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1996 J. Phys. A: Math. Gen. 29 7837

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# Hilbert space path integral representation for the reduced dynamics of matter in thermal radiation fields

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Received 20 March 1996, in final form 8 July 1996

**Abstract.** A Hilbert space path integral for the dissipative dynamics of matter in thermal radiation fields is derived from the Hamiltonian of quantum electrodynamics. This path integral represents the conditional transition probability of a stochastic Markov process as a sum over sample trajectories in Hilbert space. The realizations of the process are piecewise deterministic paths broken by instantaneous quantum jumps. It is shown that the operators which define the possible quantum jumps form a continuous family parametrized by the polarization vector of the emitted or absorbed photons. The stochastic process is shown to be representation-independent and to be invariant with respect to space rotations. The precise physical interpretation of the stochastic process is given. In particular, the expansion of the density matrix in terms of quantum jumps is derived for finite temperatures from the Hilbert space path integral.

## 1. Introduction

In many applications of quantum electrodynamics one is not interested in solving the basic equations in its full generality. Usually one would like to restrict the mathematical description to the evolution of a few number of degrees of freedom and to account for the remaining degrees of freedom by introducing dissipation and noise into the equations of motion [1]. In this method the relevant degrees of freedom constitute an open or reduced system that is coupled to an environment. For example, in quantum optics one eliminates either the matter degrees of freedom to describe the behaviour of certain radiation modes, or the degrees of freedom of the quantized radiation field in order to describe the behaviour of atoms or molecules in external driving fields. Whereas the conventional theory uses density matrix equations, it has recently been shown that it is possible to use stochastic processes for pure states to model the behaviour of reduced quantum systems. Phenomenological models based on piecewise deterministic jump processes [2–5] as well as on diffusion processes [6–10] have been suggested. It has been demonstrated that this stochastic approach yields both important conceptual insights into the dynamics, and efficient numerical simulation methods [11].

The starting point of the stochastic approach to the reduced system dynamics is the description of statistical ensembles of quantum systems in terms of probability distributions on its space of states, i.e. the underlying projective Hilbert space [12]. We write  $P[\psi, t] D\psi D\psi^*$  for the probability to find at time  $t$  the system in a state described by some wavefunction within the volume element  $D\psi D\psi^*$  around  $\psi$ . The volume element of the Hilbert space is defined by

$$D\psi D\psi^* \equiv \prod_x \frac{i}{2} d\psi(x) d\psi^*(x) \quad (1)$$

where the product is extended over a complete set of quantum numbers  $x$ . More precisely, the probability density  $P[\psi, t]$  is a distribution on the projective Hilbert space since we require that it does not depend on the phase of the wavefunction and that it vanishes outside the unit sphere in Hilbert space. The normalization of  $P[\psi, t]$  reads

$$\int D\psi D\psi^* P[\psi, t] = 1 \quad (2)$$

where the integration is extended over the whole Hilbert space. A precise mathematical formulation of probability measures on Hilbert space is given in [13, 14] and a geometrical formulation of stochastic processes in Hilbert space can be found in [15]. For example, the simplest probability distribution that describes a pure state  $\varphi$  and that fulfills these requirements takes the form (suppressing the time argument)

$$P[\psi] = \int_0^{2\pi} \frac{d\chi}{2\pi} \delta[e^{i\chi}\varphi - \psi] \quad (3)$$

where  $\delta$  denotes the Dirac measure on the Hilbert space

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

and  $\operatorname{Re}$  and  $\operatorname{Im}$  denote the real and imaginary parts, respectively. In the formulation of quantum statistical ensembles in terms of probability distributions the conventional density matrix appears as the covariance matrix of the stochastic wavefunction

$$\rho_t(x, x') \equiv \int D\psi D\psi^* \psi(x) \psi^*(x') P[\psi, t]. \quad (5)$$

For a closed quantum system with some Hamiltonian  $H$  we demand that the time evolution of the wavefunction is governed by the Schrödinger equation  $i\hbar \dot{\psi} = H\psi$ . Given some initial probability distribution  $P_0[\psi]$  the time dependence of the probability distribution is then obtained from the Liouville equation

$$P[\psi, t] = P_0[e^{iHt/\hbar}\psi] \quad (6)$$

where the unitary invariance of the measure (1) has been used. On the basis of the Liouville equation the time-dependent wavefunction  $\psi(t)$  becomes a deterministic Markov process whose realizations are solutions of the deterministic Schrödinger equation, the initial conditions being randomly distributed according to the initial distribution  $P_0[\psi]$ .

Of course, the true interest in the stochastic formulation lies in its generalization to open quantum systems that are coupled to an environment. A situation of particular interest arises when the quantum system of interest is coupled to a thermal reservoir with a large number of degrees of freedom. Invoking the Markov approximation it has been shown in [16, 17] that the dynamics of the wavefunction of the reduced system that is obtained by eliminating the degrees of freedom of the reservoir represents a piecewise deterministic stochastic jump process in the state space of the open system. The starting point of the derivation of this stochastic process is the deterministic Markov process defined by (6), where  $H$  is the Hamiltonian for the total system composed of the open system and the reservoir. The derivation in [16, 17] thus shows (i) that it is indeed possible to describe the full quantum dynamics of open systems by means of a stochastic process in Hilbert space, and (ii) that the stochastic evolution results from the unitary dynamics of the total system.

The present paper is structured as follows. It is shown in section 2 that the above derivation can be generalized to include the most general case of a bound system (an atom or molecule, for example) that interacts with a quantized radiation field in thermal equilibrium through the interaction Hamiltonian of quantum electrodynamics. The result is

a unique stochastic representation of the time evolution of the system wavefunction in terms of a piecewise deterministic Markovian jump process [18] in the state space of the reduced system. It turns out that, in contrast to the processes formulated in [2–4], the possible quantum jumps are induced by a *continuous* family of jump operators.

Furthermore, it will be shown that the stochastic process can be represented as a Hilbert space path integral. The latter gives a decomposition of the conditional transition probability in terms of the contributions from all sample paths in Hilbert space that connect the given endpoints. One finds that the Hilbert space path integral yields an expansion of the conditional transition probability of the stochastic process with respect to the number of quantum jumps.

It will be demonstrated in section 3 that the stochastic formulation of the dynamics obtained represents a fully consistent theory which admits a clear physical interpretation. In particular, it is shown that it is not necessary to apply the continuous measurement theory to supply evidence for the use of stochastic processes in the description of open quantum systems [4, 5]. Furthermore, it is proven that the stochastic process is unitarily covariant. This implies that the process does not depend on the specific representation of the state space of the open system. In addition, the stochastic process is shown to be rotationally invariant if the radiation field is isotropic. This means that realizations of the process which arise from each other by a space rotation occur with equal probability. We discuss the relation of the theory presented here to those formulations that are based on the unravelling of the quantum master equation [5] by means of various measurement schemes. The difference between these approaches is illustrated by a numerical simulation. Finally, we establish the relation of our approach to the Srinivas and Davies theory of photocounting. To this end we derive from the Hilbert space path integral representation of the propagator an expansion of the density operator in terms of the number of quantum jumps for a reduced system at finite temperature.

## 2. Hilbert space path integral for the reduced system dynamics

In this section we consider a bound quantum system, e.g. an atom or molecule, which interacts with a quantized radiation field in thermal equilibrium at temperature  $T$ . The bound system is the open or *reduced* system we are interested in, whereas the radiation field represents a thermal reservoir with an infinite number of degrees of freedom. It will be shown that on eliminating the reservoir degrees of freedom in the Markov approximation, the dynamics of the states of the reduced system is described by a stochastic process in the corresponding projective Hilbert space of the open system. The propagator of the stochastic process is then represented as a Hilbert space path integral, that is, as a sum over all sample paths of the process.

### 2.1. Microscopic theory

The atom or molecule is described by some Hamiltonian  $H_m$  that interacts with a quantized radiation field the free Hamiltonian of which may be represented as

$$H_{rad} = \sum_{\mathbf{k}, \lambda} \hbar \omega_{\mathbf{k}} (b_{\mathbf{k}\lambda}^\dagger b_{\mathbf{k}\lambda} + \frac{1}{2}). \quad (7)$$

For simplicity we have decomposed the radiation field into Fourier modes of a periodic box of volume  $V$ . These modes are labelled by the wavevector  $\mathbf{k}$  and two corresponding

polarization vectors  $\boldsymbol{\lambda}$  with  $\mathbf{k} \cdot \boldsymbol{\lambda} = 0$ . The dispersion is  $\omega_{\mathbf{k}} = c|\mathbf{k}| = ck$ , where  $c$  is the speed of light. The field operators obey the commutation relation

$$[b_{\mathbf{k}\lambda}, b_{\mathbf{k}'\lambda'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\lambda\lambda'}. \quad (8)$$

The energy eigenstates  $\varphi_\alpha$  of  $H_{rad}$  are orthonormalized Fock states

$$\varphi_\alpha = |\{N_{\mathbf{k}\lambda}^\alpha\}\rangle = |\dots, N_{\mathbf{k}\lambda}^\alpha, \dots\rangle \quad (9)$$

where  $N_{\mathbf{k}\lambda}^\alpha$  denotes the occupation number of the mode  $(\mathbf{k}, \boldsymbol{\lambda})$ . The corresponding eigenenergies are given by

$$\varepsilon_\alpha = \sum_{\mathbf{k}, \boldsymbol{\lambda}} \hbar\omega_{\mathbf{k}}(N_{\mathbf{k}\lambda}^\alpha + \frac{1}{2}). \quad (10)$$

The interaction Hamiltonian may be written

$$H_I = \frac{-e}{c} \int d^3x \mathbf{j}(\mathbf{x}) \mathbf{A}(\mathbf{x}) \quad (11)$$

where  $\mathbf{A}$  is the vector potential,  $\mathbf{j}$  the electron current, and  $e$  the electron charge. In the dipole approximation this interaction may be replaced by [19]

$$H_I = -e\mathbf{D} \cdot \mathbf{E} \quad (12)$$

where  $\mathbf{E}$  is the electric field operator in the Schrödinger picture:

$$\mathbf{E} = i \sum_{\mathbf{k}, \boldsymbol{\lambda}} \sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}} (b_{\mathbf{k}\lambda}\boldsymbol{\lambda} - b_{\mathbf{k}\lambda}^\dagger\boldsymbol{\lambda}^*) \quad (13)$$

and  $\mathbf{D}$  denotes the dipole operator of the system under consideration. Finally, the total Hamiltonian governing the coupled system of matter and radiation degrees of freedom is given by

$$H = H_m + H_{rad} + H_I. \quad (14)$$

For the derivation of the stochastic process describing the matter degrees of freedom to be given in the next subsection we need to decompose the interaction Hamiltonian  $H_I$  into eigenoperators of  $H_m$ . The latter are given by

$$\mathbf{A}^\dagger(\omega) = \mathbf{A}(-\omega) \equiv \sum_{E-E'=\hbar\omega} \Pi(E)\mathbf{D}\Pi(E'). \quad (15)$$

Here,  $\Pi(E)$  denotes the projector onto the eigenspace of  $H_m$  with energy  $E$  and the sum is extended over those energies  $E$  and  $E'$  with a fixed energy difference of  $\hbar\omega$ . Obviously we have

$$[H_m, \mathbf{A}^\dagger(\omega)] = \hbar\omega\mathbf{A}^\dagger(\omega) \quad [H_m, \mathbf{A}(\omega)] = -\hbar\omega\mathbf{A}(\omega). \quad (16)$$

The decomposition of  $H_I$  into these eigenoperators then reads

$$H_I = -e \sum_{\omega} \mathbf{A}^\dagger(\omega) \cdot \mathbf{E} = -e \sum_{\omega} \mathbf{A}(\omega) \cdot \mathbf{E}. \quad (17)$$

## 2.2. Stochastic dynamics of the matter degrees of freedom

The radiation field is assumed to be in thermal equilibrium at temperature  $T$ . The corresponding stationary probability distribution  $P_b[\psi_b]$  on the Fock space of the bath may therefore be written as [17]

$$P_b[\psi_b] = \sum_{\alpha} p_{\alpha} \int_0^{2\pi} \frac{d\chi}{2\pi} \delta_b[e^{i\chi} \varphi_{\alpha} - \psi_b] \quad (18)$$

where  $\delta_b$  denotes the Dirac measure on the Hilbert space of the bath and  $p_{\alpha} = \exp[-\varepsilon_{\alpha}/k_B T]/Z$ . ( $Z$  is the partition function and  $k_B$  the Boltzmann constant.)

The most important quantity that is to be derived in order to construct a stochastic process for the reduced system dynamics is the conditional transition probability in the interaction picture  $\tilde{T}[\psi, t|\tilde{\psi}, t_0]$  (also called propagator). This quantity gives the probability density to find at time  $t \equiv t_0 + \tau$  ( $\tau \geq 0$ ) the reduced system in the state  $\psi$  under the condition that at time  $t_0$  the state  $\tilde{\psi}$  has been given. Starting from the Liouville formulation of the total system and assuming the reduced system and the bath to be statistically independent at time  $t_0$  one obtains the following exact expression [17]:

$$\tilde{T}[\psi, t|\tilde{\psi}, t_0] = \int_0^{2\pi} \frac{d\chi}{2\pi} \sum_{\alpha, \beta} w_{\alpha\beta} p_{\beta} \delta[e^{i\chi} w_{\alpha\beta}^{-1/2} L_{\alpha\beta} \tilde{\psi} - \psi] \quad (19)$$

where

$$L_{\alpha\beta} \tilde{\psi} \equiv \langle \varphi_{\alpha} | U(t, t_0) \tilde{\psi} \varphi_{\beta} \rangle_b \quad (20)$$

and

$$w_{\alpha\beta} \equiv \|L_{\alpha\beta} \tilde{\psi}\|^2. \quad (21)$$

In equation (20)  $U(t, t_0)$  denotes the quantum mechanical time evolution operator of the total system (atom + radiation field) in the interaction picture. The index  $b$  of the angular brackets indicates that the scalar product refers only to the bath variables. In equation (21)  $\|\dots\|$  is the norm in the state space of the atomic or molecular system. Finally,  $\delta$  is the Dirac measure on this state space.

The next step consists of the derivation of the short-time behaviour of the propagator. To this end, we decompose the propagator as

$$\tilde{T}[\psi, t|\tilde{\psi}, t_0] = T_d[\psi, t|\tilde{\psi}, t_0] + T_n[\psi, t|\tilde{\psi}, t_0] \quad (22)$$

where

$$T_d[\psi, t|\tilde{\psi}, t_0] = \int_0^{2\pi} \frac{d\chi}{2\pi} \sum_{\alpha} w_{\alpha\alpha} p_{\alpha} \delta[e^{i\chi} w_{\alpha\alpha}^{-1/2} L_{\alpha\alpha} \tilde{\psi} - \psi] \quad (23)$$

$$T_n[\psi, t|\tilde{\psi}, t_0] = \int_0^{2\pi} \frac{d\chi}{2\pi} \sum_{\alpha \neq \beta} w_{\alpha\beta} p_{\beta} \delta[e^{i\chi} w_{\alpha\beta}^{-1/2} L_{\alpha\beta} \tilde{\psi} - \psi]. \quad (24)$$

We shall analyse the behaviour of the propagator  $\tilde{T}[\psi, t_0 + \tau|\tilde{\psi}, t_0]$  for small  $\tau$  in the so-called quantum optical case. In order to explain this in more detail we introduce three different time scales. The first one is the correlation time  $\tau_b$  of the quantized modes of the radiation field in thermal equilibrium, i.e.  $\tau_b$  is the time scale of the decay of the bath correlation functions. Second, we have the relaxation time  $\tau_m$  of the system which is the time scale of the approach of the open system to the thermal equilibrium state. The third time scale  $\tau_f$  is set by the inverse atomic or molecular frequencies; thus  $\tau_f$  is of the order of the period of the bound motion of the unperturbed atom or molecule. For the thermal

radiation field  $\tau_b \approx \hbar/kT$  which is of the order of  $10^{-12}/T$  s, where the temperature is measured in Kelvin [1]. The time scale  $\tau_m$  is of the order of the natural lifetime, that is,  $10^{-8}$  s or even much larger, whereas  $\tau_f$  is of the order of  $10^{-14}$  s [20]. Thus, even for low temperatures we can choose a time  $\tau$  such that

$$\tau \gg \tau_b \quad \tau \ll \tau_m \quad \tau \gg \tau_f. \quad (25)$$

The first condition justifies performing the Markov approximation for the propagator, which enables one to eliminate the bath degrees of freedom. Once the bath variables have been eliminated, the second and the third condition yield a short-time behaviour of the propagator that leads to a differential Chapman–Kolmogorov equation which represents the stochastic time evolution of the reduced system. On account of the second condition in (25) we may employ second-order perturbation theory and the third condition enables us to use the rotating-wave approximation when dealing with the bath correlation functions in the interaction representation.

In second-order perturbation theory we find

$$L_{\alpha\beta} = \delta_{\alpha\beta} + \sum_{i,\omega} f_{\alpha\beta}^i(\omega) A_i^\dagger(\omega) + \sum_{i,j,\omega,\omega'} g_{\alpha\beta}^{ij}(\omega, \omega') A_i(\omega) A_j^\dagger(\omega') \quad (26)$$

and

$$\begin{aligned} w_{\alpha\beta} = & \delta_{\alpha\beta} - \delta_{\alpha\beta} \sum_{\alpha'} \sum_{i,j,\omega,\omega'} [f_{\alpha'\alpha}^i(\omega)]^* f_{\alpha'\alpha}^j(\omega') \langle A_i(\omega) A_j^\dagger(\omega') \rangle \\ & + \sum_{i,j,\omega,\omega'} [f_{\alpha\beta}^i(\omega)]^* f_{\alpha\beta}^j(\omega') \langle A_i(\omega) A_j^\dagger(\omega') \rangle \end{aligned} \quad (27)$$

where we have defined

$$f_{\alpha\beta}^i(\omega) \equiv \frac{ie}{\hbar} \int_0^\tau ds e^{i\omega s} \langle \varphi_\alpha | E_i(s) | \varphi_\beta \rangle_b \quad (28)$$

$$g_{\alpha\beta}^{ij}(\omega, \omega') \equiv -\frac{e^2}{\hbar^2} \int_0^\tau ds \int_0^{\tau-s} ds' e^{-i\omega(s+s') + i\omega's} \langle \varphi_\alpha | E_i(s+s') E_j(s) | \varphi_\beta \rangle_b \quad (29)$$

and  $E_i(s) = \exp(iH_{rad}s/\hbar) E_i \exp(-iH_{rad}s/\hbar)$  denotes the electric field operator in the interaction picture. For notational simplicity we have introduced

$$\langle B \rangle \equiv \langle \tilde{\psi} | B | \tilde{\psi} \rangle \quad (30)$$

for any system operator  $B$  and the angular brackets denote the scalar product on the Hilbert space of the open system. On using the approximations explained above one obtains for the Fourier transform of the correlation tensor

$$\begin{aligned} \gamma_{ij}(\omega) & \equiv \frac{e^2}{\hbar^2} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \int D\psi_b D\psi_b^* \langle \psi_b | E_i(t) E_j | \psi_b \rangle_b P_b[\psi_b] \\ & = \begin{cases} \gamma(\omega) \bar{N}(\omega) \delta_{ij} & \omega > 0 \\ \gamma(\omega) (\bar{N}(\omega) + 1) \delta_{ij} & \omega < 0 \end{cases} \end{aligned} \quad (31)$$

where

$$\gamma(\omega) = \frac{4e^2|\omega|^3}{3\hbar c^3} \quad (32)$$

and  $\bar{N}(\omega)$  denotes the average number of photons of frequency  $|\omega|$ :

$$\bar{N}(\omega) = (e^{\hbar|\omega|/kT} - 1)^{-1}. \quad (33)$$

Invoking now the Markov approximation for the stochastic process in the Hilbert space of the reduced system and the rotating-wave approximation, one obtains by following the lines given in [17] for the short-time behaviour of  $T_d$

$$T_d \approx \left\{ 1 - \tau \sum_{\omega>0} \gamma(\omega) \bar{N}(\omega) \langle C_2(\omega) \rangle + \gamma(\omega) (\bar{N}(\omega) + 1) \langle C_1(\omega) \rangle \right\} \\ \times \delta \left[ \left\{ \mathbf{1} + \frac{\tau}{2} \sum_{\omega>0} \gamma(\omega) \bar{N}(\omega) (\langle C_2(\omega) \rangle - C_2(\omega)) \right. \right. \\ \left. \left. + \gamma(\omega) (\bar{N}(\omega) + 1) (\langle C_1(\omega) \rangle - C_1(\omega)) \right\} \tilde{\psi} - \psi \right] \quad (34)$$

where we have introduced

$$C_1(\omega) \equiv \mathbf{A}^\dagger(\omega) \mathbf{A}(\omega) \quad C_2(\omega) \equiv \mathbf{A}(\omega) \mathbf{A}^\dagger(\omega). \quad (35)$$

The second part of the propagator can be written in the form

$$T_n = \sum_{\alpha\beta} \left( \sum_{ij} \sum_{\omega\omega'} f_{\alpha\beta}^{i*}(\omega) f_{\alpha\beta}^j(\omega') \langle \tilde{\psi} | A_i(\omega) A_j^\dagger(\omega') | \tilde{\psi} \rangle \right) \\ \times p_\beta \delta \left[ \frac{\sum_i \sum_\omega f_{\alpha\beta}^i(\omega) A_i^\dagger(\omega) \tilde{\psi}}{\| \sum_i \sum_\omega f_{\alpha\beta}^i(\omega) A_i^\dagger(\omega) \tilde{\psi} \|} - \psi \right]. \quad (36)$$

Equation (28) yields

$$f_{\alpha\beta}^i(\omega) = -e \frac{e^{-i(\varepsilon_\beta - \varepsilon_\alpha - \hbar\omega)\tau/\hbar} - 1}{\varepsilon_\beta - \varepsilon_\alpha - \hbar\omega} \langle \varphi_\alpha | E_i | \varphi_\beta \rangle_b. \quad (37)$$

In accordance with the third condition in (25) we now assume that for a given pair  $(\alpha, \beta)$  of quantum numbers of the bath there exists precisely one  $\omega$  such that

$$\varepsilon_\beta - \varepsilon_\alpha \in I_\omega \equiv [\hbar\omega - \Delta, \hbar\omega + \Delta] \quad (38)$$

where  $\Delta \sim \hbar/\tau$  is the energy uncertainty associated with the interaction time  $\tau$ . The matrix element of the electric field operator in (38) is different from zero only if the Fock states  $\varphi_\alpha \equiv |\{N_{k\lambda}^\alpha\}\rangle$  and  $\varphi_\beta \equiv |\{N_{k\lambda}^\beta\}\rangle$  differ by  $\pm 1$  in the occupation number of precisely one mode. Thus, the only non-vanishing matrix elements are given by

$$\langle \varphi_\alpha | E_i | \varphi_\beta \rangle_b = i \sqrt{\frac{2\pi\hbar\omega_k}{V}} \sqrt{N_{k\lambda}^\beta} \lambda_i$$

for  $\varphi_\alpha = |\dots, N_{k\lambda}^\beta - 1, \dots\rangle$  and  $\varphi_\beta = |\dots, N_{k\lambda}^\beta, \dots\rangle$  and by

$$\langle \varphi_\alpha | E_i | \varphi_\beta \rangle_b = i \sqrt{\frac{2\pi\hbar\omega_k}{V}} \sqrt{N_{k\lambda}^\beta + 1} \lambda_i^*$$

for  $\varphi_\alpha = |\dots, N_{k\lambda}^\beta + 1, \dots\rangle$  and  $\varphi_\beta = |\dots, N_{k\lambda}^\beta, \dots\rangle$ .

Thus we obtain for  $\varepsilon_\beta - \varepsilon_\alpha \in I_\omega$  and  $\omega > 0$

$$\frac{\sum_{i,\omega} f_{\alpha\beta}^i(\omega) A_i^\dagger(\omega) \tilde{\psi}}{\| \sum_{i,\omega} f_{\alpha\beta}^i(\omega) A_i^\dagger(\omega) \tilde{\psi} \|} = \frac{\boldsymbol{\lambda} \cdot \mathbf{A}^\dagger(\omega) \tilde{\psi}}{\| \boldsymbol{\lambda} \cdot \mathbf{A}^\dagger(\omega) \tilde{\psi} \|}$$

and for  $\varepsilon_\beta - \varepsilon_\alpha \in I_\omega$  and  $\omega < 0$

$$\frac{\sum_{i,\omega} f_{\alpha\beta}^i(\omega) A_i^\dagger(\omega) \tilde{\psi}}{\| \sum_{i,\omega} f_{\alpha\beta}^i(\omega) A_i^\dagger(\omega) \tilde{\psi} \|} = \frac{\boldsymbol{\lambda}^* \cdot \mathbf{A}(-\omega) \tilde{\psi}}{\| \boldsymbol{\lambda}^* \cdot \mathbf{A}(-\omega) \tilde{\psi} \|}$$

where the polarization vector  $\lambda$  refers to that mode in which the occupation numbers differ by  $\pm 1$ . The important point to note is that the quotients on the right-hand sides in the above equations only depend on the energy differences and the polarization vector of the corresponding mode. This fact leads to the following expression for the non-diagonal part of the conditional transition probability:

$$T_n \approx \tau \sum_{\omega > 0} \gamma(\omega) \bar{N}(\omega) \frac{3}{8\pi} \int d\Omega_k \sum_{\lambda} \langle \lambda^* \cdot \mathbf{A}(\omega) \lambda \cdot \mathbf{A}^\dagger(\omega) \rangle \delta \left[ \frac{\lambda \cdot \mathbf{A}^\dagger(\omega) \tilde{\psi}}{\|\lambda \cdot \mathbf{A}^\dagger(\omega) \tilde{\psi}\|} - \psi \right] \\ + \tau \sum_{\omega < 0} \gamma(\omega) (\bar{N}(\omega) + 1) \frac{3}{8\pi} \int d\Omega_k \sum_{\lambda} \langle \lambda \cdot \mathbf{A}(\omega) \lambda^* \cdot \mathbf{A}^\dagger(\omega) \rangle \\ \times \delta \left[ \frac{\lambda^* \cdot \mathbf{A}^\dagger(-\omega) \tilde{\psi}}{\|\lambda^* \cdot \mathbf{A}^\dagger(-\omega) \tilde{\psi}\|} - \psi \right].$$

Here,  $d\Omega_k$  denotes the element of the solid angle around the direction of the wavevector  $\mathbf{k}$  and  $\sum_{\lambda}$  means the sum over the corresponding two independent polarizations. For the sake of a compact notation we introduce the abbreviation

$$\int d\omega(\lambda) f(\lambda) \equiv \frac{3}{8\pi} \int d\Omega_k \sum_{\lambda} f(\lambda). \quad (39)$$

Clearly the measure  $d\omega(\lambda)$  is normalized such that

$$\int d\omega(\lambda) \lambda_i^* \lambda_j = \delta_{ij}. \quad (40)$$

Moreover, for integrands  $f(\lambda)$  that have the property of phase invariance, i.e.  $f(e^{i\chi} \lambda) = f(\lambda)$ , the measure  $d\omega(\lambda)$  is rotationally invariant, that is, for any space rotation  $R$  we have

$$\int d\omega(\lambda) f(R\lambda) = \int d\omega(\lambda) f(\lambda). \quad (41)$$

We shift the summation index in the second sum in equation (36) from  $\omega$  to  $-\omega$ . This finally yields

$$T_n \approx \tau \sum_{\omega > 0} \gamma(\omega) \bar{N}(\omega) \int d\omega(\lambda) \|\lambda \cdot \mathbf{A}^\dagger(\omega) \tilde{\psi}\|^2 \delta \left[ \frac{\lambda \cdot \mathbf{A}^\dagger(\omega) \tilde{\psi}}{\|\lambda \cdot \mathbf{A}^\dagger(\omega) \tilde{\psi}\|} - \psi \right] \\ + \tau \sum_{\omega > 0} \gamma(\omega) (\bar{N}(\omega) + 1) \int d\omega(\lambda) \|\lambda^* \cdot \mathbf{A}(\omega) \tilde{\psi}\|^2 \delta \left[ \frac{\lambda^* \cdot \mathbf{A}(\omega) \tilde{\psi}}{\|\lambda^* \cdot \mathbf{A}(\omega) \tilde{\psi}\|} - \psi \right]. \quad (42)$$

Equations (34) and (42) determine completely the short-time behaviour of the conditional transition probability  $\tilde{T}$ . This short-time behaviour immediately yields the differential Chapman–Kolmogorov equation for time-dependent Schrödinger picture probability distribution  $P[\psi, t]$  of the reduced system. Proceeding in precisely the same way as has been explained in [17] we obtain the Liouville master equation

$$\frac{\partial}{\partial t} P[\psi, t] = \frac{i}{\hbar} \int dx \left\{ \frac{\delta}{\delta\psi(x)} G(\psi)(x) - \frac{\delta}{\delta\psi^*(x)} G(\psi)^*(x) \right\} P[\psi, t] \\ + \int D\tilde{\psi} D\tilde{\psi}^* \{ W[\psi|\tilde{\psi}] P[\tilde{\psi}, t] - W[\tilde{\psi}|\psi] P[\psi, t] \}. \quad (43)$$

Here, we have introduced the nonlinear operator  $G(\psi)$ ,

$$G(\psi) \equiv \hat{H}\psi + \frac{i\hbar}{2} \sum_{\omega>0} (\gamma(\omega)\bar{N}(\omega)\langle\psi|\mathbf{A}(\omega) \cdot \mathbf{A}^\dagger(\omega)|\psi\rangle)\psi + \frac{i\hbar}{2} \sum_{\omega>0} (\gamma(\omega)(\bar{N}(\omega) + 1)\langle\psi|\mathbf{A}^\dagger(\omega) \cdot \mathbf{A}(\omega)|\psi\rangle)\psi \quad (44)$$

the linear, non-Hermitian operator  $\hat{H}$ ,

$$\hat{H} \equiv H_m - \frac{i\hbar}{2} \sum_{\omega>0} (\gamma(\omega)\bar{N}(\omega)\mathbf{A}(\omega) \cdot \mathbf{A}^\dagger(\omega) + \gamma(\omega)(\bar{N}(\omega) + 1)\mathbf{A}^\dagger(\omega) \cdot \mathbf{A}(\omega)) \quad (45)$$

and the rate for a transition from  $\tilde{\psi}$  to  $\psi$  is given by

$$W[\psi|\tilde{\psi}] \equiv \sum_{\omega>0} \left\{ \gamma(\omega)\bar{N}(\omega) \int d\omega(\boldsymbol{\lambda}) \|\boldsymbol{\lambda} \cdot \mathbf{A}^\dagger(\omega)\tilde{\psi}\|^2 \delta \left[ \frac{\boldsymbol{\lambda} \cdot \mathbf{A}^\dagger(\omega)\tilde{\psi}}{\|\boldsymbol{\lambda} \cdot \mathbf{A}^\dagger(\omega)\tilde{\psi}\|} - \psi \right] \right\} + \sum_{\omega>0} \left\{ \gamma(\omega)(\bar{N}(\omega) + 1) \int d\omega(\boldsymbol{\lambda}) \|\boldsymbol{\lambda}^* \cdot \mathbf{A}(\omega)\tilde{\psi}\|^2 \delta \left[ \frac{\boldsymbol{\lambda}^* \cdot \mathbf{A}(\omega)\tilde{\psi}}{\|\boldsymbol{\lambda}^* \cdot \mathbf{A}(\omega)\tilde{\psi}\|} - \psi \right] \right\}. \quad (46)$$

Equation (43) together with these definitions defines a unique stochastic process  $\psi(t)$  in the projective Hilbert space representing the stochastic evolution of the wavefunction of the reduced (open) atomic or molecular system. As we shall explain in more detail in the next section, the realizations of this process are piecewise deterministic paths in Hilbert space, broken by instantaneous changes of the wavefunction, the so-called quantum jumps.

### 2.3. Representation as Hilbert space path integral

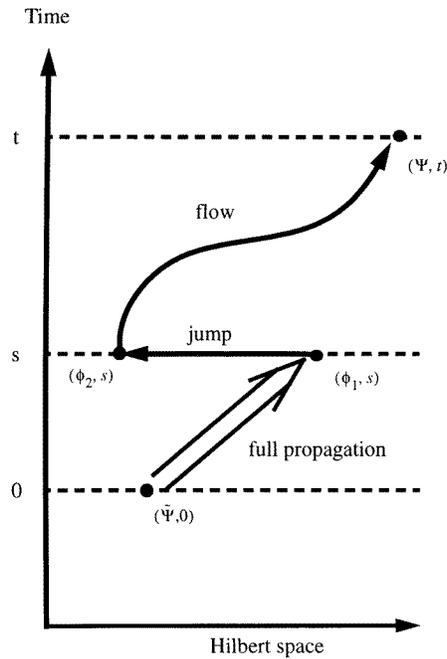
It should be clear that the realizations, or *sample paths*, of the stochastic process defined by the Liouville master equation are paths in the Hilbert space of the open system. It is therefore possible to give a Hilbert space path integral representation of the process. This representation is obtained from the Kolmogorov forward equation [21] for the conditional transition probability in the Schrödinger picture

$$T[\psi, t|\tilde{\psi}, 0] = (1 - F[\tilde{\psi}, t])\delta[\psi - g_t(\tilde{\psi})] + \int_0^t ds \int D\phi_1 D\phi_1^* \int D\phi_2 D\phi_2^* (1 - F[\phi_2, t - s])\delta[\psi - g_{t-s}(\phi_2)] \times W[\phi_2|\phi_1]T[\phi_1, s|\tilde{\psi}, 0]. \quad (47)$$

The above equation is an integral representation of the conditional transition probability of the stochastic process defined by the Liouville master equation (43). In fact, as is easily checked, the solution of (47) is the solution of the Liouville master equation corresponding to the initial condition  $T[\psi, 0|\tilde{\psi}, 0] = \delta[\psi - \tilde{\psi}]$ .

Equation (47) admits a clear physical interpretation which is also the basis for the development of a stochastic simulation algorithm: the first term on the right-hand side of (47) is the contribution to  $T[\psi, t|\tilde{\psi}, 0]$  from those trajectories that start at the Hilbert spacetime point  $(\tilde{\psi}, 0)$  and reach  $(\psi, t)$  without any quantum jump. Clearly, this contribution is given by the delta functional that describes the deterministic part of the time evolution times the probability that no jump occurs in the time interval  $[0, t]$ . Thus we see that

$$g_t(\psi) = \frac{e^{-i\hat{H}t/\hbar}\psi}{\|e^{-i\hat{H}t/\hbar}\psi\|} \quad (48)$$



**Figure 1.** Graphical representation of the Kolmogorov forward equation (47) for the conditional transition probability of the stochastic process. The total probability for reaching the Hilbert spacetime point  $(\psi, t)$  is given by integrating over all intermediate states  $\phi_1$  and  $\phi_2$  and over all intermediate times  $s$ .

is the flow corresponding to the nonlinear Schrödinger-type equation  $\dot{\psi} = -iG(\psi)/\hbar$  and

$$F[\psi, t] = 1 - \|e^{-i\hat{H}t/\hbar}\psi\|^2 \quad (49)$$

gives the probability that a jump occurs during the time interval  $[0, t]$  provided the state  $\psi$  is given at time 0. The second term on the right-hand side of (47) is the contribution to  $T[\psi, t|\tilde{\psi}, 0]$  from those trajectories that are interrupted by at least one quantum jump. The integration time  $s$  denotes the instant of the last jump. The probability of a particular realization of this type is given by the (conditional) probability  $T[\phi_1, s|\tilde{\psi}, 0]$  of being in some intermediate state  $\phi_1$  at time  $s$ , times the probability  $W[\phi_2|\phi_1] ds$  for a jump from  $\phi_1$  to  $\phi_2$  in the time interval  $[s, s + ds]$ , times the probability that no further jump occurs in the time interval from  $s$  to  $t$ . The contribution from all those paths is given by the sum over all possible jump times  $s$  and over all intermediate states  $\phi_1$  and  $\phi_2$ . The content of equation (47) is represented graphically in figure 1.

A typical realization of the stochastic process thus consists of smooth deterministic parts according to the flow given by (48). These continuous parts are broken by instantaneous changes of the wavefunction (quantum jumps)

$$\tilde{\psi} \longrightarrow \psi = \frac{\lambda \cdot \mathbf{A}^\dagger(\omega)\tilde{\psi}}{\|\lambda \cdot \mathbf{A}^\dagger(\omega)\tilde{\psi}\|} \quad (50)$$

or

$$\tilde{\psi} \longrightarrow \psi = \frac{\lambda^* \cdot \mathbf{A}(\omega)\tilde{\psi}}{\|\lambda^* \cdot \mathbf{A}(\omega)\tilde{\psi}\|}. \quad (51)$$

These jumps occur at the rates

$$d\Gamma^+[\tilde{\psi}, \lambda, \omega] = \gamma(\omega)\bar{N}(\omega) d\omega(\lambda) \|\lambda \cdot \mathbf{A}^\dagger(\omega)\tilde{\psi}\|^2$$

or

$$d\Gamma^-[\tilde{\psi}, \lambda, \omega] = \gamma(\omega)(\bar{N}(\omega) + 1) d\omega(\lambda) \|\lambda^* \cdot \mathbf{A}(\omega)\tilde{\psi}\|^2$$

respectively. The stochastic waiting time between two successive jumps is given by the distribution function (49).

In order to construct the path integral representation we define the quantities

$$\begin{aligned} \gamma[\psi, t|\tilde{\psi}] &\equiv (1 - F[\tilde{\psi}, t])\delta[\psi - g_t(\tilde{\psi})] \\ q[\psi, t|\phi_1] &\equiv \int D\phi_2 D\phi_2^* (1 - F[\phi_2, t])\delta[\psi - g_t(\phi_2)]W[\phi_2|\phi_1]. \end{aligned}$$

The quantity  $\gamma[\psi, t|\tilde{\psi}]$  is the probability that at time  $t$  the state  $\psi$  is realized and that no jump has occurred, provided at time 0 the state  $\tilde{\psi}$  has been given. The quantity  $q[\psi, t|\phi_1] ds$  represents the probability for the following event. Under the condition that at time 0 the state  $\phi_1$  is given, a jump occurs immediately afterwards in the time interval  $[0, ds]$  and then no further jump occurs until the state  $\psi$  is reached at time  $t$ . On using these quantities we may write the Kolmogorov forward equation as

$$T[\psi, t|\tilde{\psi}, 0] = \gamma[\psi, t|\tilde{\psi}] + \varepsilon \int_0^t ds \int D\phi_1 D\phi_1^* q[\psi, t-s|\phi_1]T[\phi_1, s|\tilde{\psi}, 0] \tag{52}$$

where we have introduced an expansion parameter  $\varepsilon$ . This parameter allows us to write an expansion of the propagator in terms of the number  $N$  of quantum jumps:

$$T[\psi, t|\tilde{\psi}, 0] = \sum_{N=0}^{\infty} \varepsilon^N T^{(N)}[\psi, t|\tilde{\psi}, 0]. \tag{53}$$

Inserting (53) into the Kolmogorov forward equation one obtains a recursion relation for the contributions  $T^{(N)}$ . Summing up these contributions and setting  $\varepsilon$  equal to 1 we find

$$\begin{aligned} T[\psi, t|\tilde{\psi}, 0] &= \gamma[\psi, t|\tilde{\psi}] + \sum_{N=1}^{\infty} \int_0^t ds_N \int_0^{t-s_N} ds_{N-1} \\ &\dots \int_0^{t-s_N \dots - s_2} ds_1 \int D\phi_N D\phi_N^* \int D\phi_{N-1} D\phi_{N-1}^* \\ &\dots \int D\phi_1 D\phi_1^* q[\psi, s_N|\phi_N]q[\phi_N, s_{N-1}|\phi_{N-1}] \dots q[\phi_2, s_1|\phi_1]\gamma[\phi_1, s_0|\tilde{\psi}]. \end{aligned} \tag{54}$$

Equation (54) is the Hilbert space path integral representation of the stochastic process. It represents the conditional transition probability  $T[\psi, t|\tilde{\psi}, 0]$  as a sum over all paths in Hilbert space that connect the Hilbert spacetime points  $(\tilde{\psi}, 0)$  and  $(\psi, t)$ . Each path is characterized by the number  $N$  of quantum jumps, by the time intervals  $s_1, s_2, \dots, s_N$  between successive jumps, by the time  $s_0 \equiv t - s_1 - s_2 - \dots - s_N$  until the first jump occurs, and by the intermediate states  $\phi_1, \phi_2, \dots, \phi_N$ . According to (54) the propagator is obtained by summing over the number  $N$  of quantum jumps, and by integrating over the time intervals between these jumps, as well as over the intermediate states. Again,  $\gamma[\psi, t|\tilde{\psi}]$  is the contribution of no jump.

It is important to emphasize that the Hilbert space path integral representation constructed above differs significantly from the influence functional representation of the reduced density matrix [22, 23]. The latter is a sum over paths in the underlying classical phase space and each path contributes a complex probability amplitude. In contrast, the Hilbert space path integral (54) is a sum over paths in Hilbert space and each path contributes a real and positive probability.

### 3. Discussion

We shall discuss in this section the essential properties of the stochastic process defined by the Liouville master equation (43) or, equivalently, by the Hilbert space path integral (54) and elaborate in detail on its physical interpretation.

#### 3.1. Unitary covariance

An important property is the unitary covariance of the stochastic process defined in equation (43). To be more precise, consider a unitary (canonical) transformation  $U$  of the Hilbert space of the reduced system and transform state vectors as  $\psi \mapsto \psi' = U\psi$ . By virtue of the unitary invariance of the measure  $D\psi D\psi^*$  the corresponding transformation rule for the probability distribution reads

$$P'[\psi', t] = P[\psi, t]. \quad (55)$$

Unitary covariance then means that equation (43) is form-invariant, that is, the transformed distribution  $P'$  also obeys the Liouville master equation (43) if, at the same time, the system operators  $A_i(\omega)$  and the Hamiltonian  $\hat{H}$  are transformed as

$$A_i(\omega) \mapsto A'_i(\omega) = U A_i(\omega) U^\dagger \quad \hat{H} \mapsto \hat{H}' = U \hat{H} U^\dagger. \quad (56)$$

In particular, unitary covariance implies that the stochastic formulation of the reduced system dynamics does not depend on the specific representation of the Hilbert space of the reduced system. An immediate consequence of the covariance is also that the probability distribution does not depend on the phase of the wavefunction

$$P[e^{i\chi}\psi, t] = P[\psi, t] \quad (57)$$

if the initial distribution is phase invariant, that is, if  $P[e^{i\chi}\psi, 0] = P[\psi, 0]$ . Furthermore,  $P[\psi, t]$  is concentrated on the unit sphere in Hilbert space if the initial distribution is so, since both the nonlinear evolution and the quantum jumps preserve the normalization of the wavefunction. The stochastic process defined by the Liouville master equation may therefore be considered as a stochastic process on *projective* Hilbert space.

#### 3.2. Rotational invariance of the stochastic process

In addition to canonical covariance the stochastic process defined by equation (43) is invariant under the group of rotations if the Hamiltonian of the reduced system is rotationally invariant. This means the following. We denote by  $U(\alpha)$  the unitary representation in Hilbert space of the rotation of physical space around the axis  $\alpha/\alpha$  with the angle  $\alpha \equiv |\alpha|$ . Thus, under rotations the state vectors transform as  $\psi \mapsto \psi' = U(\alpha)\psi$ . Since  $U(\alpha)$  is unitary and since the measure  $D\psi D\psi^*$  is invariant with respect to unitary transformations, the probability density is transformed as

$$P'[\psi, t] = P[U^\dagger(\alpha)\psi, t]. \quad (58)$$

Starting from an initial distribution that is rotationally invariant,  $P'[\psi, 0] = P[\psi, 0]$ , rotational invariance of the process means that  $P$  is rotationally invariant for all times, that is

$$P'[\psi, t] = P[U^\dagger(\alpha)\psi, t] = P[\psi, t]. \quad (59)$$

In other words, if  $\psi(t)$  is a realization of the process, then also  $U(\alpha)\psi(t)$  is a realization which occurs with the same probability. Note that rotational invariance is to be expected

since the reservoir, that is, the quantized radiation field, is assumed to be in thermal equilibrium and is therefore isotropic.

For a formal proof of rotational invariance it suffices to show that  $P'[\psi, t]$  and  $P[\psi, t]$  obey identical equations of motion. Since  $U(\alpha)$  is a canonical transformation we already know from the preceding subsection that  $P'$  again fulfills the Liouville master equation if the operators  $A(\omega)$  and  $\hat{H}$  are transformed according to equation (56). However, since  $H$  is assumed to be rotational invariant and since  $A(\omega)$  transforms as a vector operator under rotations, it follows immediately from the scalar nature of  $A^\dagger(\omega) \cdot A(\omega)$  and from equations (45) and (29) that neither  $\hat{H}$  nor the nonlinear operator  $G(\psi)$  change under rotations, i.e.

$$\begin{aligned} \hat{H}' &\equiv U(\alpha)\hat{H}U^\dagger(\alpha) = \hat{H} \\ G'(\psi) &\equiv U(\alpha)G(U^\dagger(\alpha)\psi) = G(\psi). \end{aligned}$$

Finally, the transition rates (46) are likewise rotationally invariant, which means

$$W'[\psi|\psi] \equiv W[U^\dagger(\alpha)\psi|U^\dagger(\alpha)\psi] = W[\psi|\psi]. \tag{60}$$

Note that this follows from the fact that the rotation of the vector operator  $A(\omega)$  can be compensated by a corresponding rotation of the polarization vector  $\lambda^*$  on using the rotational invariance of the measure  $d\omega(\lambda)$  (see equation (41)).

### 3.3. Physical interpretation of the process

The simulation algorithm described in section 2 is very similar to the algorithms proposed in [2, 3, 24]. There is, however, an essential difference. Note first that according to equation (46) for each atomic frequency  $\omega$  we have, in contrast to the usual formulation, two *continuous* families  $\lambda \cdot A^\dagger(\omega)$  and  $\lambda^* \cdot A(\omega)$  of jump operators parametrized by the polarization vector  $\lambda$ . The physical interpretation for this fact is obvious: the quantum jump with operator  $\lambda^* \cdot A(\omega)$  corresponds to the emission and the jump with operator  $\lambda \cdot A^\dagger(\omega)$  corresponds to the absorption of a photon with polarization  $\lambda$ . We shall emphasize the fact that the structure of the transition rates  $W[\psi|\psi]$  has been derived from first principles and that it is the appearance of continuous families of jump operators which ensures the rotational invariance (see section 3.2).

In order to illustrate this point we shall discuss an interesting example that has been given by Mølmer *et al* [24]. Consider a two-level atom. Both levels are three-fold degenerated forming a ( $J_g = J_e = 1$ )-multiplet, where  $J_g$  and  $J_e$  are the total angular momenta of the ground state and the excited state, respectively. We introduce the states  $|g, m_g\rangle$  and  $|e, m_e\rangle$  which are eigenstates of the  $z$ -component of the angular momentum operator with eigenvalues  $\hbar m_g$  and  $\hbar m_e$ . The operator  $A$  can then be written as

$$A = \sum_{m_g, m_e = \pm 1, 0} |g, m_g\rangle\langle g, m_g|D|e, m_e\rangle\langle e, m_e| \tag{61}$$

where we have suppressed the frequency argument since we have only one atomic frequency in this case. Since the dipole operator  $D$  is a vector operator,  $A$  can be expressed in terms of the reduced matrix element of the dipole operator and certain Clebsch–Gordan coefficients. In addition to the coupling to the vacuum of the radiation field ( $T = 0$ ) leading to spontaneous emission, the atom is subjected to a resonant laser field linearly polarized in the  $y$ -direction. The important property of this example is that there exists a state into which all trajectories of the process are ultimately trapped. This trapping state

$$\Phi = \frac{1}{\sqrt{2}}(|g, +1\rangle + |g, -1\rangle) \tag{62}$$

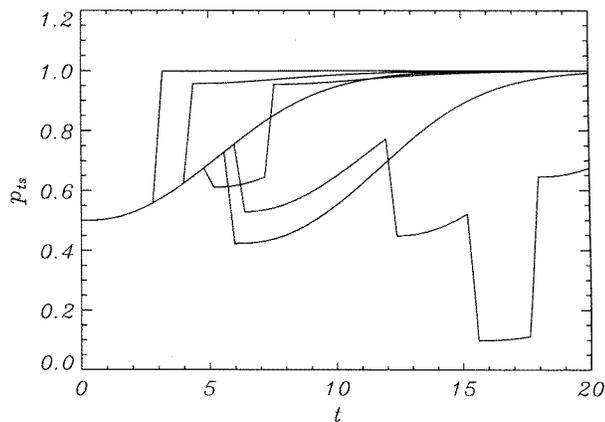
is a zero mode of the operator  $\hat{H}$ , that is,  $\hat{H}\Phi = 0$ . In [24] two different unravellings of the quantum master equation for this situation have been investigated which correspond to two different measurement schemes: first, measurement of the photon angular momentum along the  $z$ -axis and, second, measurement of the photon angular momentum along the  $y$ -axis. As has been discussed in that paper, both schemes lead to different realizations of the process. In the first case the possible transitions are  $|e, 0\rangle \rightarrow |g, -1\rangle$  for a photon which is right circularly polarized along the  $z$ -axis, and  $|e, 0\rangle \rightarrow |g, +1\rangle$  for a photon which is left circularly polarized along the  $z$ -axis. Consequently, the trapping into the state  $\Phi$  results essentially from the non-unitary evolution generated by  $\hat{H}$ . In the second case, however, we have the transitions  $|e, 0\rangle \rightarrow \Phi$  for left and right circularly polarized photons along the  $y$ -direction, and  $|e, 0\rangle \rightarrow \Phi^\perp$  for a photon that is linearly polarized in the  $y$ -direction, where  $\Phi^\perp = \frac{1}{\sqrt{2}}(|g, +1\rangle - |g, -1\rangle)$  is perpendicular to  $\Phi$ . Thus, in this case a transition can directly lead to the trapping state.

In contrast to these unravellings which are based on a measurement of the photon angular momentum along a specific axis and which therefore break the rotational invariance (as far as the coupling to the bath is concerned), in our stochastic process the photon may have any polarization along any direction in space. According to equation (46), the possible quantum jumps of the stochastic process are given by

$$|e, 0\rangle \rightarrow \cos \varphi |g, +1\rangle + \sin \varphi |g, -1\rangle \quad (63)$$

where  $\varphi$  is a stochastic angle uniformly distributed over the interval  $[0, 2\pi)$ . Thus, for  $\varphi = 0, \pi/2, \pi, 3\pi/2$  we obtain those jumps corresponding to the measurement of the photon angular momentum along the  $z$ -axis, whereas the cases  $\varphi = \pi/4, 3\pi/4, 5\pi/4, 7\pi/4$  lead to the transitions corresponding to the measurement along the  $y$ -axis. We show in figure 2 some realizations of the stochastic process defined by our Liouville master equation for this model. It is immediately clear from the figure that both types of paths of the wavefunction corresponding to the two measurement schemes discussed above occur in our stochastic process.

The conclusion to be drawn from these considerations is the following. The difference to the algorithms proposed by other authors is that a photon may be emitted or absorbed with



**Figure 2.** Six realizations of the stochastic process for a two-level system driven by a resonant laser field polarized in the  $y$ -direction. Each energy level forms a multiplet with angular momentum  $J = 1$ . For each realization  $\psi$  the figure shows, as a function of time, the probability  $p_{ts} = |\langle \Phi | \psi \rangle|^2$  for being in the trapping state  $\Phi$  (see text).

any polarization. Thus, in order to fix the stochastic process we do not need to prescribe a specific measurement scheme. The reason is that our starting point for the derivation of a stochastic dynamics for the reduced system is different from other approaches. In our derivation it is the presence of the thermal reservoir that causes the jumps of the wavefunction. These jumps appear as *instantaneous* changes of the wavefunction since the relaxation times of the reservoir are assumed to be small on the time scale of the reduced system. Also the jumps are *stochastic* since the precise state of the reservoir is not known, but only the probabilities of its various states, and since by the very procedure of the Markov approximation the bath variables have been eliminated. For this reason we do not obtain different unravellings of the corresponding quantum master equation, but rather a unique stochastic process.

These statements do not mean that the various stochastic approaches based on different unravellings, i.e. different measurement schemes are wrong. On the contrary, the stochastic process defined by our Liouville master equation subsumes those unravellings that arise from measurements of the photon angular momentum along all possible quantization axes. To state it differently, our approach is based on the assumption that only the thermodynamic properties of the state of the bath are known and that the properties of the emitted/absorbed photons are only available insofar as they can be observed by observables that refer to the reduced system, i.e. the atom. It is precisely for this reason that the integration over the polarization vector appears in the expression for the transition rates  $W[\psi|\psi]$ .

It should be clear that a specific measurement scheme leads to a different physical situation. If one wishes to perform a derivation (in the same sense as was done above) for a stochastic process in the case that a certain measurement apparatus acts on the system, one has to proceed as follows. Right from the beginning, one has to add to the microscopic Hamiltonian (see section 2.1) a Hamiltonian describing the (metastable) states for the apparatus, an interaction term describing the coupling of the system to the apparatus, and a Hamiltonian describing a heat bath and its coupling to the apparatus [25, 26]. The reduced probability distribution then describes the joint probability of the states of the atom *plus* meter [27].

### 3.4. Expansion of the density matrix

It is now interesting to establish the relationship to the conventional description of open quantum systems in terms of a quantum master equation for the reduced density matrix. This relation is straightforward if one considers that in our formalism the density matrix (5) is nothing but the covariance matrix of the stochastic wavefunction. Thus, the Hilbert space path integral representation of the propagator immediately allows the derivation of an analogous expansion of the density operator of the open system in terms of quantum jumps. The expansion of the density matrix in terms of the number of quantum jumps

$$\rho(t) = \sum_{N=0}^{\infty} \rho^{(N)}(t) \quad (64)$$

is found by inserting the expansion of the propagator (53) into the definition of the density matrix (5). The contribution  $\rho^{(0)}(t)$  to the density matrix from the path without quantum jumps is found to be

$$\rho^{(0)}(t) = S_t \rho(0) \quad (65)$$

where  $\rho(0)$  is the initial value of the density matrix. Paths with  $N$  jumps lead to the contribution

$$\rho^{(N)}(t) = \int_0^t ds_N \int_0^{t-s_N} ds_{N-1} \dots \int_0^{t-s_N-\dots-s_2} ds_1 S_{s_N} J S_{s_{N-1}} J S_{s_{N-2}} \dots J S_{s_1} J S_{s_0} \rho(0). \quad (66)$$

In the two above expressions we have introduced two super-operators  $J$  and  $S_s$  which are defined through their action on some operator  $B$  by

$$S_s B \equiv \exp\left(-\frac{i}{\hbar} \hat{H} s\right) B \exp\left(\frac{i}{\hbar} \hat{H}^\dagger s\right) \quad (67)$$

and by

$$JB \equiv \sum_{\omega>0} \gamma(\omega) \bar{N}(\omega) \int d\omega(\lambda) \lambda \cdot A^\dagger(\omega) B \lambda^* \cdot A(\omega) \\ + \sum_{\omega>0} \gamma(\omega) (\bar{N}(\omega) + 1) \int d\omega(\lambda) \lambda^* \cdot A(\omega) B \lambda \cdot A^\dagger(\omega). \quad (68)$$

The expansion of the density matrix given in equations (64)–(66) is formally identical with the expansion of the density matrix obtained by Srinivas and Davies [28] with the help of a model of a photodetector that performs continuous measurements. However, it is important to remark that the physical basis of our derivation is different: the expansion of the density matrix (64) follows directly from the expansion of the conditional transition probability of the stochastic process. The latter, in turn, has been obtained by eliminating the degrees of freedom of the thermal radiation field. Thus, the above expansion is valid at finite temperatures and no model of detection enters its derivation.

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