Wave-Function Approach to Dissipative Processes in Quantum Optics

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A novel treatment of dissipation of energy from a "small" quantum system to a reservoir is presented. We replace the usual master equation for the small-system density matrix by a wave function evolution including a stochastic element. This wave-function approach provides new insight and it allows calculations on problems which would otherwise be exceedingly complicated. The approach is applied here to a two- or three-level atom coupled to a laser field and to the vacuum modes of the quantized electromagnetic field.

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A typical model system in quantum optics consists of an atom coupled simultaneously to a laser field and to the vacuum modes of the quantized electromagnetic field. The atom-laser interaction, responsible for absorption and stimulated emission processes, is coherent, whereas the coupling between the atom and the vacuum modes, responsible for spontaneous emission processes, is fundamentally incoherent. This leads to a dissipation of energy from the "small system" (atom+laser) to the "reservoir" (vacuum field), which is usually treated by a density operator approach. A master equation, usually referred to as the optical Bloch equations (OBE's), is written for the reduced atomic density matrix ρ_A [1].

We present here an alternative approach using a wave-function treatment to describe the atomic system. The apparent incompatibility between such a wave-function approach and the inherent irreversibility of the spontaneous processes is lifted by introducing repeated "gedanken measurements" on the atomic system simulating the detection of the spontaneous photons. The random result of each of these measurements determines the atomic state afterwards, and is at the origin of the irreversibility. We show that this treatment is equivalent to the standard density matrix approach leading to the OBE's.

There are two main interests in this approach. First, it gives new insights into the processes taking place in the interaction of an atom with light. Here we will give two examples concerning the Rabi transitory regime for a two-level atom and the "dark resonance" problem. Second, it provides an efficient computational tool. If we consider an atomic system with N states, the master equation treatment requires the simultaneous solution of N^2 OBE's, while in this new approach, we deal with wave functions and we have to look for the evolution of no more than N variables. For instance, in problems related to a quantum treatment of laser cooling, N includes both the number of internal and external atomic states and can be very large. This makes the density matrix approach unwieldy except for simple one-dimensional configurations, while the wave-function approach can still be handled in the general case.

This wave-function approach can be applied to a wide class of problems involving dissipative processes [2]. For simplicity we restrict ourselves here to the simple case of a two-level atom, with a ground state g and an excited state e, coupled to a monochromatic laser field and to the quantized electromagnetic field in its ground state. The laser field is described by a classical function $\mathcal{E}(t)=\mathcal{E}_0 \times\cos\omega_L t$. The atom-laser coupling can then be written in the rotating wave approximation ($\hbar=1$):

$$H_0=-\delta S^+S^-+(\Omega/2)(S^++S^-)\,,$$

where $S^+=|e\rangle\langle g|$, $S^-=(S^+)^\dagger$. $\delta=\omega_L-\omega_A$ is the detuning between the laser and atomic frequencies; $\Omega=-d\mathcal{E}_0$ is the Rabi frequency and characterizes the coupling between the atomic dipole d and the laser electric field. Suppose that the atom–quantized-field system is described at time t by the wave function

$$|\psi(t)\rangle=|\phi(t)\rangle\otimes|0\rangle=(\alpha_g|g\rangle+\alpha_e|e\rangle)\otimes|0\rangle\,, \tag{1}$$

where $|0\rangle$ represents the ground state (no photon) of the quantized electromagnetic field. At time $t+dt$, some spontaneous photons may have been emitted; here, we choose $dt\ll\Gamma^{-1},\Omega^{-1},\delta^{-1}$, so that at most one spontaneous photon is emitted between t and $t+dt$. The wave function at time $t+dt$ can then be written as

$$|\psi(t+dt)\rangle=|\psi^{(0)}(t+dt)\rangle+|\psi^{(1)}(t+dt)\rangle\,, \tag{2a}$$

$$|\psi^{(0)}(t+dt)\rangle=(\alpha_g'|g\rangle+\alpha_e'|e\rangle)\otimes|0\rangle\,, \tag{2b}$$

$$|\psi^{(1)}(t+dt)\rangle=|g\rangle\otimes\sum_{\mathbf{k},\epsilon}\beta_{\mathbf{k},\epsilon}|\mathbf{k},\epsilon\rangle\,. \tag{2c}$$

The expressions for $|\psi^{(0)}\rangle$ and $|\psi^{(1)}\rangle$ can be obtained from the Wigner-Weisskopf approach to time-dependent perturbation theory [3]. Let us summarize here the main results. First the square of the norm of $|\psi^{(1)}\rangle$ is equal to the probability $dp=\Gamma dt\,|\alpha_e|^2=\Gamma dt\,\langle\phi(t)|S^+S^-|\phi(t)\rangle$ for a spontaneous emission during dt, and one has $\langle\psi^{(0)}|\psi^{(0)}\rangle=1-\langle\psi^{(1)}|\psi^{(1)}\rangle=1-dp$. The values of α_g'

and α_e' can be obtained from the evolution of $|\phi\rangle$ during dt with the non-Hermitian Hamiltonian $H=H_0-i\Gamma S^+S^-/2$, whose effect, in addition to H_0, is to reduce the excited-state amplitude by a factor $1-\Gamma dt/2$ [4]. In $|\psi^{(1)}\rangle$, the atom is taken in g since the probability for a reexcitation during dt after a decay can be neglected; the quantized field is in a state which contains one photon, with a probability amplitude $\beta_{\mathbf{k},\epsilon}$ that a given mode $\mathbf{k},\epsilon$ is populated after dt.

We now assume that all spontaneous photons are detected with a perfect counter and that we measure at time $t+dt$ the number of those photons. Depending on the result 0 or 1 of the measurement, we have to project $|\psi(t+dt)\rangle$ on $|\psi^{(0)}(t+dt)\rangle$ or $|\psi^{(1)}(t+dt)\rangle$ and normalize the result. In a numerical study of this process, the randomness of the measurement result is mimicked by the choice of a pseudorandom number ϵ uniformly distributed between 0 and 1. The two possible cases $\epsilon>dp$ and $\epsilon<dp$ correspond respectively to the detection of 0 and 1 photon. After this gedanken measurement process, assuming that the detected photon has been destroyed, we get for $\epsilon>dp$

$$|\psi(t+dt)\rangle=\mu(\alpha_g'|g\rangle+\alpha_e'|e\rangle)\otimes|0\rangle$$
$$=\mu(1-idtH)|\phi(t)\rangle\otimes|0\rangle \qquad (3a)$$

or, for $\epsilon<dp$,

$$|\psi(t+dt)\rangle=|g\rangle\otimes|0\rangle, \qquad (3b)$$

with $\mu=(1-dp)^{-1/2}$. In both cases we return to a wave function with the same form as (1), i.e., an atomic part times the vacuum of the field, and the whole sequence can be repeated to determine the (random) time evolution of the atomic part $|\phi(t)\rangle$ of the wave function. Note that not only the detection of a photon but also the zero measurement leads to a modification of the initial wave function [5–7].

This procedure, which we denote the Monte Carlo wave-function (MCWF) approach, is equivalent to the standard master equation approach (OBE). More precisely, we now demonstrate that the density operator $\bar{\sigma}(t)$ that one obtains by averaging $|\phi(t)\rangle\langle\phi(t)|$ over the different outcomes for the MCWF $|\phi(t)\rangle$ evolves according to the usual OBE's. This ensures that for any atomic operator B, the mean value $\langle\phi(t)|B|\phi(t)\rangle$, averaged over the different outcomes for $|\phi(t)\rangle$, is equal to the one time average $b(t)=\mathrm{Tr}(B\rho_A(t))$, where the initial density operator $\rho_A(0)$ coincides with $|\phi(0)\rangle\langle\phi(0)|$.

Consider a MCWF $|\phi(t)\rangle$; at time $t+dt$, the operator $\sigma(t+dt)=|\phi(t+dt)\rangle\langle\phi(t+dt)|$ can take two possible values corresponding to the two possible choices in (3). For a given $|\phi(t)\rangle$, the average value of $\sigma(t+dt)$ is

$$\overline{\sigma(t+dt)}=(1-dp)\mu^2(1-i\,dt\,H)|\phi(t)\rangle\langle\phi(t)|(1+i\,dt\,H^\dagger)+dp|g\rangle\langle g|$$
$$\simeq\sigma(t)-i\,dt[H\sigma(t)-\sigma(t)H^\dagger]+\Gamma dt\,S^-\sigma(t)S^+. \qquad (4)$$

We now average (4) over the different random issues for $|\phi(t)\rangle$, all starting in $|\phi(0)\rangle$ for $t=0$. It gives

$$\frac{d\bar{\sigma}}{dt}=i[\bar{\sigma},H_0]-\frac{\Gamma}{2}(S^+S^-\bar{\sigma}+\bar{\sigma}S^+S^-)+\Gamma S^-\bar{\sigma}S^+, \qquad (5)$$

which is identical to the well-known OBE's [1]. The MCWF method can also be used to calculate $\bar{\sigma}(t)$ when $\rho_A(0)$ describes a mixed state. One just has to choose among different initial MCWF's with probabilities ensuring agreement between $\bar{\sigma}(0)$ and $\rho_A(0)$.

As an example we present the derivation of the Rabi transitory regime using the MCWF approach. In Fig. 1(a) we show the population of the excited state $|\alpha_e(t)|^2$ as a function of time for a given "history" for $|\phi(t)\rangle$. The average of 100 of those sequences, all starting in g at $t=0$, is sketched in Fig. 1(b), together with the result obtained from the OBE's. It is clear from Fig. 1(b) that the decay of the Rabi oscillation towards a steady-state value results from a dephasing of the individual oscillation of each of the excited-state populations.

We now indicate how to handle situations where the states e and g have degenerate Zeeman sublevels. At each step dt, we calculate as above the probability $dp=\Gamma\pi_e\,dt$ for emitting a spontaneous photon, where π_e is the total population of the excited state e. Using dp we decide randomly whether a spontaneous photon is detected. If no photon is detected, the wave function is slightly modified according to (3a): The Hamiltonian evolution due to H_0 is taken into account, all excited-state amplitudes are reduced by a factor $1-\Gamma dt/2$, and the resulting wave function is normalized. If a photon is detected, a second random choice determines its angular momentum q_z along the quantization axis Oz ($q_z=\pm1,0$) according

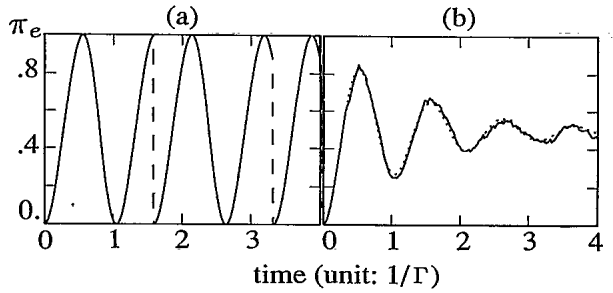

FIG. 1. (a) Time evolution of the excited-state population π_e of a two-level atom in the MCWF approach ($\Omega=3\Gamma$, $\delta=0$). The dashed lines indicate the projection of the atomic wave function onto the ground state after the detection of a spontaneous photon. (b) Average of $\pi_e(t)$ for 100 MCWF starting all in the ground state at $t=0$. The dotted line represents the result from the standard OBE treatment.

to the various excited-state populations of $|\phi(t)\rangle$ and the branching ratios from these states (square of Clebsch-Gordan coefficients). After this detection the atom is in a superposition of the ground states $|g,m_z\rangle$ (with angular momentum m_z along Oz) with amplitudes proportional to the former excited-state amplitudes $\langle e,m_z+q_z|\phi(t)\rangle$ times the Clebsch-Gordan coefficients corresponding to the transitions $e,m_z+g_z \rightarrow g,m_z$. As for the two-level case, one can show that this leads to an evolution of $\bar{\sigma}(t)$ identical to the OBE's.

As an example, consider a $g,J=1 \leftrightarrow e,J=1$ transition irradiated by two counterpropagating resonant laser fields with the same intensity and polarized $\sigma+$ and $\sigma-$ with respect to the z axis [Fig. 2(a)]. It is known from the OBE analysis that the atomic population is eventually trapped in a ground state which is not coupled to the laser field [8]. At positions where the two waves are in phase, this state is $|\phi_{NC}\rangle=(|g,m_z=-1\rangle+|g,m_z=1\rangle)/\sqrt{2}$. Consider a MCWF analysis of this situation with the atom starting for instance in $|g,m_z=\pm 1\rangle$. The atom-laser coupling leads first to an increase of the population of the excited state $|e,m_z=0\rangle$ [Fig. 2(b)]. A spontaneous photon may then be emitted which, depending on its angular momentum $q_z=\pm 1$, puts the atom back into $|g,m_z=\mp 1\rangle$. But it may also happen that no spontaneous photon is detected after a very long time, the successive steps "evolution due to H, projection onto the 0-photon state" causing a continuous rotation of the wave function from $|g,m_z=\pm 1\rangle$ into $|\phi_{NC}\rangle$, and therefore trapping the atomic population into this state [last part of the time sequence of Fig. 2(b)]. The MCWF approach offers a completely different physical picture if another gedanken measurement is considered. For instance, we could have chosen to measure the component q_y of the angular momentum of the detected photon, where the y axis is parallel to the resulting linear polarization of the laser light at the atomic position. Because of the "π polarization" of the laser excitation along the y axis, we identify the trapping state as $|\phi_{NC}\rangle=|g,m_y=0\rangle$, and after the detection of a photon with $q_y=\pm 1$, an atom decaying from the excited state $|e,m_z=0\rangle$ (superposition of the states $|e,m_y=\pm 1\rangle$) arrives directly in this trapping state. In particular no continuous rotation towards the state $|\phi_{NC}\rangle$ takes place in this picture. Let us emphasize that both detection schemes are legitimate and lead to average results equivalent to the ones given by the OBE's. The choice of a particular detection scheme should be made by considering the simplicity of the numerical calculation, or for emphasizing a particular physical aspect of the problem [9].

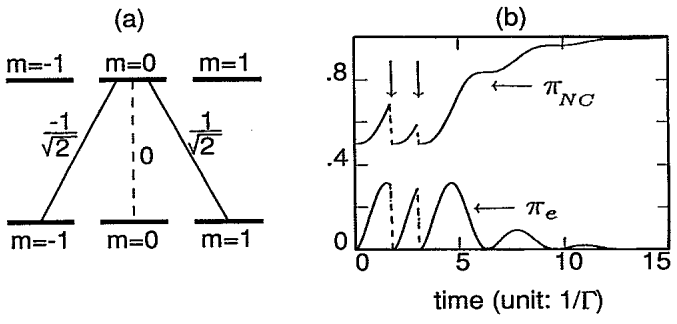

FIG. 2. (a) $g,J=1 \leftrightarrow e,J=1$ transition excited with $\sigma+-\sigma-$ light. An atom starting in $|g,m_z=\pm 1\rangle$ will remain in the subspace $\{|g,m_z=\pm 1\rangle, |e,m_z=0\rangle\}$ because of the zero transition element between $|e,m_z=0\rangle$ and $|g,m_z=0\rangle$. (b) Time evolution of the population of $|e,m_z=0\rangle$ and of $|\phi_{NC}\rangle$ for a given MCWF ($\delta=0$, $\langle e,0|H_0|g,-1\rangle=-\langle e,0|H_0|g,1\rangle=\Gamma\sqrt{2}$). The arrows indicate the detection of a spontaneous photon with angular momentum ± 1 along Oz. At $t=\infty$ the atom always ends up in $|\phi_{NC}\rangle$ (population trapping).

A number of problems require a quantum treatment of the external atomic degrees of freedom. To this purpose the detection of a spontaneously emitted photon with momentum $\hbar\mathbf{k}$ should be chosen according to the known radiation pattern for the transition. Next the polarization of the photon (perpendicular to $\hbar\mathbf{k}$) is picked up, and the atomic wave function after this detection is a superposition of atomic ground states with different values of the momentum $\mathbf{p}$, $|g,m_z,\mathbf{p}\rangle$, with amplitudes derived from the former excited-state amplitudes $\langle e,m_z',\mathbf{p}+\hbar\mathbf{k}|\phi(t)\rangle$ [10].

The MCWF approach is not limited to the calculation of one-time average values of atomic operators. Consider for instance the correlation function in a state $|\psi_0\rangle=|\phi_0\rangle \otimes|0\rangle$ of two Hermitian atomic operators A and B in the Heisenberg point of view:

$$c(t,\tau)=\langle\psi_0|A(t)B(t+\tau)+B(t+\tau)A(t)|\psi_0\rangle$$

($\tau>0$). It is usually calculated in the OBE formalism using the quantum regression theorem (QRT) [11]: One expands B on the basis $X_{ij}=|i\rangle\langle j|$, where $|i\rangle,|j\rangle$ are members of a basis set of the atomic Hilbert space; the values of the corresponding $c_{ij}(t,0)$ are one-time averages and are calculated directly from the OBE's. The τ evolution of the $c_{ij}(t,\tau)$ is then

$$\frac{\partial c_{ij}}{\partial\tau}(t,\tau)=\sum_{kl}\mathcal{L}_{ijkl}c_{kl}(t,\tau)\,, \tag{6a}$$

where the coefficients $\mathcal{L}_{ijkl}$ are shown to be the same as the ones giving the evolution of the one-time averages (QRT):

$$\frac{d\langle X_{ij}(t)\rangle}{dt}=\sum_{kl}\mathcal{L}_{ijkl}\langle X_{kl}(t)\rangle\,. \tag{6b}$$

In the MCWF approach, we first let $|\phi_0\rangle$ evolve from 0 to t. For a given outcome $|\phi_0(t)\rangle$ of this evolution, we form the two new states $|\chi_\pm(0)\rangle=\mu_\pm^{-1/2}(1\pm A)|\phi_0(t)\rangle$, where $\mu_\pm$ are normalization coefficients. Evolving now $|\chi_\pm(\tau)\rangle$, we calculate $c_r(\tau)=\langle\chi_r(\tau)|B|\chi_r(\tau)\rangle$ ($r=\pm$), and we finally obtain $c(t,\tau)=[\mu_+c_+(\tau)-\mu_-c_-(\tau)]/2$. This procedure, with an average over the different outcomes for $|\chi_\pm(\tau)\rangle$ for a given $|\phi_0(t)\rangle$, and then with a

second average over the different outcomes for $|\phi_0(t)\rangle$, gives the same results as the ones obtained from the QRT. To prove this, we check that $\tilde{c}_{ij}(\tau)$, obtained as the average of

$$\tfrac{1}{2}[\mu_+\langle\chi_+(\tau)|X_{ij}|\chi_+(\tau)\rangle-\mu_-\langle\chi_-(\tau)|X_{ij}|\chi_-(\tau)\rangle]$$

over the different outcomes of the Monte Carlo evolution, indeed equals $c_{ij}(t,\tau)$. For $\tau=0$, this is easily verified from the expression of $|\chi_\pm(0)\rangle$. Because they are linear combinations of one-time averages and therefore follow from (6b), the evolution of the $\tilde{c}_{ij}(\tau)$'s is identical to the evolution (6a) of the $c_{ij}(t,\tau)$'s, and the identity holds for any τ. Similarly, the value of $\langle[A(t),B(t+\tau)]\rangle$ can be obtained from this procedure by considering $|\chi'_\pm(0)\rangle=\mu_\pm^{\mp 1/2}(1\pm iA)|\phi_0(t)\rangle$. Using two pairs of states $\chi_\pm(\tau),\chi'_\pm(\tau)$ derived from each of 100 wave functions $|\phi_0(t)\rangle$, we have simulated the dipole correlation function, and therefore the fluorescence spectrum of a laser driven two-level atom and we have obtained a satisfactory agreement [same type as in Fig. 1(b)] with the OBE result.

Finally, we discuss the connection of our approach with previous wave-function approaches to quantum optics problems. In the pioneering work of Mollow [12] the total atom+field wave function was used to keep track of all emitted photons, and to derive quantities such as the frequency spectrum of the fluorescence light. In contrast, our purpose has been to eliminate the field and to derive a stochastic evolution of only the atomic part of the wave function. A wave-function approach has also been fruitful in studies of the quantum jump phenomenon [13,14]. It gives access to the delay function characterizing the statistical distribution of the time between two successive spontaneous emissions. This delay function can also generate a very efficient Monte Carlo analysis of the process, where the choice of a single random number determines the time of emission of each spontaneous photon. This has been used to demonstrate the existence of dark periods in a "quantum jump situation" [14], and to explore the cooling produced by velocity selective coherent population trapping [15]. The MCWF method is not as fast as the ones based on the delay function, since many random numbers are needed before the detection of a single photon ($dt\ll\Gamma^{-1}$), but on the other hand it does not require any precalculated delay function, and it can be used for atomic transitions with arbitrarily large numbers of levels. The MCWF treatment may also be useful for the inclusion of dissipation in the generation and evolution of "nonclassical" field states. Here, however, its effectiveness should be judged by a comparison with the methods specifically developed for this type of problem, e.g., the generalized P distribution [16].

To summarize, we have presented a general wave-function approach to the problem of dissipation of energy from a coherently excited quantum-mechanical system. This approach provides new physical pictures which may be particularly valuable in situations dealing with a single quantum system instead of an assembly [17]. It can also greatly simplify the calculations when a large number of quantum levels are involved; the quantum treatment of collisions of slow atoms irradiated with quasiresonant laser fields and the description of 3D laser cooling and trapping processes in a regime where the semiclassical approach [18] is not valid anymore are examples of problems which could benefit from such an approach.

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Note added.—Since the submission of the manuscript, it has been brought to our attention that a similar procedure has been developed in the context of nonclassical field generation [19].

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