Stochastic dynamics of quantum jumps

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The dynamics of an open quantum system coupled to an external reservoir is studied on the basis of a recently proposed formulation of quantum statistical ensembles in terms of probability distributions on projective Hilbert space. The previous result is generalized to include interaction Hamiltonians of the form $\sum_i A_i \otimes B_i$, where A_i and B_i are operators acting on the Hilbert space of the reduced system and of the reservoir, respectively. The differential Chapman-Kolmogorov equation governing the dynamics of the conditional transition probability of the reduced system is derived from the underlying microscopic theory based on the Schrödinger equation for the total system. The stochastic process turns out to be a piecewise deterministic Markovian jump process in the projective Hilbert space of the reduced system. The sample paths are derived and shown to be similar to those of the Monte Carlo wave function simulation methods proposed in the literature. Finally, a diffusion-noise expansion of the Liouville master equation is performed and demonstrated to yield a stochastic differential equation for the state vector of the open system.

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I. INTRODUCTION

The dynamics of open quantum systems is conventionally described by means of the reduced density operator, which is obtained from the density operator of the total system by tracing over the variables of the external reservoir. In order to eliminate the reservoir variables from the equation of motion, various approximations are performed, leading to a closed equation of motion for the density operator of the reduced system [1,2]. The most famous approximation of this type is the Markov approximation, which yields under some additional assumptions the so-called quantum Markovian master equation [3–6] generating a quantum dynamical semigroup [7–10] in the space of statistical operators.

In recent years various interesting models have been proposed that allow the formulation of the physics of open quantum systems from a completely different point of view. These models suggest that the dynamics of open quantum systems may be described in terms of a stochastic process on the Hilbert space pertaining to the reduced system. The basic idea is then to represent the wave function of the reduced system as a random variable in the Hilbert space and to interpret its covariance matrix as the density operator. Consequently, the dynamics of the time-dependent wave function is defined by a stochastic process in Hilbert space that is constructed such that the equation of motion governing its covariance matrix is just the quantum Markovian master equation for the reduced density operator.

It is clear that the basic principle just described does not lead to a unique stochastic representation of the reduced system dynamics. This is due to the obvious fact that the dynamic equation for the two-point correlation function of a stochastic process alone does not fix uniquely this process. This is true even if the Markovian assumption is made. In fact, the most general form for a Markov process on a given phase space consists of a smooth deterministic time evolution, a discontinuous jump process, and a diffusion process [11]. Accordingly, the stochastic models discussed in the literature may be subdivided into the class of diffusion-type processes with continuous drift and the class of piecewise deterministic jump processes.

The so-called quantum state diffusion model, for example, belongs to the first type of models. Following the work of Pearle [12], Gisin [13] and Gisin and Percival [14] have developed this model, which is defined by a stochastic differential equation for the state vector with nonlinear drift and multiplicative noise. This stochastic differential equation is equivalent to a certain (functional) Fokker-Planck equation [15] on the underlying Hilbert space. The stochastic dynamics of the wave function may also be described in terms of a stochastic differential equation with linear drift [16].

In contrast to these diffusion-type processes there exists the possibility to represent the dynamics of the open system wave function as a stochastic process whose realizations are piecewise deterministic paths [17]. The first such method has been developed by Dalibard, Castin, and Mølmer [18] and applied to some simple models of quantum optics. This was a major step forward since it offered a natural theoretical description of quantum jumps that have been distinctly observed in experiments with individual ions in radio-frequency traps [19–21] and with single terrylene molecules [22] (see also the review article [23] on quantum jumps by Cook). A short time later Dum, Zoller, and Ritsch [24] suggested a Monte Carlo simulation method of the quantum master equation, which is essentially the same algorithm as that of Dalibard, Castin, and Mølmer, and formulated it in a most general form in Ref. [25]. Independently, the idea of

complementary unravelings of the quantum master equation in terms of different types of stochastic processes has been developed by Carmichael [26]. Wiseman and Milburn [27] have traced back three different unravelings of the quantum optical master equation to three different measurement schemes, i.e., to direct photodetection, homodyne, and heterodyne detection. For the example of a two-level atom, they have formulated the corresponding stochastic processes by means of differential Chapman-Kolmogorov equations on the Bloch sphere. In Ref. [28] a stochastic process for the open system wave function has been formulated by means of a Liouville master equation for the corresponding probability distribution. Finally, a piecewise deterministic stochastic process has been constructed by Blanchard and Jadczyk [29] describing the coupling of a quantum system to a classical system.

The great variety of these approaches clearly demonstrates, as mentioned before, that it is not possible to obtain a unique stochastic representation of the reduced state vector only on the basis of the equation for the reduced density matrix. The question then arises whether it is possible to derive a unique stochastic process for the open system dynamics directly from the underlying microscopic theory without referring to the density operator description. It is the aim of the present paper to show that this is indeed possible. For a special case this derivation is given in [30], whereas a short exposition of the method is outlined in [31].

In Sec. II we shall first develop a formulation of quantum ensembles in terms of probability distributions on projective Hilbert space. This formulation provides a classical statistical theory on the phase space that is given by the space of rays of the Hilbert space of the system under study. Within this formulation the dynamics of closed systems is given by the Liouville equation, which describes the unitary flow corresponding to Schrödinger's equation and is a first-order functional differential equation for the probability distribution. Moreover, as will be shown, the combination of two subsystems and the reduction of a system to one of its subsystems may be defined in terms of probability distributions on the projective Hilbert spaces of the corresponding systems.

On the basis of this formal setting we shall derive in Sec. III an exact equation for the conditional transition probability of the reduced system by starting from the Liouville equation for the total (closed) system. Employing the Markov approximation of classical probability theory, we then show that the conditional transition probability obeys a differential Chapman-Kolmogorov equation that defines a unique stochastic Markov process in projective Hilbert space. This Markov process is, in fact, a piecewise deterministic jump process. The continuous flow is described by the Liouville part of the Chapman-Kolmogorov equation corresponding to a nonlinear, norm-preserving Schrödinger-type equation, whereas the jump process is defined in terms of a gain-and-loss master equation for the probability distribution of the reduced system. Furthermore, it is shown that the realizations of the stochastic process correspond essentially to the realizations generated by the algorithms of the Monte Carlo wave function simulation methods mentioned above.

We investigate furthermore the diffusion approximation of the differential Chapman-Kolmogorov equation. It is shown that, under certain conditions, the differential Chapman-Kolmogorov equation admits an asymptotic expansion, which yields a functional Fokker-Planck equation. The latter is then transformed to a stochastic Schrödinger-type equation that is of the same form as that of the quantum state diffusion model.

Finally, in Sec. IV we summarize our results.

II. PROBABILITY DISTRIBUTIONS ON PROJECTIVE HILBERT SPACE

In this section we shall develop a general formal setting for the description of ensembles of quantum systems in terms of probability distributions on the underlying projective Hilbert space. In Sec. II A we deal with ensembles of closed quantum systems and introduce the basic notions of probability theory on Hilbert space. In particular, we shall formulate three postulates that imply that these probability distributions are, in fact, distributions on *projective* Hilbert space. In Sec. II B we derive a kind of tensor product for probability distributions that gives the probability distribution of a system that is combined from two subsystems. Furthermore, a reduction formula is constructed that defines the probability distribution of a reduced system in terms of the distribution of the total system. These expressions will enable us to derive in Sec. III the stochastic process of the reduced system dynamics.

A. Closed systems

Consider a closed quantum mechanical system S, the states of which are given by wave functions ψ in some Hilbert space $\mathcal{H}$. We write $\psi = \psi(x)$, where x denotes a complete set of quantum numbers of the system under study. The scalar product on $\mathcal{H}$ is written as

$$\langle\psi|\varphi\rangle \equiv \int dx\ \psi^*(x)\varphi(x) \tag{1}$$

and the corresponding norm is denoted by $||\psi|| \equiv \langle\psi|\psi\rangle^{1/2}$.

Assume that we have an ensemble that consists of a large number of copies of the system S each member of which is described by its own wave function. This ensemble may be characterized by a probability distribution on the Hilbert space $\mathcal{H}$ in the following way. The functional volume element on $\mathcal{H}$ is defined by

$$\begin{aligned} D\psi D\psi^* &\equiv \prod_x d[\mathrm{Re}\psi(x)]d[\mathrm{Im}\psi(x)] \\ &= \prod_x \frac{i}{2} d\psi(x)d\psi^*(x)\ , \end{aligned} \tag{2}$$

where $\mathrm{Re}\psi(x)$ and $\mathrm{Im}\psi(x)$ are the real and the imaginary part of $\psi(x)$, respectively, and the product $\prod_x$ ex-

tends over all possible values of x, e.g., over all points of position space. The probability density $P[\psi]$ corresponding to the above ensemble may then be introduced by defining $P[\psi]D\psi D\psi^*$ to be the probability of finding the system in the volume element $D\psi D\psi^*$ around ψ. It should be clear that in the case of an infinite-dimensional Hilbert space $P[\psi]$ is a functional on Hilbert space and (2) is a functional measure. From a mathematical point of view, our presentation will be rather formal. However, we remark that a mathematically rigorous definition of probability measures on Hilbert space and the construction of the underlying Borel algebra has been given in a series of papers by Bach [32] (see also Ref. [33]).

It is important to note that the measure (2) is invariant with respect to linear unitary transformations $U:\mathcal{H} \longrightarrow \mathcal{H}$. This fact may be expressed by the equation

$$\delta[U\psi] = \delta[\psi] \,, \tag{3}$$

where

$$\delta[\psi(x)] \equiv \prod_x \delta(\mathrm{Re}\psi(x))\delta(\mathrm{Im}\psi(x)) \tag{4}$$

denotes the functional δ function on the Hilbert space $\mathcal{H}$ [$\delta(\,)$ is the ordinary δ function]. According to the general principles of quantum mechanics, the physical state of a system S is completely described by a normalized wave function and wave functions that differ by a phase factor are equivalent. It is thus natural to require that $P[\psi]$ fulfills the following three postulates:

(i) P is normalized

$$\int D\psi D\psi^* P[\psi] = 1 \,; \tag{5}$$

(ii) the probability distribution is concentrated on the unit sphere in Hilbert space defined by $\langle\psi|\psi\rangle \equiv ||\psi||^2 = 1$, that is, there exists a functional $Q[\psi]$ such that

$$P[\psi] = \delta(||\psi|| - 1)Q[\psi] \,; \tag{6}$$

(iii) the probability distribution does not depend upon the phase of the wave function, i.e., we have for all $\phi \in [0, 2\pi)$

$$P[e^{i\phi}\psi] = P[\psi] \,. \tag{7}$$

A representation of the projective Hilbert space is obtained by taking the unit sphere in $\mathcal{H}$ and by identifying those points on this sphere that differ by a phase factor. Thus, by conditions (6) and (7), $P[\psi]$ can in fact be regarded as a probability density on the space of rays, that is, as a probability density on projective Hilbert space.

In terms of $P[\psi]$ the expectation value of any physical observable represented by a self-adjoint operator A is defined by the expectation of the quantum mechanical expectation value

$$\begin{aligned}\langle A\rangle &\equiv \langle\langle\psi|A|\psi\rangle\rangle \\ &\equiv \int D\psi D\psi^* \int dx\; \psi^*(x)A\psi(x)P[\psi] \,.\end{aligned} \tag{8}$$

We now turn to the description of the dynamics. We require that for the closed quantum system under consideration each member of the ensemble evolves according to the Schrödinger equation

$$i\frac{\partial\psi}{\partial t} = H\psi \,, \tag{9}$$

where H is the Hamiltonian of the system and choosing appropriate units we have assumed $\hbar = 1$. By the introduction of an initial probability distribution $P_0[\psi]$, which describes the initial state of the ensemble, ψ becomes a deterministic Markov process that is governed by a Liouville equation. Denoting the time-dependent probability distribution by $P = P[\psi, t]$ we write

$$P[\psi, t] = \int D\psi_0 D\psi_0^*\; \delta[e^{-iHt}\psi_0 - \psi]P_0[\psi_0] \,. \tag{10}$$

This equation expresses the fact that any initial ψ_0 drawn from the initial distribution P_0 evolves according to Schrödinger's equation. Using (3) we obtain from Eq. (10) by integrating over ψ_0

$$P[\psi, t] = P_0[e^{iHt}\psi] \,. \tag{11}$$

Differentiating (11) with respect to time and using the fact that H is self-adjoint, we find the differential form of the Liouville equation, which is a first-order functional differential equation for the probability distribution:

$$\frac{\partial}{\partial t}P[\psi, t] = i\int dx \left\{\frac{\delta P}{\delta\psi(x)}H\psi(x) - \psi^*(x)H\frac{\delta P}{\delta\psi^*(x)}\right\} \,, \tag{12}$$

where $\delta/\delta\psi(x)$ and $\delta/\delta\psi^*(x)$ are functional Wirtinger derivatives. Since the linear time-evolution operator $\exp(-iHt)$ is unitary, it is easily seen that the Liouville equation (12) preserves the basic conditions (5)–(7), i.e., if $P_0[\psi]$ is a probability density on projective Hilbert space so is $P[\psi, t]$ for all $t > 0$.

Another concept that will be important in the following sections is provided by the interaction representation of the time-dependent probability distribution on Hilbert space. Assume that the total Hamiltonian takes the form

$$H = H_0 + H_I \,, \tag{13}$$

where H_0 describes some free evolution and H_I denotes the interaction Hamiltonian. We define the probability distribution $\tilde{P}[\psi, t]$ in the interaction representation by

$$\tilde{P}[\psi, t] \equiv P[e^{-iH_0(t-t_0)}\psi, t] \,. \tag{14}$$

At time $t = t_0$ the Schrödinger and the interaction representation coincide, that is, we have $\tilde{P}[\psi, t_0] = P[\psi, t_0]$. The time evolution in the interaction representation is therefore given by

$$\tilde{P}[\psi, t] = \tilde{P}[U_I^\dagger(t, t_0)\psi, t_0] \,, \tag{15}$$

where $U_I(t, t_0)$ is the time-evolution operator in the interaction picture.

B. Combination and reduction of systems

This subsection is devoted to a formulation of the combination of statistically independent subsystems and of the reduction of a system to one of its subsystems in terms of probability distributions on projective Hilbert space. The physical situation we have in mind is the following one. Suppose that we have two systems S_1 and S_2 with corresponding Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. Wave functions in $\mathcal{H}_1$ are written as $\psi_1(x_1)$ and wave functions in $\mathcal{H}_2$ are denoted by $\psi_2(x_2)$. Furthermore, throughout the paper (unless stated otherwise) we use the convention that all quantities that refer to system S_i carry an index i, where $i = 1, 2$. For example, $\langle|\rangle_2$ denotes the scalar product on $\mathcal{H}_2$ and $||\,||_1$ is the norm in $\mathcal{H}_1$. According to the general principles of quantum mechanics, the Hilbert space $\mathcal{H}$ underlying the combined system $S = S_1 + S_2$ is given by the tensor product

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \,. \tag{16}$$

We first assume that we have two statistically independent subsystems S_1 and S_2 described by their distributions $P_1[\psi_1]$ and $P_2[\psi_2]$, respectively. The probability density $P[\psi]$ for the wave function $\psi \in \mathcal{H}$ is then obtained by averaging over all possible ways to represent ψ as a product $\psi = \psi_1\psi_2$, that is, we have the equation

$$\begin{aligned} P[\psi] &= (P_1 \otimes P_2)[\psi] \\ &= \int D\psi_1 D\psi_1^* \int D\psi_2 D\psi_2^*\, \delta[\psi - \psi_1\psi_2] P_1[\psi_1] \\ &\quad \times P_2[\psi_2] \,, \end{aligned} \tag{17}$$

where $\delta[\psi]$ denotes the Dirac measure on $\mathcal{H}$ [see Eq. (4)]. This expression may be called a tensor product of probability distributions. It implies that for any self-adjoint operator A on $\mathcal{H}$ of the form $A = A_1 \otimes A_2$, the following equation holds:

$$\langle A\rangle_{P_1\otimes P_2} = \langle A_1\rangle_{P_1} \langle A_2\rangle_{P_2} \,, \tag{18}$$

where the probability distributions by which the different expectation values are defined have been indicated as indices of the angular brackets. Equation (18) means that for statistically independent systems S_1 and S_2 the expectation value in the combined system S of any product of operators is equal to the product of the expectation values of S_1 and S_2. In order to prove Eq. (18) we insert the definition (17) for the tensor product into the expression (8) for the expectation value of A to obtain

$$\begin{aligned} \langle A\rangle_{P_1\otimes P_2} &= \int D\psi D\psi^* \int D\psi_1 D\psi_1^* \int D\psi_2 D\psi_2^*\, \langle\psi|A|\psi\rangle \\ &\quad \times \delta[\psi - \psi_1\psi_2] P_1[\psi_1] P_2[\psi_2] \,. \end{aligned} \tag{19}$$

On integrating over ψ we find

$$\begin{aligned} \langle A\rangle_{P_1\otimes P_2} &= \int D\psi_1 D\psi_1^* \int D\psi_2 D\psi_2^* \\ &\quad \times \langle\psi_1\psi_2|A_1 \otimes A_2|\psi_1\psi_2\rangle P_1[\psi_1] P_2[\psi_2] \\ &= \left(\int D\psi_1 D\psi_1^*\, \langle\psi_1|A_1|\psi_1\rangle_1 P_1[\psi_1]\right) \\ &\quad \times \left(\int D\psi_2 D\psi_2^*\, \langle\psi_2|A_2|\psi_2\rangle_2 P_2[\psi_2]\right) \,, \end{aligned}$$

which is identical to Eq. (18).

Let us check whether the basic conditions (5)–(7) are fulfilled for the tensor product. First, condition (5) follows from Eq. (18) by setting $A_1 = A_2 = \mathbf{1}$, where $\mathbf{1}$ denotes the identity operator on the respective Hilbert spaces. Condition (6) is obvious from the fact that $P[\psi]$ is nonzero only if ψ is the product of two normalized wave functions. Finally, also condition (7) is fulfilled since on using (3) for the unitary transformation given by the multiplication with the phase factor $\exp(i\phi)$ we obtain

$$\begin{aligned} P[e^{i\phi}\psi] &= \int D\psi_1 D\psi_1^* \int D\psi_2 D\psi_2^*\, \delta[\psi - e^{-i\phi}\psi_1\psi_2] \\ &\quad \times P_1[\psi_1] P_2[\psi_2] \\ &= \int D\psi_1 D\psi_1^* \int D\psi_2 D\psi_2^*\, \delta[\psi - \psi_1\psi_2] \\ &\quad \times P_1[e^{i\phi}\psi_1] P_2[\psi_2] \end{aligned}$$

and thus $P[\psi]$ is phase invariant if $P_1[\psi_1]$ is so.

Let us turn to the reduction of a system to one of its subsystems. Given a probability distribution $P[\psi]$ for the combined system S on $\mathcal{H}$, the reduced probability distribution $P_1[\psi_1]$ on $\mathcal{H}_1$ for the system S_1 can be obtained as follows. If the total system S is in a pure state $\psi \in \mathcal{H}$, quantum mechanics tells us that the reduced system S_1 can be described by a mixture of the normalized states (in $\mathcal{H}_1$) given by

$$\chi_\alpha[\psi](x_1) = w_\alpha^{-1/2}[\psi] \int dx_2\, \varphi_\alpha^*(x_2)\psi(x_1, x_2) \tag{20}$$

with corresponding weights

$$w_\alpha[\psi] = \int dx_1 \left| \int dx_2\, \varphi_\alpha^*(x_2)\psi(x_1, x_2)\right|^2 \,, \tag{21}$$

where $\{\varphi_\alpha\}$ is a complete orthonormal basis of $\mathcal{H}_2$. Thus, in the most general case, the reduced probability distribution on $\mathcal{H}_1$ is obtained by averaging over the probability distribution of the total system leading to the expression

$$P_1[\psi_1] = \int D\psi D\psi^* \sum_\alpha w_\alpha[\psi]\, \delta_1\left[\chi_\alpha[\psi] - \psi_1\right] P[\psi] \,, \tag{22}$$

where $\delta_1[\psi_1]$ is the Dirac measure on the Hilbert space $\mathcal{H}_1$ of the reduced system. It should be clear that the reduced probability distribution (22) depends on the choice of the basis φ_α. This dependence can, however, be removed by integrating the right-hand side of Eq. (22) over the group $\mathcal{U}$ of unitary transformations $U: \mathcal{H}_2 \mapsto \mathcal{H}_2$ and dividing out a normalization factor N, that is, by replacing the above reduction formula by

$$P_1[\psi_1] = \frac{1}{N}\int_U DU \int D\psi D\psi^* \sum_\alpha w_\alpha[\psi] \times \delta_1[\chi_\alpha[\psi] - \psi_1] P[(\mathbf{1}\otimes U)\psi] \,. \tag{23}$$

In order to keep things as simple as possible we will not use here this basis-invariant form.

Again, it is easy to check that the basic conditions (5)–(7) are fulfilled for the reduced probability distribution provided they are satisfied for the distribution of the total system. Furthermore, we have for any operator A_1 acting on $\mathcal{H}_1$:

$$\langle A_1\rangle_{P_1} = \langle A_1 \otimes \mathbf{1}\rangle_P \,. \tag{24}$$

In order to prove this relation we write the left-hand side explicitly as

$$\begin{aligned}\langle A_1\rangle_{P_1} &= \int D\psi_1 D\psi_1^* \int dx_1\ \psi_1^*(x_1) A_1 \psi_1(x_1) P_1[\psi_1] \\ &= \int D\psi_1 D\psi_1^* \int D\psi D\psi^* P[\psi] \\ &\quad \times \int dx_1\ \psi_1^*(x_1) A_1 \psi_1(x_1) \\ &\quad \times \sum_\alpha w_\alpha[\psi]\delta_1[\chi_\alpha[\psi] - \psi_1] \,.\end{aligned}$$

On integrating over ψ_1 we find

$$\begin{aligned}\langle A_1\rangle_{P_1} &= \int D\psi D\psi^* P[\psi] \int dx_1 \sum_\alpha w_\alpha[\psi]\chi_\alpha^*[\psi](x_1) A_1 \chi_\alpha[\psi](x_1) \\ &= \int D\psi D\psi^* P[\psi] \int dx_1\, dx_2\, dx_2'\ \psi^*(x_1,x_2) A_1 \left(\sum_\alpha \varphi_\alpha(x_2)\varphi_\alpha^*(x_2')\right)\psi(x_1,x_2') \\ &= \int D\psi D\psi^* P[\psi] \int dx_1\, dx_2\ \psi^*(x_1,x_2)(A_1\otimes\mathbf{1})\psi(x_1,x_2) \\ &= \langle A_1\otimes\mathbf{1}\rangle_P \,,\end{aligned}$$

where in the penultimate step the completeness (in $\mathcal{H}_2$) of the set $\{\varphi_\alpha\}$ has been used.

Finally, we mention the following fact (the proof can be found in Ref. [30]). Suppose that we have given two distributions P_1 and P_2 on their respective Hilbert spaces and that we form the tensor product $P = P_1 \otimes P_2$ according to Eq. (17). Applying then the reduction formula Eq. (22), the original distribution P_1 is recovered. Thus the above equations yield a consistent description of the combination and the reduction of quantum systems in terms of probability distributions on Hilbert space.

III. REDUCED SYSTEM DYNAMICS AS STOCHASTIC PROCESS IN PROJECTIVE HILBERT SPACE

In this section we shall investigate the dynamics of an open system that is coupled to an external reservoir. We start from a microscopic representation of the dynamics by means of the Liouville equation for the probability distribution of the total system. Employing the basic principles formulated in Sec. II, it is then possible to derive within the Markov approximation an equation of motion for the time-dependent probability distribution pertaining to the reduced system. This derivation leads to a unique stochastic process in the projective Hilbert space of the reduced system.

A. Derivation of the differential Chapman-Kolmogorov equation

In the following we use the same notation as in Sec. II B. The system S_1 (Hilbert space $\mathcal{H}_1$, wave functions ψ_1) is considered to be the system of interest (simply referred to as *the system*), whereas S_2 (Hilbert space $\mathcal{H}_2$, wave functions ψ_2) is the external reservoir. The Hamiltonian H of the combined system S acting on the Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ is written as $H = H_0 + H_I$, where H_I is the interaction Hamiltonian and

$$H_0 = H_1 \otimes \mathbf{1} + \mathbf{1} \otimes H_2 \tag{25}$$

represents the free dynamics of the two subsystems S_1 (Hamiltonian H_1) and S_2 (Hamiltonian H_2). The most general interaction Hamiltonian H_I takes the form

$$H_I = \sum_i A_i \otimes B_i \,, \tag{26}$$

where A_i and B_i are operators acting on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. In order to simplify the presentation we assume in the following that the operators A_i are eigenoperators of H_1 (which can always be achieved) with a discrete, nondegenerate spectrum ω_i. This means that we assume that the interaction Hamiltonian in the interaction picture can be written as

$$H_I(s) \equiv e^{iH_0 s} H_I e^{-iH_0 s} = \sum_i e^{i\omega_i s} A_i \otimes B_i(s) \,, \tag{27}$$

where $B_i(s) \equiv \exp(iH_2 s) B_i \exp(-iH_2 s)$ and $\omega_i \neq \omega_j$ for $i \neq j$. Furthermore, we require that the diagonal elements of B_i in the H_2 representation vanish.

The external reservoir is described by a probability density $P_2[\psi_2]$ on $\mathcal{H}_2$ given by

$$P_2[\psi_2] = \int_0^{2\pi} \frac{d\phi}{2\pi} \sum_\alpha p_\alpha\, \delta_2[\varphi_\alpha - e^{i\phi}\psi_2] \,, \tag{28}$$

where $\{\varphi_\alpha\}$ is an orthonormal eigenbasis of H_2, $H_2\varphi_\alpha = \varepsilon_\alpha\varphi_\alpha$, and $p_\alpha \geq 0$, $\sum_\alpha p_\alpha = 1$. Thus $P_2[\psi_2]$ represents a probability density that is concentrated on the eigenstates φ_α of H_2 with corresponding weigths p_α and is constant along rays $\exp(i\phi)\psi_2$. The latter property implies that P_2 is a stationary solution of the Liouville equation (12) for the reservoir.

We now fix an arbitrary initial time t_0 and a positive time interval τ, writing $t = t_0+\tau$. According to Eq. (15), the probability distribution $\tilde{P}[\psi, t]$ in the interaction representation is given by

$$\tilde{P}[\psi, t] \equiv P[e^{-iH_0\tau}\psi, t] = \tilde{P}[U_I^\dagger(t, t_0)\psi, t_0] \,. \tag{29}$$

The interaction picture time-evolution operator reads

$$U_I(t, t_0) = \mathcal{T} \exp\left(-i\int_0^\tau ds H_I(s)\right) \,, \tag{30}$$

where $H_I(s)$ is defined by Eq. (27) and $\mathcal{T}$ indicates time ordering. Assuming the initial condition $P[\psi, t_0] = P_1[\psi_1, t_0] \otimes P_2[\psi_2]$, we find from Eq. (29)

$$\tilde{P}[\psi, t] = \int D\tilde{\psi}_1 D\tilde{\psi}_1^* \int D\tilde{\psi}_2 D\tilde{\psi}_2^* \, \delta\left[U_I^\dagger(t, t_0)\psi - \tilde{\psi}_1\tilde{\psi}_2\right] \times P_1[\tilde{\psi}_1, t_0]P_2[\tilde{\psi}_2] \,. \tag{31}$$

The reduced probability distribution $\tilde{P}_1[\psi_1, t]$ in the interaction picture in then obtained by applying the reduction formula (22) to Eq. (31). On using the reservoir distribution (28) we have

$$\tilde{P}_1[\psi_1, t] = \int D\tilde{\psi}_1 D\tilde{\psi}_1^* \, T[\psi_1, t|\tilde{\psi}_1, t_0]\tilde{P}_1[\tilde{\psi}_1, t_0] \,, \tag{32}$$

where the functional kernel T is given by

$$T[\psi_1, t|\tilde{\psi}_1, t_0] = \int_0^{2\pi} \frac{d\phi}{2\pi} \sum_{\alpha,\beta} w_{\alpha\beta}p_\beta \, \delta_1\left[e^{i\phi}w_{\alpha\beta}^{-1/2}L_{\alpha\beta}\tilde{\psi}_1 - \psi_1\right] \,. \tag{33}$$

For any pair (α, β) the linear operator $L_{\alpha\beta}$:$\mathcal{H}_1 \mapsto \mathcal{H}_1$ is defined by

$$L_{\alpha\beta}\tilde{\psi}_1(x_1) \equiv \int dx_2 \, \varphi_\alpha^*(x_2)U_I(t, t_0)\tilde{\psi}_1(x_1)\varphi_\beta(x_2) \tag{34}$$

and

$$w_{\alpha\beta} \equiv ||L_{\alpha\beta}\tilde{\psi}_1||_1^2 \equiv \int dx_1 \left|\int dx_2 \, \varphi_\alpha^*(x_2)U_I(t, t_0)\tilde{\psi}_1(x_1)\varphi_\beta(x_2)\right|^2 \,. \tag{35}$$

Note that we have chosen the eigenbasis φ_α of H_2 in the reduction formula (22). This choice is justified by the following. We have transformed the probability distribution to the interaction representation and will transform back to the Schrödinger representation later on. The exact dynamics of the reduced probability distribution turns out to be unaffected by these transformations if the basis entering the reduction formula is identical to the eigenbasis of the Hamiltonian of the reservoir.

Obviously, the kernel $T[\psi_1, t|\tilde{\psi}_1, t_0]$ can be interpreted as the conditional probability density for a transition from the ray $e^{i\phi}\tilde{\psi}_1$ to the ray $e^{i\phi}\psi_1$ during the time interval $[t_0, t]$ under the condition that at time t_0 the ray $e^{i\phi}\tilde{\psi}_1$ is given. Since $\sum_\alpha w_{\alpha\beta} = 1$ and $\lim_{\tau\to 0} w_{\alpha\beta} = \delta_{\alpha\beta}$ it is easy to verify that

$$\int D\psi_1 D\psi_1^* \, T[\psi_1, t|\tilde{\psi}_1, t_0] = 1 \tag{36}$$

and

$$\lim_{\tau\to 0} T[\psi_1, t_0 + \tau|\tilde{\psi}_1, t_0] = \int_0^{2\pi} \frac{d\phi}{2\pi}\delta_1\left[e^{i\phi}\tilde{\psi}_1 - \psi_1\right] . \tag{37}$$

These equations express the fact that the total probability for a transition to any state is equal to 1 and that at time t_0 the ray $e^{i\phi}\tilde{\psi}_1$ is given. Note that by definition the functional kernel $T[\psi_1, t|\tilde{\psi}_1, t_0]$ acts on phase invariant distributions that are concentrated on the unit sphere in $\mathcal{H}_1$. Thus one can always assume that $||\tilde{\psi}_1||_1 = 1$ and in the following we may omit the integration over ϕ in Eq. (33), keeping in mind that we have for all $\phi \in [0, 2\pi)$

$$T[e^{i\phi}\psi_1, t|\tilde{\psi}_1, t_0] = T[\psi_1, t|e^{i\phi}\tilde{\psi}_1, t_0] = T[\psi_1, t|\tilde{\psi}_1, t_0] \,. \tag{38}$$

Up to now everything is exact. However, the expression that is obtained for the conditional transition probability T involves, of course, the reservoir variables. In order to eliminate the latter we now invoke the Markov approximation. To this end, it is assumed that there exists a time scale τ such that $\tau_B \ll \tau \ll \tau_S$, where τ_B is of the order of the reservoir correlation time and τ_S is of the order of the relaxation time of the reduced system. The condition $\tau_B \ll \tau$ implies that after a time interval of order τ, any reference to the precise initial value at time t_0 has been wiped out and that, therefore, at time $t = t_0 + \tau$ the conditional transition probability T takes on the same form as at time t_0 (random phase approximation). In other words, it follows that the wave function ψ_1 of the reduced system represents a stochastic Markov process (in the interaction representation) that is completely defined in terms of the conditional transition probability $T[\psi_1, t_2|\tilde{\psi}_1, t_1]$ for arbitrary times $t_2 \geq t_1$. On the other hand, in view of the second condition $\tau \ll \tau_S$ it suffices to study, once the reservoir variables have been eliminated, the short-time behavior of the conditional transition probability $T[\psi_1, t_2|\tilde{\psi}_1, t_1]$.

Employing second-order perturbation theory (weak coupling assumption) we obtain

$$L_{\alpha\beta} = \delta_{\alpha\beta} + \sum_i f_{\alpha\beta}^i A_i + \sum_{i,j} g_{\alpha\beta}^{ij} A_i^\dagger A_j \tag{39}$$

and

$$w_{\alpha\beta} = \delta_{\alpha\beta}\left\{1 - \sum_{i,j}\sum_{\alpha'} f^{i*}_{\alpha'\alpha} f^{j}_{\alpha'\alpha}\,\langle\tilde{\psi}_1|A_i^\dagger A_j|\tilde{\psi}_1\rangle_1\right\} + \sum_{i,j} f^{i*}_{\alpha\beta} f^{j}_{\alpha\beta}\langle\tilde{\psi}_1|A_i^\dagger A_j|\tilde{\psi}_1\rangle_1\,, \tag{40}$$

where we have defined the quantities

$$f^i_{\alpha\beta} \equiv -i\int_0^\tau ds e^{i\omega_i s}\langle\varphi_\alpha|B_i(s)|\varphi_\beta\rangle_2, \tag{41}$$

$$g^{ij}_{\alpha\beta} \equiv -\int_0^\tau ds\int_0^{\tau-s} ds' e^{-i\omega_i(s+s')+i\omega_j s} \times \langle\varphi_\alpha|B_i^\dagger(s+s')B_j(s)|\varphi_\beta\rangle_2\,. \tag{42}$$

Note that, since the diagonal elements of B_i in the H_2 representation are assumed to vanish, we have $f^i_{\alpha\alpha} = 0$ for all i and α. We decompose the conditional transition probability T into a diagonal part T_d and a nondiagonal part T_n as

$$T[\psi_1, t|\tilde{\psi}_1, t_0] = T_d[\psi_1, t|\tilde{\psi}_1, t_0] + T_n[\psi_1, t|\tilde{\psi}_1, t_0]\,, \tag{43}$$

where

$$T_d = \sum_\alpha w_{\alpha\alpha}p_\alpha\delta_1[w^{-1/2}_{\alpha\alpha}L_{\alpha\alpha}\tilde{\psi}_1 - \psi_1]\,, \tag{44}$$

$$T_n = \sum_{\alpha\neq\beta} w_{\alpha\beta}p_\beta\delta_1[w^{-1/2}_{\alpha\beta}L_{\alpha\beta}\tilde{\psi}_1 - \psi_1]\,. \tag{45}$$

As will be demonstrated next, T_d and T_n exhibit a different short-time behavior corresponding to a deterministic drift and a discontinuous jump process, respectively.

Equation (44) may be interpreted as follows. For each α the transition $\tilde{\psi}_1 \longrightarrow \psi_1$ occurs within the time interval $[t_0, t]$ with probability $w_{\alpha\alpha}p_\alpha$. Since the size of these transitions becomes infinitesimally small for infinitesimal τ [see Eq. (39)] it is justified to replace the whole set of these possible transitions by a single transition given by the weighted sum

$$\tilde{\psi}_1 \longrightarrow \psi_1 = \sum_\alpha p_\alpha w^{-1/2}_{\alpha\alpha}L_{\alpha\alpha}\tilde{\psi}_1 \tag{46}$$

with corresponding transition probability $\sum_\alpha w_{\alpha\alpha}p_\alpha$. This means that we approximate (for τ small on the time scale of the system dynamics) the diagonal part of the conditional transition probability by the expression

$$T_d = \left(\sum_\alpha w_{\alpha\alpha}p_\alpha\right)\delta_1\left[\sum_\alpha p_\alpha w^{-1/2}_{\alpha\alpha}L_{\alpha\alpha}\tilde{\psi}_1 - \psi_1\right]\,. \tag{47}$$

It is shown in the Appendix that for $\tau_B \ll \tau$

$$\Gamma_{ij} \equiv \sum_{\alpha',\alpha} f^{i*}_{\alpha'\alpha}f^{j}_{\alpha'\alpha}p_\alpha \approx \tau\gamma_i\delta_{ij} \tag{48}$$

and hence

$$\sum_\alpha w_{\alpha\alpha}p_\alpha \approx 1 - \tau\sum_i \gamma_i\langle\tilde{\psi}_1|A_i^\dagger A_i|\tilde{\psi}_1\rangle_1\,. \tag{49}$$

Similarly, we find to second order in the interaction

$$\sum_\alpha p_\alpha w^{-1/2}_{\alpha\alpha}L_{\alpha\alpha} \approx \mathbf{1} + \frac{\tau}{2}\sum_i\gamma_i\langle\tilde{\psi}_1|A_i^\dagger A_i|\tilde{\psi}_1\rangle_1 + \sum_{i,j}\sum_\alpha g^{ij}_{\alpha\alpha}A_i^\dagger A_j p_\alpha\,. \tag{50}$$

In the Appendix it is shown that for $\tau_B \ll \tau$ we have

$$\tilde{\Gamma}_{ij} \equiv \sum_\alpha g^{ij}_{\alpha\alpha}p_\alpha \approx -\tau\left(\frac{1}{2}\gamma_i + iS_i\right)\delta_{ij}\,, \tag{51}$$

where the γ_i are real and non-negative and the S_i are real [10]. Thus we find

$$\sum_\alpha p_\alpha w^{-1/2}_{\alpha\alpha}L_{\alpha\alpha} \approx \mathbf{1} + \frac{\tau}{2}\sum_i\gamma_i\left(\langle\tilde{\psi}_1|A_i^\dagger A_i|\tilde{\psi}_1\rangle_1 - A_i^\dagger A_i\right) - i\tau\sum_i S_i A_i^\dagger A_i\,. \tag{52}$$

This finally yields the following expression for the short-time behavior of the diagonal part of the conditional transition probability:

$$T_d \approx \left\{1 - \tau\sum_i\gamma_i\langle\tilde{\psi}_1|A_i^\dagger A_i|\tilde{\psi}_1\rangle_1\right\} \times\delta_1\left[\left\{\mathbf{1} + \frac{\tau}{2}\sum_i\gamma_i\left(\langle\tilde{\psi}_1|A_i^\dagger A_i|\tilde{\psi}_1\rangle_1 - A_i^\dagger A_i\right) - i\tau\sum_i S_i A_i^\dagger A_i\right\}\tilde{\psi}_1 - \psi_1\right]\,. \tag{53}$$

On using Eq. (39) and (40) we obtain for the nondiagonal part (45) to leading order

$$T_n = \sum_{\alpha,\beta}\left(\sum_{i,j} f^{i*}_{\alpha\beta}f^{j}_{\alpha\beta}\,\langle\tilde{\psi}_1|A_i^\dagger A_j|\tilde{\psi}_1\rangle_1\right) \times p_\beta\,\delta_1\left[\frac{\sum_i f^i_{\alpha\beta}A_i\tilde{\psi}_1}{||\sum_i f^i_{\alpha\beta}A_i\tilde{\psi}_1\,||_1} - \psi_1\right]\,. \tag{54}$$

According to Eq. (41) we have

$$f^i_{\alpha\beta} = \frac{e^{-i(\varepsilon_\beta - \varepsilon_\alpha - \omega_i)\tau} - 1}{\varepsilon_\beta - \varepsilon_\alpha - \omega_i}\langle\varphi_\alpha|B_i|\varphi_\beta\rangle_2\,. \tag{55}$$

Thus the secular terms in the sum over i in the argument of the functional δ function in Eq. (54) are precisely those terms that fulfill the energy conservation $\varepsilon_\beta = \varepsilon_\alpha + \omega_i$. Recall that we are considering the interaction time τ, which is large (on the time scale of the reservoir) but finite. Consequently, we have a finite energy uncertainty Δ of order $\Delta \sim 1/\tau$. As mentioned before, we assume that the frequency spectrum ω_i is nondegenerate. We now impose the additional assumption that for times of order τ the energy intervals

$$I_i \equiv [\omega_i - \Delta, \omega_i + \Delta] \tag{56}$$

do not overlap and are well separated. Physically, this means that for interaction times of order τ, the corresponding energy uncertainty is much smaller than the differences between the frequencies ω_i. In other words, within interaction times of order τ it is possible to identify uniquely that interaction term that contributes to a given transition of the reservoir. Note that the very same assumption $\omega_j - \omega_i \gg 1/\tau$ is needed for the determination of the correlation functions (see the Appendix). It is therefore justified to take into account in (54) only those terms (α, β) that satisfy the condition

$$\varepsilon_\beta - \varepsilon_\alpha \in I_k \tag{57}$$

for some k. If this condition is fulfilled the kth term in the sum over i in the argument of the δ functional in Eq. (54) dominates and, due to the normalization factor, the argument of the functional δ function in (54) becomes

$$\frac{f^k_{\alpha\beta}}{|f^k_{\alpha\beta}|}\frac{A_k\tilde{\psi}_1}{||A_k\tilde{\psi}_1||_1} - \psi_1 \,. \tag{58}$$

Since the first factor is a pure phase factor it can be omitted by invoking the phase invariance of the transition probability [see Eq. (38)]. In other words, this factor is irrelevant since we are working in projective Hilbert space. Thus we see that the argument of the δ functional becomes time independent. We emphasize that it is precisely this time independence that ensures that the short-time behavior of the conditional transition probability yields a differential Chapman-Kolmogorov equation leading to a Markovian jump process. Note that the use of a projective Hilbert space enters the argument in an essential manner.

Summarizing these arguments we find for the nondiagonal part of the conditional transition probability

$$T_n \approx \sum_{i,j,k} \Gamma^k_{ij} \langle\tilde{\psi}_1|A_i^\dagger A_j|\tilde{\psi}_1\rangle_1 \, \delta_1\left[\frac{A_k\tilde{\psi}_1}{||A_k\tilde{\psi}_1||_1} - \psi_1\right] , \tag{59}$$

where

$$\Gamma^k_{ij} \equiv \sum_{\varepsilon_\beta - \varepsilon_\alpha \in I_k} f^{i*}_{\alpha\beta} f^j_{\alpha\beta} p_\beta \,. \tag{60}$$

It is shown in the Appendix that under the conditions explained above

$$\Gamma^k_{ij} \approx \tau\gamma_i\delta_{ij}\delta_{ik} \,. \tag{61}$$

Hence we find

$$T_n \approx \tau\sum_i \gamma_i \langle\tilde{\psi}_1|A_i^\dagger A_i|\tilde{\psi}_1\rangle_1 \, \delta_1\left[\frac{A_i\tilde{\psi}_1}{||A_i\tilde{\psi}_1||_1} - \psi_1\right] . \tag{62}$$

Combining Eqs. (53) and (62) we finally obtain the following short-time behavior of the conditional transition probability:

$$\begin{aligned} T[\psi_1, t|\tilde{\psi}_1, t_0] \approx & \left\{1 - \tau\sum_i \gamma_i \langle\tilde{\psi}_1|A_i^\dagger A_i|\tilde{\psi}_1\rangle_1\right\} \\ & \times\delta_1\left[\left\{\mathbf{1} + \frac{\tau}{2}\sum_i \gamma_i\left(\langle\tilde{\psi}_1|A_i^\dagger A_i|\tilde{\psi}_1\rangle_1 - A_i^\dagger A_i\right) - i\tau\sum_i S_i A_i^\dagger A_i\right\}\tilde{\psi}_1 - \psi_1\right] \\ & + \tau\sum_i \gamma_i \langle\tilde{\psi}_1|A_i^\dagger A_i|\tilde{\psi}_1\rangle_1 \, \delta_1\left[\frac{A_i\tilde{\psi}_1}{||A_i\tilde{\psi}_1||_1} - \psi_1\right] . \end{aligned} \tag{63}$$

As can be seen from this expression, the short-time behavior of the conditional transition probability has in fact the appropriate form that leads to a differential Chapman-Kolmogorov equation. The second term represents the gain term of a discontinuous jump process whereas the first term exhibits the short-time structure of a deterministic flow and of the loss term corresponding to the jump process. Note that the exact relations (36) and (37) remain true for the approximate expression derived above.

Our final step consists of transforming to the Schrödinger picture and deriving from the above short-time structure of the conditional transition probability the equation of motion for the reduced probability distribution $P_1[\psi_t, t]$. On using Eqs. (63) and (32) we obtain to first order in τ

$$\begin{aligned} \tilde{P}_1[\psi_1, t_0 + \tau] - \tilde{P}_1[\psi_1, t_0] = & -\frac{\tau}{2}\int dx_1 \left\{\frac{\delta}{\delta\psi_1}\sum_i\left(\gamma_i\langle\psi_1|A_i^\dagger A_i|\psi_1\rangle_1 - \gamma_i A_i^\dagger A_i - 2iS_i A_i^\dagger A_i\right)\psi_1 P_1[\psi_1, t_0] + \text{c.c.}\right\} \\ & + \tau\int D\tilde{\psi}_1 D\tilde{\psi}_1^* \left\{W[\psi_1|\tilde{\psi}_1]P_1[\tilde{\psi}_1, t_0] - W[\tilde{\psi}_1|\psi_1]P_1[\psi_1, t_0]\right\} , \end{aligned} \tag{64}$$

where c.c. means complex conjugated and we have introduced the transition functional

$$W[\psi_1|\tilde{\psi}_1] = \sum_i \gamma_i ||A_i\tilde{\psi}_1||_1^2 \, \delta_1\left[\frac{A_i\tilde{\psi}_1}{||A_i\tilde{\psi}_1||_1} - \psi_1\right] . \tag{65}$$

In the Schrödinger representation the reduced probability distribution $P_1[\psi_1, t]$ on the Hilbert space $\mathcal{H}_1$ of the reduced system is given by

$$P_1[\psi_1, t] = \tilde{P}_1[e^{iH_1\tau}\psi_1, t] \,. \tag{66}$$

Inserting this equation into Eq. (64), dividing by τ, and performing the limit $\tau \longrightarrow 0$ finally yields the Liouville master equation for the probability distribution $P_1[\psi_1, t]$ of the reduced system:

$$\frac{\partial}{\partial t}P_1[\psi_1,t] = i\int dx_1 \left\{ \frac{\delta}{\delta\psi_1(x_1)}G(\psi_1)(x_1) - \frac{\delta}{\delta\psi_1^*(x_1)}[G(\psi_1)]^*(x_1)\right\}P_1[\psi_1,t] + \int D\tilde{\psi}_1 D\tilde{\psi}_1^* \left\{ W[\psi_1|\tilde{\psi}_1]P_1[\tilde{\psi}_1,t] - W[\tilde{\psi}_1|\psi_1]P_1[\psi_1,t]\right\} . \quad (67)$$

Here we have introduced the nonlinear and non-Hermitian operator $G{:}\mathcal{H}_1 \mapsto \mathcal{H}_1$ defined by

$$G(\psi_1) = \hat{H}_1\psi_1 + \frac{i}{2}\sum_i \gamma_i ||A_i\psi_1||_1^2\psi_1 , \quad (68)$$

where the linear, non-Hermitian operator $\hat{H}_1$ is given by

$$\hat{H}_1 = H_1 + h_1 - \frac{i}{2}\sum_i \gamma_i A_i^\dagger A_i . \quad (69)$$

$\hat{H}_1$ is made up of three parts: the free Hamiltonian H_1 of the system, a Hermitian part $h_1 = \sum_i S_i A_i^\dagger A_i$ induced by the coupling to the reservoir (Lamb shift), and a non-Hermitian part describing dissipation of energy into the reservoir degrees of freedom [34].

As is easily verified, the above Liouville master equation (67) preserves the basic conditions formulated in Sec. II A, i.e., normalization, concentration on the unit sphere in Hilbert space, and phase invariance. Thus it uniquely defines a stochastic process on the projective Hilbert space of the reduced system.

Moreover, we note that the Liouville master equation is invariant with respect to unitary (canonical) transformations $U{:}\mathcal{H}_1 \mapsto \mathcal{H}_1$. To be more precise, if we transform state vectors as $\psi_1 \mapsto \psi_1' = U\psi_1$, by virtue of the unitary invariance of the measure $D\psi_1 D\psi_1^*$ the corresponding transformation rule for the probability distribution reads

$$P_1'[\psi_1', t] = P_1[\psi_1, t] . \quad (70)$$

As is easily shown, the transformed distribution P_1' also obeys the Liouville master equation (67) if, at the same time, the system operators A_i and the Hamiltonian $\hat{H}_1$ are transformed as

$$A_i \mapsto A_i' = UA_iU^\dagger , \quad \hat{H}_1 \mapsto \hat{H}_1' = U\hat{H}_1U^\dagger . \quad (71)$$

B. Construction of the realizations of the stochastic process

The Liouville part of Eq. (67) given by the first term on the right-hand side describes the rate of change of P_1 due to the flow induced by the nonlinear (deterministic) Schrödinger-type equation

$$i\frac{\partial}{\partial t}\psi_1 = G(\psi_1) = \hat{H}_1\psi_1 + \frac{i}{2}\sum_i \gamma_i ||A_i\psi_1||_1^2\psi_1 . \quad (72)$$

As is easily checked, the solution of Eq. (72) corresponding to the normalized initial value $\psi_1(0) = \tilde{\psi}_1$ is given by

$$\psi_1(t) = \frac{e^{-i\hat{H}_1 t}\tilde{\psi}_1}{||e^{-i\hat{H}_1 t}\tilde{\psi}_1||_1} . \quad (73)$$

Thus we see that the time evolution is generated by the non-Hermitian operator $\hat{H}_1$ and that the nonlinear term in Eq. (72) induces the constraint $||\psi_1||_1 = 1$.

The master part of Eq. (67) (given by the second term on the right-hand side) describes the rate of change of P_1 due to discontinuous quantum jumps. The gain term represents the probability density per unit time for a transition from any state into the state ψ_1, whereas the loss term gives the probability density per unit time for a transition from the state ψ_1 into any other state. The total rate for transitions from a *given* state $\tilde{\psi}_1$ to any other state is therefore

$$\Gamma[\tilde{\psi}_1] = \int D\psi_1 D\psi_1^* W[\psi_1|\tilde{\psi}_1] = \sum_i \gamma_i ||A_i\tilde{\psi}_1||_1^2 . \quad (74)$$

Let us assume that the state $\tilde{\psi}_1$ was reached through a jump at time t. Due to the continuous time evolution between the jumps, the total rate Γ for the next transition depends upon the time τ elapsed since the time t. Inserting Eq. (73) (with t replaced by τ) into Eq. (74) we obtain after some algebra

$$\Gamma[\tilde{\psi}_1, \tau] = -\frac{d}{d\tau}\ln ||e^{-i\hat{H}_1\tau}\tilde{\psi}_1||_1^2 . \quad (75)$$

According to the general theory of Markov processes (see, e.g., Ref. [35]), the distribution function of the random waiting time τ is given by

$$F[\tilde{\psi}_1, \tau] = 1 - \exp\left(-\int_0^\tau ds\Gamma[\tilde{\psi}_1, s]\right) = 1 - ||e^{-i\hat{H}_1\tau}\tilde{\psi}_1||_1^2 . \quad (76)$$

This waiting time distribution function $F[\tilde{\psi}_1, \tau]$ represents the probability that the next jump occurs within the time interval $[t, t+\tau)$. Obviously, we have $F[\tilde{\psi}_1, 0] = 0$. Since the norm in Eq. (76) is a monotonously decreasing function of τ, the limit

$$\lim_{\tau\to\infty} ||e^{-i\hat{H}_1\tau}\tilde{\psi}_1||_1^2 \equiv q \quad (77)$$

exists and thus $F[\tilde{\psi}_1, \infty] = 1 - q$. In general, we have $0 \le q \le 1$. For $q = 0$ it follows that $F[\tilde{\psi}_1, \infty] = 1$. This means that the next jump occurs with probability 1 in some finite time. However, if the non-Hermitian part of $\hat{H}_1$ has a zero mode it is possible that $q > 0$. In

this case, the so-called defect q [36] is to be interpreted as the probability that after time t *no* further quantum jump occurs. We remark that this can be formulated mathematically by adding the point ∞ to the set $\mathbb{R}^+$ of non-negative reals. This means that the space underlying the random variable τ becomes $\Omega = \mathbb{R}^+ \cup \{\infty\}$ and the defect q is the probability of the event $\tau = \infty$.

The quantity $W[\psi_1|\tilde{\psi}_1]$ denotes the probability density per unit time for a transition from $\tilde{\psi}_1$ to ψ_1. Since this transition rate is given by a discrete sum of functional δ functions [see Eq. (65)] we have a discrete set of possible transitions: Under the condition that the state just before the jump is given by $\tilde{\psi}_1$, the transition

$$\tilde{\psi}_1 \longrightarrow \psi_1 = \frac{A_i\tilde{\psi}_1}{||A_i\tilde{\psi}_1||_1} \tag{78}$$

takes place with probability $p_i = \gamma_i||A_i\tilde{\psi}_1||_1^2/\Gamma[\tilde{\psi}_1]$. Note that $\sum_i p_i = 1$.

Summarizing, we obtain a realization $\psi_1(t)$ of the stochastic process defined by the Liouville master equation (67) by means of the following algorithm:

(i) Assume that the state $\tilde{\psi}_1$ was reached by a jump at time t, that is, we have $\psi_1(t) = \tilde{\psi}_1$.

(ii) Determine a random waiting time τ according to the distribution function (76). This can be done, for example, by drawing a random number η that is uniformly distributed over the interval $[0,1)$ and by determining τ from the equation $\eta = F[\tilde{\psi}_1, \tau]$. For $\eta < 1 - q$ there exists a unique solution. For $\eta \geq 1 - q$ we set $\tau = \infty$. Within the time interval $[t, t+\tau)$ the realization is then determined by the continuous time evolution

$$\psi_1(t+s) = \frac{e^{-i\hat{H}_1 s}\tilde{\psi}_1}{||e^{-i\hat{H}_1 s}\tilde{\psi}_1||_1}\,, \quad 0 \leq s < \tau\,. \tag{79}$$

For $\tau = \infty$ the algorithm terminates here.

(iii) At time $t + \tau$ (if τ is finite) one of the possible jumps labeled by the index i [see Eq. (78)] occurs. Select a specific jump of type i with probability

$$p_i = \gamma_i||A_i\psi_1(t+\tau-\varepsilon)||_1^2/\Gamma[\psi_1(t+\tau-\varepsilon)] \tag{80}$$

and set

$$\psi_1(t+\tau) = \frac{A_i\psi_1(t+\tau-\varepsilon)}{||A_i\psi_1(t+\tau-\varepsilon)||_1}\,, \tag{81}$$

where the limit $\varepsilon \longrightarrow 0+$ is understood.

(iv) Repeat these steps until the desired final time is reached.

It should be clear that once an ensemble of realizations has been generated according to this algorithm, any statistical quantity can be estimated as ensemble average. As has been emphasized [37], the numerical implementation of this or similar algorithms may serve as a very efficient method for simulating the dynamics of open quantum systems. In fact, as has been demonstrated in a different context [38], the stochastic simulation method of complex systems described by master equations leads to numerical algorithms that can easily be vectorized and parallelized.

It is important to note that the above stochastic simulation algorithm derived from the Liouville master equation (67) is very similar to the Monte Carlo wave function simulation method proposed in Refs. [18,24–26]. The difference to these methods is that the realizations of the stochastic process defined by our Liouville master equation are strictly confined to the unit sphere in Hilbert space. This is due to the fact that we have introduced, right from the beginning, the projective Hilbert space as the phase space underlying the stochastic process. For the same reason the continuous part of the time evolution is nonlinear in our case, the nonlinearity being responsible for the normalization of the state vector.

Apart from this different normalization, our analysis thus implies that the piecewise deterministic quantum jump methods proposed in the literature can be justified from a general microscopic ansatz for the interaction of the open system with the external reservoir. Note that this has been achieved without referring to an equation of motion for the density matrix of the reduced system. In contrast, the equation governing the dynamics of the reduced density operator can be *derived* from the above Liouville master equation as the equation of motion for the covariance matrix

$$\rho_t(x_1, x_1') = \int D\psi_1 D\psi_1^*\ \psi_1(x_1)\psi_1^*(x_1')P_1[\psi_1, t]\,. \tag{82}$$

In fact, differentiating (82) with respect to time and invoking the Liouville master equation (67) we obtain

$$\begin{aligned}\frac{\partial}{\partial t}\rho_t = &-i\,[H_1 + h_1, \rho_t] \\ &+ \sum_i \gamma_i \left(A_i\rho_t A_i^\dagger - \frac{1}{2}A_i^\dagger A_i\rho_t - \frac{1}{2}\rho_t A_i^\dagger A_i\right)\,.\end{aligned} \tag{83}$$

This equation is exactly of the Lindblad form of the quantum Markovian master equation [7,8] with Lindblad operators A_i and Hamiltonian $H_1 + h_1$.

C. Diffusion-noise approximation

We shall demonstrate in this subsection that under certain conditions the diffusion limit of the Liouville master equation (67) exists and yields a Fokker-Planck equation that is equivalent to a stochastic Schrödinger-type equation. For the sake of a simple notation we assume in the following that we have only one Lindblad operator A and we omit the index 1 from all quantities that refer to the reduced system S_1. Furthermore, the Lamb shift is included in the system Hamiltonian.

According to the general theory of stochastic processes, a diffusion expansion of a given master equation can be performed if the size of the transitions among the states becomes arbitrarily small and if, at the same time, the number of transitions in any finite time interval becomes arbitrarily large. In order to formulate these conditions we introduce a small (dimensionless) parameter ε and write the Lindblad operator as

$$A = \mathbf{1} + \varepsilon C \,, \tag{84}$$

where $\mathbf{1}$ denotes the identity operator and the operator C is independent of ε. Our aim is to investigate the behavior of the Liouville master equation in the limit $\varepsilon \longrightarrow 0$. On using Eq. (84) we obtain to second order in ε

$$G(\psi) = H\psi - \frac{i}{2}\gamma\left\{\mathbf{1} + \varepsilon(C^\dagger + C) + \varepsilon^2 C^\dagger C\right\}\psi + \frac{i}{2}\gamma\left\{\mathbf{1} + \varepsilon\langle C^\dagger + C\rangle_\psi + \varepsilon^2\langle C^\dagger C\rangle_\psi\right\}\psi \tag{85}$$

and

$$W[\psi_1|\tilde{\psi}_1] = \gamma\left(1 + \varepsilon\langle C^\dagger + C\rangle_{\tilde{\psi}} + \varepsilon^2\langle C^\dagger C\rangle_{\tilde{\psi}}\right) \times \delta[\tilde{\psi} - \psi + \varepsilon M(\tilde{\psi}) + \varepsilon^2 N(\tilde{\psi})] \,, \tag{86}$$

where we have introduced the abbreviation $\langle\cdots\rangle_\psi \equiv \langle\psi|\cdots|\psi\rangle$ and defined the nonlinear operators

$$M(\psi) \equiv \left\{C - \frac{1}{2}\langle C^\dagger + C\rangle_\psi\right\}\psi \,,$$

$$N(\psi) \equiv -\frac{1}{2}\left\{\langle C^\dagger C\rangle_\psi - \frac{3}{4}\langle C^\dagger + C\rangle_\psi^2 + \langle C^\dagger + C\rangle_\psi C\right\}\psi.$$

Inserting these expressions into the Liouville master equation we obtain to second order

$$\frac{\partial}{\partial t}P[\psi,t] = i\int dx\left\{\frac{\delta}{\delta\psi(x)}K(\psi)(x) - \frac{\delta}{\delta\psi^*(x)}[K(\psi)]^*(x)\right\}P[\psi,t] + \frac{1}{2}\gamma\varepsilon^2\int dx\int dx'\left\{\frac{\delta^2}{\delta\psi(x)\delta\psi(x')}M(\psi)(x)M(\psi)(x') + \frac{\delta^2}{\delta\psi^*(x)\delta\psi^*(x')}[M(\psi)]^*(x)[M(\psi)]^*(x') + 2\frac{\delta^2}{\delta\psi(x)\delta\psi^*(x')}M(\psi)(x)[M(\psi)]^*(x')\right\}P[\psi,t] \,. \tag{87}$$

This is obviously a functional Fokker-Planck equation for the reduced probability distribution. The nonlinear drift operator $K(\psi)$ takes the form

$$K(\psi) = H\psi + \frac{i}{2}\gamma\varepsilon\left\{C - C^\dagger\right\}\psi + i\gamma\varepsilon^2\left\{\frac{1}{2}\langle C^\dagger + C\rangle_\psi C - \frac{1}{8}\langle C^\dagger + C\rangle_\psi^2 - \frac{1}{2}C^\dagger C\right\}\psi \,. \tag{88}$$

As can be seen from Eq. (87), the diffusion part of the Fokker-Planck equation involving the second-order functional derivatives scales as $\gamma\varepsilon^2$. Thus, in order to obtain a nonvanishing and finite diffusive contribution in the limit $\varepsilon \longrightarrow 0$, we assume that the ε dependence of the relaxation time γ reads

$$\gamma = \varepsilon^{-2}\bar{\gamma} \,. \tag{89}$$

On the other hand, the drift operator (88) contains a term that is proportional to $\gamma\varepsilon = \bar{\gamma}\varepsilon^{-1}$. This term diverges in the limit $\varepsilon \longrightarrow 0$ unless we impose the condition that the operator C is self-adjoint, that is, $C = C^\dagger$. Using this condition we obtain for the drift operator

$$K(\psi) = H\psi + i\bar{\gamma}\left\{\langle C\rangle_\psi C - \frac{1}{2}\langle C\rangle_\psi^2 - \frac{1}{2}C^2\right\}\psi \tag{90}$$

and the operator $M(\psi)$ takes the form

$$M(\psi) = (C - \langle C\rangle_\psi)\,\psi \,. \tag{91}$$

The Fokker-Planck equation (87) is equivalent to a certain stochastic Schrödinger-type equation. The noise term of the latter is multiplicative since the Fokker-Planck equation is nonlinear. Employing standard techniques from probability theory we find that, under the conditions just described, the Ito stochastic differential equation corresponding to the Fokker-Planck equation (87) is given by

$$i\frac{d}{dt}\psi = H\psi + i\bar{\gamma}\left\{\langle C\rangle_\psi C - \frac{1}{2}\langle C\rangle_\psi^2 - \frac{1}{2}C^2\right\}\psi + i\bar{\gamma}^{1/2}\left\{C - \langle C\rangle_\psi\right\}\psi\eta(t) \,, \tag{92}$$

where $\eta(t)$ is a *real* and Gaussian white-noise process with zero mean and correlation function

$$\langle\eta(t)\eta(t')\rangle = \delta(t - t') \,. \tag{93}$$

It is interesting to note that Eq. (92) is of the same form as the stochastic differential equation of the quantum state diffusion model proposed by Gisin and Percival [14] for the case of a self-adjoint Lindblad operator. The only difference is that in our case the stochastic differential equation contains a real instead of a complex Wiener process (it has already been remarked in Ref. [39] that the quantum state diffusion model also works with a real Wiener process). The appearance of a real instead of a complex white-noise process in the stochastic Schrödinger equation indicates the fact that the diffusion part of the Fokker-Planck equation (87) differs from that of the Fokker-Planck equation given by Diósi [15].

Summarizing, we have shown that the piecewise deterministic jump process defined by our Liouville master equation leads, in fact, under certain conditions to a well-defined diffusion limit. These conditions are the condition of small jumps (84), the scaling (89), and that the Lindblad operator is self-adjoint. Of course, it is possible to formulate other conditions and to perform different expansions of the Liouville master equation. Furthermore,

we remark that, if several different Lindblad operators are present, the diffusion limit may be valid only for a certain subset of the them. In this case, the differential Chapman-Kolmogorov equation takes on its most general form containing a Liouville-master-Fokker-Planck operator.

IV. SUMMARY

The question that has motivated the investigation presented in this paper was the following one. Is it possible to formulate a set of basic physical postulates and assumptions that enables one to derive, directly from the underlying microscopic dynamics and without referring to a density operator description, a unique stochastic process governing the dynamics of the states of the open system? It has been shown above that this in indeed possible. Let us summarize the basic postulates and assumptions that have led to this conclusion.

(i) The starting point was a formulation of quantum ensembles of closed and open systems in terms of probability distributions on projective Hilbert space. The latter may be obtained by taking the unit sphere in Hilbert space and identifying states that differ by a pure phase factor. Consequently, we have introduced probability densities $P[\psi]$ on Hilbert space that satisfy the three basic postulates given at the beginning of Sec. II and may thus be regarded as distributions on projective Hilbert space.

(ii) When dealing with open systems that are considered as subsystems of some larger system, we need a unique prescription that tells us how to compose two statistically independent subsystems and how to reduce a given system to one of its subsystems. This composition and reduction has been formulated in terms of probability distributions on projective Hilbert space. The obtained equations take into account the basic rules of quantum mechanics and they guarantee that the distributions for the combined and for the reduced system are again distributions on the corresponding projective Hilbert spaces.

(iii) The basic assumptions for the derivation of the reduced system dynamics are the weak coupling assumption and the validity of the Markov approximation. Note that the latter is understood in the sense of classical probability theory, that is, it means essentially the truncation of the hierarchy of multitime joint probability distributions on the level of the two-time joint probability distribution.

(iv) We have made some technical assumptions, i.e., that the system operators of the interaction Hamiltonian are eigenoperators of the system Hamiltonian with a nondegenerate spectrum and that the diagonal elements of the reservoir operators vanish in the representation of the reservoir Hamiltonian.

All in all, these postulates and assumptions then led to the conclusion that (i) the short-time structure of the conditional transition probability implies the existence of a differential Chapman-Kolmogorov equation and that (ii) the latter takes on the form of a Liouville master equation. The Liouville master equation uniquely defines a stochastic process on the projective Hilbert space of the reduced system. The realizations of this stochastic process, which have been constructed in Sec. III, are piecewise deterministic paths interrupted by discontinuous quantum jumps. As is also explained in Sec. III, these realizations are very similar to those generated by the Monte Carlo wave function simulation methods proposed in Refs. [18,24–26]. Moreover, the equation of motion for the reduced density operator is given by the equation governing the two-point correlation function of the stochastic process.

The mathematical formulation of the stochastic process in terms of a differential Chapman-Kolmogorov equation allows us to perform definite asymptotic expansions. As an example, we have presented a diffusion approximation of the Liouville master equation. This yields a functional Fokker-Planck equation, which, in turn, is equivalent to a stochastic Schrödinger-type equation. The latter closely resembles the stochastic differential equation of the quantum state diffusion model.

Concluding, we point out the following interpretation of the stochastic theory developed here. The starting point of our derivation has been the unitary time evolution according to the Schrödinger equation of the total (closed) system. The essential step towards a stochastic description is the enlargement of the formal setting through the introduction of probability distributions on projective Hilbert space. This enlargement immediately leads to a Liouville equation for the probability distribution of closed systems. Our derivation then demonstrates that the dynamics of an open subsystem is approximated by a differential Chapman-Kolmogorov equation, which defines a piecewise deterministic jump process for pure states. This fact clearly reveals that the stochastic dynamics of the open system wave function is the synthesis of the continuous Schrödinger-type evolution and the discontinuous quantum jumps of the Bohr picture.

APPENDIX: DETERMINATION OF THE RESERVOIR CORRELATION FUNCTIONS

In this appendix we shall determine the reservoir correlation functions

$$\Gamma_{ij} \equiv \sum_{\alpha,\beta} f^{i*}_{\alpha\beta} f^{j}_{\alpha\beta} p_\beta \,, \tag{A1}$$

$$\tilde{\Gamma}_{ij} \equiv \sum_{\alpha} g^{ij}_{\alpha\alpha} p_\alpha \,, \tag{A2}$$

$$\Gamma^{k}_{ij} \equiv \sum_{\varepsilon_\beta - \varepsilon_\alpha \in I_k} f^{i*}_{\alpha\beta} f^{j}_{\alpha\beta} p_\beta \,. \tag{A3}$$

On using (41) we find

$$\Gamma_{ij} = \int_0^\tau ds \int_0^\tau ds' e^{i(\omega_j s' - \omega_i s)} \langle B_i^\dagger(s - s') B_j \rangle \,,$$

where the angular brackets denote the reservoir average

$$\langle B_i^\dagger(s) B_j \rangle \equiv \sum_\alpha p_\alpha \langle \varphi_\alpha | B_i^\dagger(s) B_j | \varphi_\alpha \rangle_2 \,.$$

Transforming to new time variables $t = s - s'$, $t' = s'$ we obtain

$$\Gamma_{ij} = \int_0^\tau dt' \int_{-t'}^{\tau - t'} dt e^{i(\omega_j - \omega_i)t' - i\omega_i t} \langle B_i^\dagger(t) B_j \rangle \ .$$

Since $\tau \gg \tau_B$ the correlation function vanishes very fast outside a small strip along the t' axis. Thus we may approximate

$$\Gamma_{ij} \approx \left(\int_0^\tau dt' e^{i(\omega_j - \omega_i)t'} \right) \left(\int_{-\infty}^{\infty} dt e^{-i\omega_i t} \langle B_i^\dagger(t) B_j \rangle \right) \ .$$

If we assume that the frequency differences $\omega_j - \omega_i$ are large compared to $\Delta \sim 1/\tau$, the first factor on the right-hand side of this equation averages to $\tau \delta_{ij}$. Thus we find

$$\Gamma_{ij} \approx \tau \gamma_i \delta_{ij} \ , \tag{A4}$$

where the inverse relaxation times are given by

$$\gamma_i \equiv \int_{-\infty}^{\infty} dt e^{-i\omega_i t} \langle B_i^\dagger(t) B_i \rangle \ . \tag{A5}$$

Similarly, we find, on using Eq. (42),

$$\tilde{\Gamma}_{ij} = - \int_0^\tau dt' \int_0^{\tau - t'} dt e^{i(\omega_j - \omega_i)t' - i\omega_i t} \langle B_i^\dagger(t) B_j \rangle \ .$$

On using the same arguments as above we obtain

$$\tilde{\Gamma}_{ij} \approx -\tau \left(\frac{1}{2} \gamma_i + i S_i \right) \delta_{ij} \ , \tag{A6}$$

where γ_i is given in Eq. (A5) and S_i is defined by

$$\int_0^{+\infty} dt e^{-i\omega_i t} \langle B_i^\dagger(t) B_i \rangle = \frac{1}{2} \gamma_i + i S_i \ . \tag{A7}$$

Finally, we find

$$\Gamma_{ij}^k = \int_0^\tau dt' \int_{-t'}^{\tau - t'} dt e^{i(\omega_j - \omega_i)t' - i\omega_i t} C_{ij}^k(t) \ ,$$

where

$$C_{ij}^k \equiv \sum_{\varepsilon_\beta - \varepsilon_\alpha \in I_k} \langle \varphi_\beta | B_i^\dagger(t) | \varphi_\alpha \rangle \langle \varphi_\alpha | B_j | \varphi_\beta \rangle p_\beta \ .$$

Assuming again that C_{ij}^k is sharply concentrated around a small strip along the t' axis, we have

$$\Gamma_{ij}^k \approx \tau \delta_{ij} \int_{-\tau}^{\tau} e^{-i\omega_i t} C_{ii}^k(t) \ . \tag{A8}$$

Performing the time integration we find

$$\int_{-\tau}^{\tau} e^{-i\omega_i t} C_{ii}^k(t) = \sum_{\varepsilon_\beta - \varepsilon_\alpha \in I_k} 2\pi D_\tau(\varepsilon_\beta - \varepsilon_\alpha - \omega_i) \times \langle \varphi_\beta | B_i^\dagger | \varphi_\alpha \rangle \langle \varphi_\alpha | B_i | \varphi_\beta \rangle p_\beta \ ,$$

where

$$D_\tau(\omega) \equiv \frac{1}{\pi} \frac{\sin \omega\tau}{\omega} \ .$$

Obviously, $\lim_{\tau \to \infty} D_\tau(\omega) = \delta(\omega)$ and for large but finite τ the function $D_\tau(\omega)$ is concentrated around $\omega = 0$ with an effective width of order $1/\tau \sim \Delta$. By virtue of the assumption that the different intervals I_k are well separated (see Sec. III) we thus obtain

$$\int_{-\tau}^{\tau} e^{-i\omega_i t} C_{ii}^k(t) \approx \delta_{ik} \sum_{\alpha,\beta} 2\pi D_\tau(\varepsilon_\beta - \varepsilon_\alpha - \omega_i) \langle \varphi_\beta | B_i^\dagger | \varphi_\alpha \rangle \langle \varphi_\alpha | B_i | \varphi_\beta \rangle p_\beta \ .$$

On the other hand, we have directly from its definition

$$\gamma_i \approx \int_{-\tau}^{\tau} e^{-i\omega_i t} \langle B_i^\dagger(t) B_i \rangle = \sum_{\alpha,\beta} 2\pi D_\tau(\varepsilon_\beta - \varepsilon_\alpha - \omega_i) \times \langle \varphi_\beta | B_i^\dagger | \varphi_\alpha \rangle \langle \varphi_\alpha | B_i | \varphi_\beta \rangle p_\beta \ .$$

Comparing the last two equations gives

$$\int_{-\tau}^{\tau} e^{-i\omega_i t} C_{ii}^k(t) = \delta_{ik} \gamma_i \ ,$$

which, on inserting into (A8), finally yields

$$\Gamma_{ij}^k \approx \tau \gamma_i \delta_{ij} \delta_{ik} \ . \tag{A9}$$

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