larger heat bath at given temperature, while the coupling to the system is switched off. The environment is allowed

to thermalize until $t = 0$ when the super-bath is removed and the system-coupling is instantly tuned as given by Eq. (1.2). The choice of a pure state projector for the system in Eq. (1.32) is merely for convenience; in contrast we cannot drop its product form. Therefore a initial thermal state of the system and bath with respect to H_{tot} cannot be treated with the NMSSE due to entanglement.

1.5.1. Thermo Field Method

Thermo field dynamics was introduced as a real-time approach to quantum fields at finite temperature [?]. It is favored over other methods in application to the NMSSE since it does not change the equation of motion [DGS98] as shown below. In the course of this section we follow the slightly more detailed accounts of Yu and Strunz [Yu04, Str01].

The main idea is to introduce a second fictitious bath of oscillators, which is independent from the physical environment and does not interact with the system. Expressing its degrees of freedom in ladder operators b_λ and $b_\lambda^\dagger$ gives us the new Hamiltonian in the Schrödinger picture

$$H_{\mathrm{tot}} = H \otimes \mathrm{I} + \sum_\lambda (g_\lambda^* L \otimes a_\lambda^\dagger + g_\lambda L^\dagger \otimes a_\lambda) + \mathrm{I} \otimes \sum_\lambda \omega_\lambda (a_\lambda^\dagger a_\lambda - b_\lambda^\dagger b_\lambda). \tag{1.33}$$

Although this Hamiltonian is not bounded from below due to negative frequencies of the fictitious oscillators, there are no stability problems since they do not interact with the physical degrees of freedom. For the same reason the reduced dynamics obtained from Eq. (1.33) are identical to the original microscopical model (1.4). Therefore both yield equal reduced density matrices for our system provided we choose an initial state that reproduces Eq. (1.32) upon tracing of the unphysical degrees of freedom. Since these are given by a product the choice of a total initial state is independent from the system and is equivalent to demand

$$\mathrm{Tr_b}\, \tilde{\rho} = \rho(\beta) \tag{1.34}$$

for the density matrix of both environments. Here $\mathrm{Tr_b}$ denotes the partial trace with respect to the fictitious degrees of freedom.

Remarkably a solution $\tilde{\rho}$ of Eq. (1.34) is given by the pure state projector on a vacuum state with respect to new annihilation operators A, B. They are connected

to the old ladder operators by a temperature dependent Bogoliubov transformation

$$A_\lambda = \sqrt{\bar{n}_\lambda + 1}\, a_\lambda + \sqrt{\bar{n}_\lambda}\, b_\lambda^\dagger$$
$$B_\lambda = \sqrt{\bar{n}_\lambda}\, a_\lambda^\dagger + \sqrt{\bar{n}_\lambda + 1}\, b_\lambda,$$

with $\bar{n}_\lambda = (\exp(\beta\omega_\lambda) - 1)^{-1}$ denoting the mean thermal occupation number of the (physical) oscillator mode λ. An extensive but elementary calculation reveals that $|0_{AB}\rangle\langle 0_{AB}|$ with $|0_{AB}\rangle = |0_A\rangle \otimes |0_B\rangle$ defined by $A_\lambda|0_{AB}\rangle = B_\lambda|0_{AB}\rangle = 0$ satisfies Eq. (1.34).

The doubling in degrees of freedom ensures that the reduced density matrix obtained from an initial pure state $|\tilde{\Psi}_0\rangle = |\psi_0\rangle \otimes |0_{AB}\rangle$ in the enlarged Hilbert space coincides with the original one lacking unphysical bath oscillators. Expressed in these new coordinates the total Hamiltonian (1.33) reads

$$\begin{aligned} H_{\text{tot}} = H \otimes \mathrm{I} &+ \sum_\lambda \sqrt{\bar{n}_\lambda + 1}\, \left(g_\lambda^* L \otimes A_\lambda^\dagger + g_\lambda L^\dagger \otimes A_\lambda \right) \\ &+ \sum_\lambda \sqrt{\bar{n}_\lambda}\, \left(g_\lambda L^\dagger \otimes B_\lambda^\dagger + g_\lambda^* L \otimes B_\lambda \right) \\ &+ \mathrm{I} \otimes \sum_\lambda \omega_\lambda \left(A_\lambda^\dagger A_\lambda - B_\lambda^\dagger B_\lambda \right). \end{aligned} \tag{1.35}$$

Our new Hamiltonian is identical to the zero-temperature model except for the system coupling to two separate oscillator baths instead of one; therefore we need two independent processes Z_t^* and W_t^* for a stochastic version of Eq. (1.35) in general:

$$\begin{aligned} \partial_t \psi_t = -\mathrm{i}H\psi_t + LZ_t^*\psi_t - L^\dagger \int_0^t \alpha_1(t-s) \frac{\delta \psi_t}{\delta Z_s^*}\, \mathrm{d}s \\ + L^\dagger W_t^* \psi_t - L \int_0^t \alpha_2(t-s) \frac{\delta \psi_t}{\delta W_s^*}\, \mathrm{d}s. \end{aligned} \tag{1.36}$$

All effects of the original thermal initial state are now encoded in the correlation functions

$$\alpha_1(t) = \sum_\lambda (\bar{n}_\lambda + 1)\, |g_\lambda|^2\, \mathrm{e}^{-\mathrm{i}\omega_\lambda t} \quad \text{and} \quad \alpha_2(t) = \sum_\lambda \bar{n}_\lambda\, |g_\lambda|^2\, \mathrm{e}^{\mathrm{i}\omega_\lambda t}$$

for Z_t^* and W_t^* respectively. Since both are Gaussian, their independence is equivalent

to the vanishing of all their mutual correlations $\mathbb{E}\left(Z_t^* W_s\right) = \mathbb{E}\left(Z_t W_s\right) = 0$.

As we doubled the bath degrees of freedom merely to cope with a thermal initial state it is quite natural that the zero-temperature result from **??** with a single driving process is recovered in the limit $T \to 0 \ldots$

The thermo field approach to our non-Markovian Schrödinger equation turns out to be especially simple in the case of self-adjoint coupling operators $L^\dagger$: From Eq. (1.36) we see how both driving processes Z_t^* and W_t^* can be combined into a single one, which we will denote by Z_t^* again. Since we took them to be mutually independent we find for our new sum process using $2\bar{n}_\lambda + 1 = \coth \frac{\beta\omega_\lambda}{2}$:

$$\mathbb{E}\left(Z_t Z_s^*\right) = \sum_\lambda \left(|g_\lambda|^2 \coth \frac{\beta\omega_\lambda}{2} \cos\omega_\lambda(t-s) - \mathrm{i}\sin\omega_\lambda(t-s) \right). \tag{1.37}$$

Consequently the finite temperature NMSSE takes the form identical to zero temperature theory. They only differ in how the correlation function is obtained from a microscopical model or rather from a spectral density. It is not surprising that our combined correlation function (1.37) agrees with the result of Feynman and Vernon [FV63] derived in the path integral formalism for quantum Brownian motion. But our approach is much more general since it can tackle any kind of open quantum system with linear coupling.

1.5.2. unitary noise

As shown in the last section we can treat classical thermal noise on the same footing as quantum noise under certain circumstances just by using a modified correlation function (1.37). It is worth noticing how the influence of thermal fluctuations modify only the real part of α, a feature that explicitly distinguishes noisy classical perturbations [FHS10]. Therefore it is quite instructive to present a different method for treating non-zero temperature within the non-Markovian quantum state diffusion.

We start off by expanding the thermal bath state in a coherent state basis [WM08]

$$\rho(\beta) = FILLIN$$

which is quite reminiscent of the expansion for a pure state projector that lead to our stochastic Schrödinger equation. The corresponding pure initial states are a product

involving all environmental oscillators

$$|\Psi_0(\xi)\rangle = \mathrm{e}^{-\frac{|\boldsymbol{\xi}|^2}{2}} |\psi_0\rangle \bigotimes_\lambda |\xi_\lambda\rangle$$

where the additional prefactor is usually absorbed by using normalized coherent states. A simple shift for the creation and annihilation operators $A_\lambda^\dagger = a_\lambda^\dagger - \xi_\lambda^*$ and $A_\lambda = a_\lambda - \xi_\lambda$ respectively maps the environmental part of the initial state above onto the vacuum. Therefore we can apply our zero-temperature derivation to the total Hamiltonian expressed in A and $A_\lambda^\dagger$. The resulting NMSSE reads

$$\partial_t \psi_t(Z^*, \xi) = \left(-\mathrm{i}H + L\xi_t^* + L^\dagger \xi_t + LZ_t^* - L^\dagger \int_0^t \alpha(t-s) \frac{\delta}{\delta Z_s^*} \,\mathrm{d}s \right) \psi_t(Z^*, \xi, \xi^*) \tag{1.38}$$

with a classical driving process $\xi_t = \sum_\lambda g_\lambda \xi_\lambda \mathrm{e}^{-\mathrm{i}\omega_\lambda t}$ and its familiar quantum counterpart Z_t^*. The former's properties are once again fixed by its correlations

$$\mathbb{E}\,\xi_t = 0, \quad \mathbb{E}\,\xi_t \xi_s = 0, \quad \text{and} \quad \mathbb{E}\,\xi_t \xi_s^* = 2 \sum_\lambda \bar{n}_\lambda \,|g_\lambda|^2 \cos \omega_\lambda (t-s).$$

Recovering the reduced density matrix not only requires an average over Z^* but also over all realizations of the thermal noise process ξ_t. Since all thermal occupation numbers $\bar{n}_\lambda$ tend to zero for $T \to 0$, we obtain the zero temperature limit simply by setting $\xi_t = 0$. This amounts to the trivial decomposition $\rho(T=0) = |\mathbf{0}\rangle\langle\mathbf{0}|$ of the zero temperature environmental state.

1.6. Dissipative Two-level System

$$\partial_t \psi_t = -\mathrm{i}\frac{\omega}{2}\sigma_z \psi_t + c\sigma_- Z_t^* \psi_t - c\sigma_+ \int_0^t \alpha(t-s) \frac{\delta \psi_t}{\delta Z_s^*} \,\mathrm{d}s \tag{1.39}$$

1.6.1. O-Operator Method

As elaborated in Sect. 1.2.2 we can simplify the NMSSE (1.39) by replacing the functional derivative with an operator $O(t, s, Z^*)$. We try to solve the consistency condition (1.18) by a noise-independent ansatz

$$O(t,s) = cf(t,s)\sigma_-, \tag{1.40}$$

hence all non-Markovian feedback from the environment is now encoded in the function $f(t,s)$ to be determined. Plugging this ansatz into the evolution equation for O yields

$$\partial_t c f(t,s)\sigma_- = \left[-\mathrm{i}\frac{\omega}{2}\sigma_z - c^2 F(t)\sigma_+\sigma_-, cf(t,s)\sigma_-\right] \tag{1.41}$$

with a shorthand notation $F(t) := \int_0^t \alpha(t-s)f(t,s)\,\mathrm{d}s$. From its definition (1.17) we see that F is also the prefactor for the integrated operator $\bar{O}(t) = cF(t)\sigma_-$. Since the operator algebra in Eq. (1.41) closes, our ansatz solves the equation of motion for O provided f evolves according to

$$\partial_t f(t,s) = \left(\mathrm{i}\omega + c^2 F(t)\right)\, f(t,s) \quad (s \le t).$$

Appropriate initial conditions follow trivially from Eq. (1.19); they read $f(s,s) = 1$. In the special case of an exponential bath correlation function $\alpha(t) = g\mathrm{e}^{-\gamma|t| - \mathrm{i}\Omega t}$ we can also derive a differential equation that is closed in F

$$\partial_t F(t) = g + (\mathrm{i}(\omega - \Omega) - \gamma)F(t) + c^2 F(t)^2.$$

Such correlation functions play a major role in the subsequent work.

As shown in Sect. 1.2.3, a convolutionless NMSEE with noise independent O-operator can be transformed into a master equation without any approximation. For the model under consideration it turns out to closely resemble a Lindblad-type equation except for time-dependent coefficients

$$\partial_t \rho_t = -\mathrm{i}\frac{\omega}{2}[\sigma_z, \rho_t] + c^2[\sigma_-, \rho_t\sigma_+] + c^2 F(t)[\sigma_-\rho_t, \sigma_+].$$

1.6.2. Noise-Expansion Method

In this section we propose a different method for solving Eq. (1.39): It is based on the expansion discussed in **??**, which allows us to express the quantum trajectories $\psi_t(Z^*)$ in a functional Taylor series with respect to the noise process. Due to the particular coupling structure of the model we can neglect all terms higher than linear order in Z_t^*. As further elaborated in Sect. B.1, our NMSSE (1.39) reduces to a

$\mathbb{C}$-valued integro-differential equation

$$\dot{\psi}^+(t) = -\mathrm{i}\frac{\omega}{2}\psi^+(t) - c^2\int_0^t \alpha(t-s)\mathrm{e}^{\mathrm{i}\frac{\omega}{2}(t-s)}\psi^+(s)\,\mathrm{d}s, \tag{1.42}$$

which is nevertheless quite involved—even from a numerical point of view. The situation is noticeably simpler for an exponential correlation function for which we calculate an analytic solution in the appendix as well.

But even without an explicit solution for $\psi^+(t)$ we may still discover some illuminating consequences concerning the O-operator from the last section. With $\psi^-(t) = \psi^-(0)\exp(\mathrm{i}\omega t/2)$ the full quantum trajectory reads

$$\psi_t(Z^*) = \begin{pmatrix} \psi^+(t) \\ \psi^-(t) \end{pmatrix} + c\int_0^t \begin{pmatrix} 0 \\ \mathrm{e}^{\mathrm{i}\frac{\omega}{2}(t-s)}\psi^+(s) \end{pmatrix} Z_s^*\,\mathrm{d}s. \tag{1.43}$$

This allows us to calculate the functional derivative with respect to the driving process explicitly; for $0 \le s \le t$ we find[6]

$$\frac{\delta\psi_t(Z^*)}{\delta Z_s^*} = c\begin{pmatrix} 0 \\ \mathrm{e}^{\mathrm{i}\frac{\omega}{2}(t-s)}\psi^+(s), \end{pmatrix}$$

which agrees with out ansatz (1.40) in case we choose

$$f(t,s) = \frac{\psi^+(s)}{\psi^+(t)}\,\mathrm{e}^{-\mathrm{i}\frac{\omega}{2}(s-t)}. \tag{1.44}$$

A similar structure for the O-operator has been obtained by Strunz [Str01] within a Heisenberg-operator method.

[6] For $s = t$ there is no additional prefactor $\frac{1}{2}$ from integrating a δ-function localized at the upper integral boundary as explained in the footnote on page 25.

A. Mathematical Preliminaries

We will now substantiate the claim of Sect. 1.4.2, that the linear Non-Markovian Stochastic Schrödinger Equation

$$\partial\psi_t = -\mathrm{i}h\psi_t + LZ_t^*\psi_t - L^\dagger \int_0^t \alpha(t-s)\frac{\delta\psi_t}{\delta Z_s^*}\,\mathrm{d}s \tag{A.1}$$

can also be understood as a Schrödinger equation for the closed system, consisting of the system and a generalized environment. Our investigation will proceed as follows: First we will be concerned with the kinematic structure and provide an explicit construction of the underlying bath Hilbert space; subsequently we will explore how the noise process Z_t^* and the functional derivative in Eq. (A.1) can be realized as operators on this Hilbert space.

In this section we will not attempt to present a mathematical rigorous treatment of the NMSSE, but provide the basic idea, how Eq. (A.1) fits into the established framework of *White Noise Analysis*. Therein we will follow the spirit of [Hid80, ?].

A.1. Hilbert Space of "Time Oscillators"

Let us first recall some basic terminology from probability theory (see e.g. [Sch05]): A C-valued *random variable* X is a measurable map from a measure space $(\Omega, \mathcal{A}, \mathbb{P})$ to the measurable space $(C, \mathcal{B})$. Here Ω, C denote sets, $\mathcal{A}$, $\mathcal{B}$ are σ-algebras of Ω and C respectively, and $\mathbb{P}$ is a probability measure on $(\Omega, \mathcal{A})$.[1] Expectation values, variances, etc., may then be expressed as integrals of X with respect to $\mathbb{P}$.

It is important to mention, that — versions... Therefore we may always use the microscopical version of Z_t^* defined in ??, where $\Omega = \mathbb{C}^N$ and $\mathbb{P} = \mathrm{e}^{-|\boldsymbol{z}|^2}\,\mathrm{d}^N z$. But since this is—strictly speaking—valid only for a finite number N of bath oscillators,

[1] In what follows, we will consider only Borel-σ-algebras and therefore not mention them any further.

we will take a different route: Using only the *bath correlation function*

$$\alpha(t) = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}\omega t}\, J(\omega)\, \mathrm{d}\omega, \tag{A.2}$$

we establish a suitable measure space, which will be used to support our new environmental Hilbert space afterwards. Here $J(\omega)\,\mathrm{d}\omega$ denotes the *spectral density*, which is a positive, bounded measure, i.e. $J \geq 0$ and $\int J(\omega)\,\mathrm{d}\omega < \infty$. This restriction excludes the important Markovian limit $J = 1 \iff \alpha(t) \sim \delta(t)$, but... Such a unified approach has the advantage of only making reference to the bath correlation function, stressing that it is the only property of the environment relevant within our model.

As a first step, we will fix our space Ω, which will be used as domain for our random variables later. Its physical interpretation will be more clearly after we have developed our formalism. In what follows the *Schwartz space* $\mathcal{S}$ of real valued, infinitely often differtiable functions on $\mathbb{R}$ with rapid decrease will play an important role—see [Rud91, 184-188] for its definition and properties. The reason for its importance is found in the following theorem.

Theorem 1 (Minlos's Theorem, [?, Thm. 1.1]). *Let $\mathcal{F}$ be a characteristic functional on $\mathcal{S}$, i.e. $\mathcal{F}\colon \mathcal{S} \to \mathbb{R}$ with the properties*

i) $\mathcal{F}$ is continous on $\mathcal{S}$,

ii) $\mathcal{F}$ is positive definite,

iii) $\mathcal{F}(0) = 1$.

Then there exists a unique probability measure $\mathbb{P}$ on $\mathcal{S}^*$ (the dual space of $\mathcal{S}$), such that for all $f \in \mathcal{S}$

$$\int_{\mathcal{S}^*} \mathrm{e}^{\mathrm{i}\,(\xi, f)}\, \mathrm{d}\mu(\xi) = \mathcal{F}(f). \tag{A.3}$$

Here (ξ, f) denotes the dual pairing of $\mathcal{S}/\mathcal{S}^*$, which can formally be written as $(\xi, f) = \int_{\mathbb{R}} \xi(t) f(t)\, \mathrm{d}t$. We also recall that a function f is called *positive definite*, if... In [?] they take advantage of this theorem to construct a real valued White Noise processes on $\mathcal{S}^*$ with the choice $\mathcal{F}(f) = \exp(-\int_{\mathbb{R}} f(t)^2\, \mathrm{d}t)$. This can be rephrased as $\mathcal{F}(f) = \exp(-\mathcal{C}(f))$ with the *variance functional* $\mathcal{C}(f) = \int f(t)^2\, \mathrm{d}t$.

Lemma 2 (Fourier transform, [Rud91, Thm. 7.7]). *Let $\mathcal{S}_{\mathbb{C}} = \mathcal{S} + \mathrm{i}\mathcal{S}$ denote the complexified space of test-functions. The Fourier transform is a continuous, linear one-to-one mapping of $\mathcal{S}_{\mathbb{C}}$ onto $\mathcal{S}_{\mathbb{C}}$.*

But since we are interested in complex processes with memory, we have to generalize these results. The reformulation at the end of the last paragraph points us into the right direction; first of all we define an appropriate covariance functional by

$$\mathcal{C}(f) = \int_{\mathbb{R}^2} \alpha(t-s) f(t) f(s) \,\mathrm{d}t \,\mathrm{d}s \quad (f \in \mathcal{S}). \tag{A.4}$$

Lemma 3.

Proof. Since $|\alpha(t)| \leq \int J(\omega)\,\mathrm{d}\omega = A < \infty$ for $t \in \mathbb{R}$, we have for $f, g \in \mathcal{S}_{\mathbb{C}}$

$$|\mathcal{C}(f,g)| \leq \iint |\alpha(t-s) f(t)^* g(s)| \,\mathrm{d}s \,\mathrm{d}t \leq A \int |f(t)| \,\mathrm{d}t \int |g(s)| \,\mathrm{d}s < \infty,$$

where we used that all test-functions in $\mathcal{S}_{\mathbb{C}}$ are also integrable. Continuity also follows from this inequality, since convergence in the $\mathcal{S}_{\mathbb{C}}$-sense implies convergence in the L^1-sense. The linearity and conjugate-symmetry are trivial; therefore we only need to check that $\mathcal{C}(f,f) = 0$ implies $f = 0$. For this matter we use the well-known fact, that the Fourier transform is a one-to-one, continuous and linear mapping of $\mathcal{S}_{\mathbb{C}}$ onto $\mathcal{S}_{\mathbb{C}}$ (see [Rud91, Theorem 7.7]). Consequently for $f \in \mathcal{S}_{\mathbb{C}}$ with $\mathcal{C}(f,f) = 0$, there is a $\check{f} \in \mathcal{S}_{\mathbb{C}}$ with $\int \mathrm{e}^{-\mathrm{i}\omega t} \check{f}(\omega)\,\mathrm{d}\omega = f(t)$. A short calculation then reveals

$$\begin{aligned}
\mathcal{C}(f,f) &= \iint \alpha(t-s) f(t)^* f(s) \,\mathrm{d}t \,\mathrm{d}s \\
&= \iint \int \mathrm{e}^{-\mathrm{i}\Omega(t-s)} J(\Omega)\,\mathrm{d}\Omega \int \mathrm{e}^{\mathrm{i}\omega t} \check{f}(\omega)^* \,\mathrm{d}\omega \int \mathrm{e}^{-\mathrm{i}\omega' s} \check{f}(\omega')\,\mathrm{d}\omega' \,\mathrm{d}s \,\mathrm{d}t \\
&= \iiint \left(\int \mathrm{e}^{-\mathrm{i}(\Omega-\omega)t} \,\mathrm{d}t \int \mathrm{e}^{\mathrm{i}(\Omega-\omega)s} \,\mathrm{d}s \right) \check{f}(\omega)^* \check{f}(\omega') J(\Omega)\,\mathrm{d}\Omega \,\mathrm{d}\omega \,\mathrm{d}\omega' \\
&\sim \int \left|\check{f}(\Omega)\right|^2 J(\Omega)\,\mathrm{d}\Omega.
\end{aligned}$$

Therefore $\mathcal{C}(f,f) = 0$ implies $\check{f} = 0$, leading to the conclusion $f = 0$. □

Remark. For the Markovian regime the statement holds true as well, since $\mathcal{C}$ coincides with the L^2-scalar product in that case.

However, we cannot apply Theorem 1 directly to $\mathcal{F}(f) = \mathrm{e}^{-\mathcal{C}(f,f)}$ because it does not apply to the complexified space $\mathcal{S}_{\mathbb{C}}$. Instead we will follow the strategy in [Hid80]: first we restrict $\mathcal{C}$ to $\mathcal{S}$, where it does not necessarily have the form **??**.

We want complex Hilbert space, Minlos only works with real. First define complex one, read of "real" sp, complexify again. Define α as FT, Define complex Pre-Hilbert space; define Complexification of $\mathcal{S}$

Lemma 4. *$\langle \cdot, \cdot \rangle$ is well defined scalar product, continous on $\mathcal{S}_{\mathbb{C}}$*

Complete $\mathcal{S}_{\mathbb{C}}$; Hilbert Space $\mathcal{H}_{\mathbb{C}}$

Lemma 5. *$\mathcal{H}_{\mathbb{C}}$ is seperable*

Go over to $\mathcal{S}$, what is scalar product, use polarisation; show that complexified scalar product gives back old scalar product

Theorem 6. *On $(\mathcal{S}_{\mathbb{C}}{}^*, \mathcal{B})$ there exists a Gauss Measure μ such that for $f \in \mathcal{S}_{\mathbb{C}}$*

$$\int_{\mathcal{S}_{\mathbb{C}}{}^*} \exp(\mathrm{i}\,\Re(\xi, f))\,\mathrm{d}\mu(\xi) = \exp(-\frac{1}{4}\|f\|_{\mathcal{H}}) \tag{A.5}$$

Define (L^2); scalar product; In the language of probability theory we have prop space $(\mathcal{S}_{\mathbb{C}}{}^*, \mathcal{B}, \mu)$. For $f, g \in \mathcal{S}$ we have random variables $(\cdot, f)^*$ and $(\cdot, g)$ such that $\mathbb{E}\ldots$. Can be continued to $\mathcal{H}$; later $Z_t := (\cdot, \delta_t)$; Formally

$$(\xi, f) = \int \xi(t) f(t)\,\mathrm{d}t = \int\int \xi(s)\delta(s-t)\,\mathrm{d}s f(t)\,\mathrm{d}t = \int (\cdot, \delta_t) f(t)\,\mathrm{d}t$$

Therefore $(\cdot, f) = \int Z_t f(t)\,\mathrm{d}t$; Formal scalar product; Example Brownian motion,

Theorem 7. *(L^2) has the following ONB...*

Symmetric Fock Space, how to recover microscopical model

A.2. Noise Creation- and Anhilation Operators

On all elements with finite expansion, $f \in \mathcal{H}$ define Z_f; calculate Adjoint, Formal notation, define Z_t

B. Analytic Solution of Dissipative Two-level System

B.1. General Solution

Here we present in full detail the analytic solution of the dissipative two-level system introduced in Sect. 1.6. The relevant NMSSE can always be written in terms of a single process

$$\partial_t \psi_t = -\mathrm{i}\frac{\omega}{2}\sigma_z \psi_t + c\sigma_- Z_t^* \psi_t - c\sigma_+ \int \alpha(t-s)\frac{\delta \psi_t}{\delta Z_s^*}\,\mathrm{d}s. \tag{B.1}$$

As already mentioned we employ an ansatz for the quantum trajectory at most linear in Z_s^*

$$\psi_t(Z^*) = \psi(t) + \int_0^t \psi_s(t) Z_s^*\,\mathrm{d}s. \tag{B.2}$$

Here we already incorporate that $\psi_t(Z^*)$ needs to be independent of Z_s^* for $s < 0$ and $s > t$ by using a bounded integral domain.[1] We use a basis for $\psi_t(Z^*)$ which renders σ_z diagonal and denote the corresponding components by "+" and "-". The "+"-component of our NMSSE with the ansatz (B.2) reads

$$\begin{aligned}\dot{\psi}^+(t) + \psi_t^+(t) Z_t^* + \int_0^t \dot{\psi}_s^+ Z_s^*\,\mathrm{d}s \\ = -\mathrm{i}\frac{\omega}{2}\left(\psi^+(t) + \int_0^t \psi_s^+(t) Z_s^*\,\mathrm{d}s\right) - c\int_0^t \alpha(t-s)\psi_s^-(t)\,\mathrm{d}s.\end{aligned} \tag{B.3}$$

[1] A consistent treatment of these independence-conditions is more tricky than it seems at first glance, since we are mixing a distributional object Z_s^* with a discontinuous function $s \mapsto \psi_s(t)$. As $\delta\psi_t(Z^*)/\delta Z_s^* = 0$ translates to $\psi_s(t) = 0$ the correct integral boundary reads $\int_{0-\varepsilon}^{t+\varepsilon}$ with $\varepsilon > 0$ but arbitrary otherwise.

In order to separate contributions of different order in Z_s^*, we apply the functional derivative $\delta/\delta Z_s^*$ with arbitrary s to the last equation

$$\psi_t^+(t)\delta(t-s) + \int_0^t \dot{\psi}_{s'}^+(t)\delta(s-s')\,\mathrm{d}s' = -\mathrm{i}\frac{\omega}{2}\int_0^t \psi_{s'}^+(t)\delta(s-s')\,\mathrm{d}s'. \tag{B.4}$$

Choosing $s \in (0,t)$ leaves us with a simple ordinary differential equation with solution $\psi_s^+(t) = C_s \mathrm{e}^{-\mathrm{i}\omega t/2}$. By further investigating the singular term in Eq. (B.4) we find that $\psi_s^+(s)$ and therefore the constant C_s must vanish. This amounts formally to integrating (B.4) over a small interval $(t-\varepsilon, t+\varepsilon)$ with respect to s. In the limit $\varepsilon \to 0$ all terms except the first go to zero. On the other hand we can isolate all terms independent of Z_s^* in Eq. (B.3) simply by taking the expectation value. The resulting equation

$$\dot{\psi}^+(t) = -\mathrm{i}\frac{\omega}{2}\psi^+(t) - c\int_0^t \alpha(t-s)\psi_s^-(t)\,\mathrm{d}s \tag{B.5}$$

is treated later, once we have an explicit expression for $\psi_s^-(t)$.

The "-" component of Eq. (B.1) is quite similar to (B.3)

$$\begin{aligned}\dot{\psi}^-(t) + \psi_t^-(t)Z_t^* + \int_0^t \dot{\psi}_s^-(t)Z_s^*\,\mathrm{d}s& \\ = \mathrm{i}\frac{\omega}{2}\left(\psi^-(t) + \int_0^t \psi_s^-(t)Z_s^*\right) + c\psi^+(t)Z_t^*,&\end{aligned} \tag{B.6}$$

where we already used that $\psi_s^+(t) = 0$. The solution

$$\psi^-(t) = \psi^-(0)\,\mathrm{e}^{\mathrm{i}\frac{\omega}{2}t} \tag{B.7}$$

can be read off Eq. (B.6) directly by comparing all terms independent of Z_t^*. In the same manner as we derived Eq. (B.4) we can treat all terms proportional to Z_t^*. Again we find a solution of the form $\psi_s^-(t) = C_s \mathrm{e}^{\mathrm{i}\omega t/2}$; the only difference is an additional singular term due to the driving process in Eq. (B.1). It gives rise to the boundary condition $\psi_t^-(t) = c\psi^+(t)$. Together with **??** we obtain a closed equation for $\psi^+(t)$

$$\dot{\psi}^+(t) = -\mathrm{i}\frac{\omega}{2}\psi^+(t) - c^2\int_0^t \alpha(t-s)\mathrm{e}^{\mathrm{i}\frac{\omega}{2}(t-s)}\psi^+(s)\,\mathrm{d}s. \tag{B.8}$$

Hence we may replace the original NMSSE (B.1) by a $\mathbb{C}$-valued equation similar in structure.

B.2. Exponential Correlation Function

As Eq. (B.8) still contains a memory integral there is no analytic solution in general. The situation is noticeably simpler for a bath correlation of the form

$$\alpha(t-s) = \sum_{j=1}^{N} g_j \, \mathrm{e}^{-\gamma_j |t-s| - \mathrm{i}\Omega_j (t-s)}. \tag{B.9}$$

Since ψ^+ only depends on values of $\alpha(t)$ for $t \geq 0$ we can assume $\gamma = 0$ without loss of generality. Similar to our hierarchical equations of motion elaborated in **??** we absorb the problematic terms into auxiliary functions

$$\phi_j(t) := \int_0^t \alpha_j(t-s) \mathrm{e}^{\mathrm{i}\frac{\omega}{2}(t-s)} \psi^+(s) \, \mathrm{d}s. \tag{B.10}$$

This allows us to rewrite Eq. (B.8) as a system of $(N+1)$ ordinary differential equations with constant coefficients

$$\begin{aligned} \dot{\psi}^+(t) &= -\mathrm{i}\frac{\omega}{2}\psi^+(t) - c^2 \sum_{j=1}^{N} \phi_j(t) \\ \dot{\phi}_j(t) &= g_j \psi^+(t) + \mathrm{i}\left(\frac{\omega}{2} - \Omega\right) \phi_j(t). \end{aligned}$$

and initial conditions $\phi_j(0) = 0$. In the special case $N = 1$ the diagonalization can be carried out analytically. With the shorthand notation $\tilde{\Omega} = \sqrt{(\omega - \Omega)^2 + 4c^2 g}$ the solution to Eq. (B.8) reads

$$\psi^+(t) = \frac{\psi^+(0)}{2\tilde{\Omega}} \left((\omega - \Omega + \tilde{\Omega}) \, \mathrm{e}^{-\mathrm{i}\frac{\Omega+\tilde{\Omega}}{2}t} - (\omega - \Omega - \tilde{\Omega}) \, \mathrm{e}^{-\mathrm{i}\frac{\Omega-\tilde{\Omega}}{2}t} \right). \tag{B.11}$$

C. Numerical Implementaion

Bibliography

[Bar61] V. Bargmann. On a hilbert space of analytic functions and an associated integral transform part i. *Communications on Pure and Applied Mathematics*, 14(3):187–214, 1961.

[BG09] Alberto Barchielli and Matteo Gregoratti. *Quantum trajectories and measurements in continuous time: the diffusive case*, volume 782. Springer, 2009.

[Car93] H. Carmichael. *An Open Systems Approach to Quantum Optics: Lectures Presented at the Université Libre de Bruxelles, October 28 to November 4, 1991.* Lecture Notes in Computer Science. Springer Berlin Heidelberg, 1993.

[CL83] A.O Caldeira and A.J Leggett. Quantum tunnelling in a dissipative system. *Annals of Physics*, 149(2):374 – 456, 1983.

[DGS98] Lajos Diósi, Nicolas Gisin, and Walter T. Strunz. Non-markovian quantum state diffusion. *Phys. Rev. A*, 58:1699–1712, Sep 1998.

[DS97] Lajos Diósi and Walter T. Strunz. The non-markovian stochastic schrödinger equation for open systems. *Physics Letters A*, 235(6):569 – 573, 1997.

[DS11] William L Dunn and J Kenneth Shultis. *Exploring Monte Carlo Methods.* Access Online via Elsevier, 2011.

[FHS10] R.P. Feynman, A.R. Hibbs, and D.F. Styer. *Quantum Mechanics and Path Integrals.* Dover books on physics. Dover Publications, Incorporated, 2010.

[FV63] Richard Phillips Feynman and Frank Lee Vernon. The theory of a general quantum system interacting with a linear dissipative system. *Annals of physics*, 24:118–173, 1963.

[G+85] Crispin W Gardiner et al. *Handbook of stochastic methods*, volume 3. Springer Berlin, 1985.

[Hid80] T. Hida. *Brownian motion*. Applications of mathematics. Springer-Verlag, 1980.

[Nov65] EA Novikov. Functionals and the random-force method in turbulence theory. *Sov. Phys. JETP*, 20(5):1290–1294, 1965.

[Øks03] Bernt Øksendal. *Stochastic differential equations*. Springer, 2003.

[Rud91] W. Rudin. *Functional analysis*. International series in pure and applied mathematics. McGraw-Hill, 1991.

[Sch05] R.L. Schilling. *Measures, Integrals and Martingales*. Number Bd. 13 in Measures, integrals and martingales. Cambridge University Press, 2005.

[Sch11] Wolfgang P Schleich. *Quantum optics in phase space*. Wiley. com, 2011.

[Str01] Walter T. Strunz. Stochastic schrödinger equation approach to the dynamics of non-Markovian open quantum systems. Habilitation thesis, June 2001.

[Wei99] U. Weiss. *Quantum Dissipative Systems (Second Edition)*. Series in Modern Condensed Matter Physics. World Scientific Publishing Company Incorporated, 1999.

[WM08] Daniel F Walls and G Gerard J Milburn. *Quantum optics*. Springer, 2008.

[YDGS99] Ting Yu, Lajos Diósi, Nicolas Gisin, and Walter T. Strunz. Non-markovian quantum-state diffusion: Perturbation approach. *Phys. Rev. A*, 60:91–103, Jul 1999.

[YDGS00] Ting Yu, Lajos Diosi, Nicolas Gisin, and Walter T Strunz. Post-markov master equation for the dynamics of open quantum systems. *Physics Letters A*, 265(5):331–336, 2000.

[Yu04] Ting Yu. Non-markovian quantum trajectories versus master equations: Finite-temperature heat bath. *Physical Review A*, 69(6):062107, 2004.