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The non-Markovian stochastic Schrödinger equation for open systems

Lajos Diósi [a,b,1], Walter T. Strunz [a,c,2]

[a] *Department of Physics, Queen Mary and Westfield College, University of London, Mile End Road, London E1 4NS, UK*
[b] *KFKI Research Institute for Particle and Nuclear Physics, H-1525 Budapest 114, PO Box 49, Hungary*
[c] *Fachbereich Physik, Universität GH Essen, D-45117 Essen, Germany*

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Abstract

We present the non-Markovian generalisation of the widely used stochastic Schrödinger equation. Our result allows one to describe open quantum systems in terms of stochastic state vectors rather than density operators, without Markov approximation. Moreover, it unifies two recent independent attempts towards a stochastic description of non-Markovian open systems, based on path integrals on the one hand and coherent states on the other. The latter approach utilises the analytical properties of coherent states and enables a microscopic interpretation of the stochastic states. The alternative first approach is based on the general description of open systems using path integrals as originated by Feynman and Vernon. © 1997 Elsevier Science B.V.

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In the last few years the description of open quantum systems in terms of stochastic Schrödinger equations has received remarkable attention. They are now widely used in different fields (measurement theory, quantum optics, quantum chaos, solid states [1-7]), wherever quantum irreversibility matters. They do not only serve as a fruitful theoretical concept but also as a practical method for computations in the form of quantum trajectories. Up to now, however, the Markov approximation was believed to be essential for a stochastic description [3].

For systems where non-Markovian effects are inevitable, as for non-equilibrium relativistic fields, especially in quantum cosmology [4], or solid state physics [10] [5], an advantageous stochastic pure state description was missing. This Letter presents an exact non-Markovian stochastic Schrödinger equation.

1 E-mail: diosi@rmki.kfki.hu.
2 E-mail: walter.strunz@uni-essen.de.

3 An exact non-Markovian stochastic quantum-Langevin equation for the Heisenberg coordinate operator was derived in Ref. [8]. This result anticipated that a closed stochastic Schrödinger equation, desired for a long time, exists for the state vector.

4 Non-Markovian environmental effects in quantum cosmology have been taken into account stochastically, using coloured noise, in Ref. [9]. This effective approach, however, lacks a closed evolution equation for the state vector of the system.

5 For the electron-phonon interaction the memory effects of the phonons were approximated by a Markovian stochastic Schrödinger equation for an enlarged hypothetical system in Ref. [11].

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Traditionally, open systems are described by the reduced density operator $\hat{\rho}_{\rm sys}(t) = {\rm Tr}_{\rm env}(\hat{\rho}_{\rm tot}(t))$, obtained from the total density operator by tracing over the environmental degrees of freedom. In the Markov approximation, it is well known that the system dynamics can either be described by a master equation for the reduced density operator $\hat{\rho}_{\rm sys}(t)$, or alternatively, by a stochastic Schrödinger equation for state vectors $|\psi_Z(t)\rangle$ [1-7]. In the latter approach, the reduced density operator is recovered as the ensemble average over these stochastic pure states,

$$\hat{\rho}_{\rm sys}(t) = M_Z[|\psi_Z(t)\rangle\langle\psi_Z(t)|]. \tag{1}$$

Here, $|\psi_Z(t)\rangle$ indicates the solution of the stochastic Schrödinger equation with a particular realisation of the - in this case Wiener - stochastic process $Z(t)$; the mean $M_Z[\dots]$ refers to the ensemble average over these processes. The states $|\psi_Z(t)\rangle$ may or may not be normalised depending on whether one utilises the non-linear [2] or linear [4] version of the stochastic Schrödinger equation. Both the linear and the non-linear equation leads to the correct reduced density operator according to Eq. (1) and they are mathematically equivalent by virtue of a redefinition of the stochastic processes $Z(t)$ [12].

It is the aim of this Letter to demonstrate that a stochastic decomposition just like (1) also holds in the general case, without any approximation, in particular without the Markov approximation. We derive the linear version of the relevant non-Markovian stochastic Schrödinger equation, the corresponding non-linear, norm preserving theory can be found in a way similar to the Markovian case [13].

Our result can be based on two recent independent approaches to a stochastic description of non-Markovian open systems [14,15]. One approach [14] uses coherent states and has the advantage of offering an interpretation of the solutions of the stochastic Schrödinger equation from first principles. The other [15] is based on the Feynman-Vernon approach to open systems using path integrals [16] and is valid for arbitrary temperatures.

To be specific, we use a standard model of open system quantum mechanics, a system coupled linearly via position coupling to an environment of harmonic oscillators [16]

$$\hat{H}_{\rm tot} = H_{\rm sys}(\hat{q},\hat{p}) - \hat{q}\sum_i \chi_i\hat{Q}_i + \sum_i\left(\frac{\hat{P}_i^2}{2\,m_i} + \tfrac{1}{2}m_i\omega_i^2\hat{Q}_i^2\right), \tag{2}$$

where we also introduce $\hat{F} = \sum_i \chi_i\hat{Q}_i$ for later purposes, the force acting on the system as induced by the environment. We assume a factorised total initial density operator $\hat{\rho}_{\rm tot}(0) = |\psi_0\rangle\langle\psi_0| \otimes \hat{\rho}_T$. The environment oscillators are assumed to be in a thermal initial state $\hat{\rho}_T$ at temperature T, and, for simplicity, the system is assumed to be in a pure state $|\psi_0\rangle\langle\psi_0|$. The time evolution of the total system is determined by the unitary von Neumann equation $\dot{\hat{\rho}}_{\rm tot} = -{\rm i}[\hat{H}_{\rm tot}, \hat{\rho}_{\rm tot}]$.

Without any approximation, the reduced density operator $\hat{\rho}_{\rm sys}(t)$ of the model (2) can be represented as the ensemble average (1) of stochastic pure states $|\psi_Z(t)\rangle$. They are the solutions of the following non-Markovian stochastic Schrödinger equation,

$$|\dot{\psi}_Z(t)\rangle = -{\rm i}H_{\rm sys}(\hat{q},\hat{p})|\psi_Z(t)\rangle + {\rm i}\hat{q}Z(t)|\psi_Z(t)\rangle + {\rm i}\hat{q}\int_0^t {\rm d}s\,\alpha(t,s)\frac{\delta|\psi_Z(t)\rangle}{\delta Z(s)}, \tag{3}$$

which is the main result of this Letter. Eq. (3) is a stochastic equation, since it depends on a stochastic process $Z(t)$ as specified below. It is also non-Markovian due to a memory term involving the dependence of the current state $|\psi_Z(t)\rangle$ on earlier noise $Z(s)$, describing the (delayed) back reaction of the environment on the system.

The dynamical properties and the temperature of the environment determine the memory kernel $\alpha(t,s) = \sum_i(\chi_i^2/2\ m_i\omega_i)[\coth(\hbar\omega_i/2k_{\rm B}T)\cos\omega_i(t-s) - {\rm i}\sin(t-s)]$ [16]. It can be regarded as the force correlation function $\alpha(t,s) = {\rm Tr}(\hat{F}(t)\hat{F}(s)\hat{\rho}_T)$, where $\hat{F}(t)$ is the Heisenberg operator of the force of the model (2) of the undisturbed environment. This memory kernel also determines the probability distribution of the stochastic processes $Z(t)$ entering the non-Markovian stochastic Schrödinger equation (3). They are coloured complex Gaussian processes with properties

$$M_Z[Z(t)] = 0, \quad M_Z[Z(t)Z(s)] = 0,$$
$$M_Z[Z(t)Z^*(s)] = \alpha^*(t,s), \tag{4}$$

designed in such a way as to mimic the effect of the quantum force $\hat{F}(t)$.

In the next two parts we will prove the central assertion of this Letter: The solutions $|\psi_Z(t)\rangle$ of the non-Markovian stochastic Schrödinger equation (3) reproduce the exact reduced density operator $\hat{\rho}_{\rm sys}(t)$ if one takes the ensemble average over the stochastic processes $Z(t)$ according to (1).

The first proof uses path integrals. The propagator $J(t;0)$ of the reduced density operator of the model (2) can be found in Feynman and Vernon's original original paper [16],

$$J(q,q',t;q_0,q_0',0) = \int \mathcal{D}[q] \int \mathcal{D}[q'] \times \exp\{\mathrm{i}S_{\rm sys}[q] - \mathrm{i}S_{\rm sys}[q']\}\mathcal{F}[q,q'], \tag{5}$$

with the influence functional $\mathcal{F}[q,q']$ encoding the effects of the environment on the system. It has been shown recently [15] that the propagator (5) allows for an exact stochastic decomposition using the coloured complex Gaussian stochastic processes [6] $Z(t)$ with properties (4),

$$J(q,q',t;q_0,q_0',0) = M_Z[G_Z(q,t;q_0,0)G_Z^*(q',t;q_0',0)]. \tag{6}$$

In Ref. [15], the stochastic propagators $G_Z(t;0)$ were given by their path integral representation

$$G_Z(q,t;q_0,0) = \int \mathcal{D}[q] \exp\left(\mathrm{i}S_{\rm sys}[q] + \mathrm{i}\int_0^t \mathrm{d}\tau\, q_\tau Z(\tau) - \int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\sigma\, q_\tau \alpha(\tau,\sigma) q_\sigma\right), \tag{7}$$

where we concluded that the states

$$|\psi_Z(t)\rangle = G_Z(t;0)|\psi_0\rangle \tag{8}$$

recover the reduced density operator $\hat{\rho}_{\rm sys}(t)$ according to (1).

Now we derive the Schrödinger equation corresponding to the stochastic propagator (7): first we take the time derivative on both sides of Eq. (8). The action $S_{\rm sys}[q]$ in the exponent of the path integral expression (7) leads to the system Hamilton operator $\hat{H}_{\rm sys}$ in the Schrödinger equation, the stochastic integral $\int \mathrm{d}\tau\, q_\tau Z(\tau)$ adds the stochastic driving term $\hat{q}Z(t)$ in Eq. (3). The only complication arises from the contribution of the double time integral in the exponent of the action in the path integral expression (7). Using functional differentiation, it is straightforward to show that it leads to the remaining memory term in Eq. (3). This completes the desired proof of the equivalence of the stochastic propagator (7) and the non-Markovian stochastic Schrödinger equation (3). With Eq. (6) we conclude that the solutions $|\psi_Z(t)\rangle$ of our equation (3) do in fact recover the reduced density operator of the model (2) by taking the ensemble average (1) over the processes $Z(t)$.

It is easy to show – see also Ref. [15] – that our equation (3) reduces to the well-known (linear) Markovian stochastic Schrödinger equation with complex Wiener noise in the limit of white noise.

An alternative derivation of the non-Markovian stochastic Schrödinger equation (3) uses a coherent state basis for the environmental degrees of freedom. This route to a stochastic description of non-Markovian open systems was taken in Ref. [14]. We use the non-normalised Bargmann coherent states $|a\rangle$ [17] which are analytical in a and satisfy the completeness relation $\int \mathrm{d}^2a\, \mathrm{e}^{-|a|^2}|a\rangle\langle a| = \mathbf{1}$, where $\mathrm{d}^2a \equiv \mathrm{d}\,\mathrm{Re}\,a\ \mathrm{d}\,\mathrm{Im}\,a/\pi$. Assume an expansion of the total state vector using a Bargmann basis $|a\rangle \equiv |a_1\rangle \otimes |a_2\rangle \otimes \ldots$ for the environmental degrees of freedom $a = (a_1, a_2, \ldots)$,

$$|\Psi_{\rm tot}(t)\rangle = \int \mathrm{d}^2a\, \mathrm{e}^{-|a|^2}|\psi_{a^*}(t)\rangle \otimes |a\rangle. \tag{9}$$

The states $|\psi_{a^*}(t)\rangle$ of the system correspond to a particular "configuration" $|a\rangle$ of the environment. Tracing over the environment, and using the representation (9) for the total state, we find that the reduced density operator takes the form

$$\hat{\rho}_{\rm sys}(t) = \int \mathrm{d}^2a\, \mathrm{e}^{-|a|^2}|\psi_{a^*}(t)\rangle\langle\psi_{a^*}(t)| = M_a[|\psi_{a^*}(t)\rangle\langle\psi_{a^*}(t)|]. \tag{10}$$

For the last expression we regard the coherent state variables a as classical stochastic variables with Gaus-

[6] In Ref. [15] we used $-\mathrm{i}Z(t)$ instead of $Z(t)$. Our theory, however, is invariant under phase changes of the stochastic processes $Z(t)$, which is why both choices are equivalent.

sian distribution $M_a[\ldots] = \int d^2a[\ldots] \exp\{-|a|^2\}$.

We now turn our attention to the time evolution of the total state using the coherent state representation (9). First, we rewrite the total Hamilton operator (2) in terms of the creation and annihilation operators $\hat{a}_i^\dagger$ and $\hat{a}_i$ of the environment oscillators, and also change to a Heisenberg representation of the environmental part of the total Hamiltonian. Then we find that the system part $|\psi_{a^*}(t)\rangle$ of the total state obeys the Schrödinger equation [17]

$$|\dot{\psi}_{a^*}(t)\rangle = -\mathrm{i}\hat{H}_{\mathrm{sys}}|\psi_{a^*}(t)\rangle + \mathrm{i}\hat{q}\sum_i \frac{\chi_i}{\sqrt{2\,m_i\omega_i}} \times \left(\mathrm{e}^{\mathrm{i}\omega_i t}a_i^* + \mathrm{e}^{-\mathrm{i}\omega_i t}\frac{\partial}{\partial a_i^*}\right)|\psi_{a^*}(t)\rangle. \tag{11}$$

We now restrict ourselves to the zero temperature case ($T = 0$), for which the initial condition $|\psi_{a^*}(0)\rangle = |\psi_0\rangle$ holds for all configurations a. In this coherent state approach, the non-zero temperature case is non-trivial and will be treated elsewhere [13].

In Eq. (10) the reduced density operator is expressed naturally as an ensemble average over the pure states $|\psi_{a^*}(t)\rangle$. Accordingly, the evolution equation (11) represents the stochastic Schrödinger equation for these states.

Remarkably, this construction is identical to the non-Markovian stochastic Schrödinger equation (3). To see the equivalence, we *define* stochastic processes

$$Z_a(t) \equiv \sum_i \frac{\chi_i}{\sqrt{2\,m_i\omega_i}} a_i^* \mathrm{e}^{\mathrm{i}\omega_i t}. \tag{12}$$

A simple calculation shows that these processes are – for zero temperature – realisations of the coloured complex Gaussian stochastic processes (4),

$$M_a[Z_a(t)] = 0, \quad M_a[Z_a(t)Z_a(s)] = 0,$$
$$M_a[Z_a(t)Z_a^*(s)] = \alpha_{T=0}^*(t,s). \tag{13}$$

Moreover, using the chain rule we find

$$\sum_i \frac{\chi_i}{\sqrt{2\,m_i\omega_i}} \mathrm{e}^{-\mathrm{i}\omega_i t}\frac{\partial}{\partial a_i^*} = \int \mathrm{d}s \sum_i \frac{\chi_i^2}{2\,m_i\omega_i} \mathrm{e}^{-\mathrm{i}\omega_i(t-s)} \frac{\delta}{\delta Z_a(s)} = \int \mathrm{d}s\, \alpha_{T=0}(t,s)\frac{\delta}{\delta Z_a(s)}. \tag{14}$$

Replacing the expressions (12) and (14) in the coherent state stochastic Schrödinger equation (11), we recover the non-Markovian stochastic Schrödinger equation (3), our basic result.

According to Eq. (9), the solutions $|\psi_Z(t)\rangle$ of the non-Markovian stochastic Schrödinger equation (3) represent the part of the total state which corresponds to a certain classical "configuration" a of the environment. The link between the process $Z(t)$ and the configuration a is given by Eq. (12). The interpretation of the classical "configuration" a of the environment (and thus of the stochastic processes $Z(t)$ too) can be given in the broader framework of hybrid densities [18].

We have presented the non-Markovian stochastic Schrödinger equation. It allows for the description of open quantum systems in terms of stochastic state vectors rather then density operators, without relying on the Markov approximation.

Two alternative derivations are given. First, we establish the connection to the path integral approach to open systems as initiated by Feynman and Vernon. The non-Markovian stochastic Schrödinger equation reflects a stochastic decomposition of the propagator for the reduced density operator into stochastic propagators for state vectors. Secondly, we establish the connection to a coherent state description of the environment, allowing a microscopic interpretation of the stochastic states $|\psi_Z(t)\rangle$.

Our theory is exact and the model (or some straightforward generalisation of it) appears in many areas of physics (electron–phonon interaction, the spin–boson model, the whole of quantum optics, relativistic field theories as relevant as QED). These problems can now be phrased in the language of stochastic evolution equations in Hilbert space, without approximation. The success of quantum trajectory methods in the Markovian case suggests that our result also represents a promising step towards an effective numerical algorithm for non-Markovian reduced dynamics. As a fundamental concept, stochastic pure state representations no longer depend on the Markov assumption. Starting from our exact result, approximations like perturbation expansions are possible, further simplifying the description of non-Markovian reduced dynamics.

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