Monte Carlo simulation of the atomic master equation for spontaneous emission

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A Monte Carlo simulation of the atomic master equation for spontaneous emission in terms of atomic wave functions is developed. Realizations of the time evolution of atomic wave functions are constructed that correspond to an ensemble of atoms driven by laser light undergoing a sequence of spontaneous emissions. The atomic decay times are drawn according to the photon count distribution of the driven atom. Each quantum jump of the atomic electron projects the atomic wave function to the ground state of the atom. Our theory is based on a stochastic interpretation and generalization of Mollow's pure-state analysis of resonant light scattering, and the Srinivas-Davies theory of continuous measurements in photodetection. An extension of the theory to include mechanical light effects and a generalization to atomic systems with Zeeman substructure are given. We illustrate the method by simulating the solutions of the optical Bloch equations for two-level systems, and laser cooling of a two-level atom in an ion trap where the center-of-mass motion of the atom is described quantum mechanically.

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I. INTRODUCTION

Simulation methods are becoming an increasingly important tool in studying the effect of noise in complex nonlinear systems. [1]. Recently, there has been considerable interest in formulating simulation techniques for quantum noise in problems of quantum optics [2–4]. In quantum mechanics the effect of damping and fluctuations of a system coupled to a reservoir can be described by a master equation for the reduced system density matrix. This corresponds to the assumption of a quantum Markov process for the system variables [2]. A simulation of quantum noise must therefore be based on simulating solutions of the quantum master equation.

Of particular interest in quantum optics are damping and noise in (cavity) modes of the radiation field and of atomic systems. For the reservoir one typically assumes a bath of harmonic oscillators in a vacuum, thermal, or squeezed state [2]. Monte Carlo (MC) techniques for solving density-matrix equations of damped cavity modes have been proposed that are based on transforming the master equation to a c-number equation for a (quasi-) probability distribution (using a Wigner, a Q, a P, or a generalized P representation) [1,2]. In many cases of interest this gives a Fokker-Planck equation that can be solved by simulating the associated Langevin equations [2–4]. This is particularly interesting in situations corresponding to generation of nonclassical states of light [2–4]. In the present work we will focus on the development of a wave-function simulation to solve the master equation. The system we will consider is an atom driven by laser light that is undergoing a sequence of spontaneous emissions. Thus we will develop a scheme that is based on simulating the time evolution of an atom in terms of atomic wave functions where the atom undergoes "quantum jumps" at random times drawn according to the photon statistics of spontaneous emission.

An atom driven by laser light and coupled to empty vacuum modes of the radiation field is described by the optical Bloch equations (master equation) for the reduced atomic density operator. The price to be paid for eliminating the radiation field variables is that one has to work with an atomic density matrix, i.e., in general there is no (atomic) wave-function description for the atomic dynamics damped by spontaneous emission. In a system with N atomic degrees of freedom the atomic density matrix has N^2 elements, while an *atomic* wave function has only N components. In systems with large N this difference is significant, and the following question arises. Can one replace the solution of the master equation for the atomic density matrix by a stochastic simulation of spontaneous emission in terms of atomic wave functions? An example of a system involving a large number of atomic degrees of freedom is laser cooling [5,6] in the case where, in addition to the internal atomic degrees of freedom, the center-of-mass motion of the atom has to be treated quantum mechanically—a problem which becomes even more challenging in two- and three-dimensional models [7].

In the present paper we will develop an *atomic wave-function simulation* procedure for the atomic master equation, based on a stochastic interpretation and generalization of Mollow's pure-state analysis of resonant light scattering for two-level atoms [8], as well as on the theory of continuous measurements in photodetection as given by Srinivas and Davies [9]. Mollow has shown that the reduced atomic density matrix $\rho_A(t)$ for a two-level system at time t can be represented in terms of atomic

wave functions $|\Psi(t|t_n,\ldots,t_1)\rangle$ describing an atomic ensemble that has emitted $n=0,1,2,\ldots$ photons at times $t_n>\cdots>t_1$ [10]. The relation between Mollow's n-photon atomic wave amplitudes and n-photon detection probabilities of the Srinivas-Davies theory has been established by us in our work on quantum jumps [11].

In previous work [11] we employed the above formalism to study photon statistics in two- and three-level systems and illustrated the phenomenon of quantum jumps [12–14] by deriving a simulation procedure for single-atom realizations of photon count sequences. In the present work we extend these ideas to calculate a MC approximation of the atomic density matrix in terms of atomic wave functions. By simulating a sequence of spontaneous photon emissions, we construct single-atom realizations of atomic MC wave functions, which are found by integrating Mollow's equation for the atomic amplitudes with decay times drawn according to corresponding photon emission probabilities. An ensemble average over these stochastic wave functions then provides us with the system density matrix. Following our earlier work on simulations of laser coolings [15], it is possible to extend this formalism to include mechanical light effects (laser cooling and atomic beam deflection) and multilevel systems (Zeeman substructure). Our work is related to the procedure of simulating the atomic master equation which was proposed by Dalibard and Mølmer [16]. These authors have suggested a MC integration of the master equation based on propagating a Wigner-Weisskopf wave function over time steps much shorter than the natural decay time, and simulating a sequence of photon-count–no-photon-count measurements in each time interval [14].

The paper is organized as follows. In Sec. II we review Mollow's pure-state analysis of resonant light scattering for a two-level system and point out its relation to the Srinivas-Davies theory of photon counting. This leads us to formulate our MC simulation. In Sec. III we generalize the simulation approach to mechanical light effects and illustrate the method by applying it to laser cooling in one-dimensional ion traps and comparing the simulation results with the predictions of the Javanainen-Lindberg-Stenholm theory [17]. Finally, we present a generalization to multilevel systems with Zeeman structure in Sec. IV.

II. WAVE-FUNCTION REPRESENTATION AND SIMULATION OF THE ATOMIC DENSITY MATRIX FOR A TWO-LEVEL SYSTEM

In this section we give a summary of Mollow's pure-state analysis [8] of resonant light scattering from two-level systems (TLS's), and point out the relation to the Srinivas-Davies theory of continuous measurements in photodetection [9,12]. This will lay the foundations for a simulation procedure of the optical Bloch equations (OBE's) in terms of atomic wave functions. A simulation of photon statistics of two- and three-level systems has been described in the context of our treatment of quantum jumps [11].

A. n-photon contributions to the atomic density matrix

The dynamics of a TLS with ground state $|g\rangle$ and excited state $|e\rangle$ which is driven by a classical light field and coupled to a reservoir of vacuum modes of the radiation field is described by a Schrödinger equation

$$i\frac{d}{dt}|\Psi_{AF}(t)\rangle=H|\Psi_{AF}(t)\rangle \tag{1}$$

with state vector $|\Psi(t)\rangle$ and Hamiltonian

$$H=H_{0A}+H_{0F}+H_1(t) \tag{2}$$

(we scale the Hamiltonian by dividing by $\hbar$). Here $H_{0A}=\omega_{eg}a^\dagger a$ is the free atomic Hamilton operator with ω_{eg} the transition frequency and $a=|g\rangle\langle e|$ the atomic lowering operator. H_{0F} is the Hamiltonian of the free radiation field, and $H_1(t)$ denotes the interaction part,

$$H_1(t)=-\boldsymbol{\mu}_{eg}^*\cdot[\mathcal{E}_R^\dagger(\mathbf{x}=)+\mathcal{E}_{\rm cl}^*(\mathbf{x}=0,t)]a \\ -a^\dagger\boldsymbol{\mu}_{eg}\cdot[\mathcal{E}_R(\mathbf{x}=0)+\mathcal{E}_{\rm cl}(\mathbf{x}=0,t)]\,, \tag{3}$$

with $\boldsymbol{\mu}_{eg}$ the atomic dipole matrix element, $\mathcal{E}_R(\mathbf{x}=0)$ the positive frequency part of the electric field operator, and $\mathcal{E}_{\rm cl}(\mathbf{x}=0,t)=\mathcal{E}_0\boldsymbol{\epsilon}e^{-i\omega t}$ the positive frequency part of the electric field of the laser. The state vector $|\Psi_{\rm AF}(t)\rangle$ of the combined atom-field system has an expansion of the form

$$|\Psi_{\rm AF}(t)\rangle=|\Psi\rangle\otimes|{\rm vac}\rangle+\sum_\lambda\int d^3k\,|\Psi_{\mathbf{k},\lambda}(t)\rangle\otimes b_{\mathbf{k},\lambda}^\dagger|{\rm vac}\rangle \\ +\frac{1}{\sqrt{2!}}\sum_{\lambda_1,\lambda_2}\int d^3k_1\int d^3k_2\,|\Psi_{\mathbf{k}_1,\lambda_1;\mathbf{k}_2,\lambda_2}(t)\rangle\otimes b_{\mathbf{k}_1,\lambda_1}^\dagger b_{\mathbf{k}_2,\lambda_2}^\dagger|{\rm vac}+\cdots\,, \tag{4}$$

which describes the presence of $n=0,1,2,\ldots$ scattered photons in the field. Note that $\Psi_{\rm AF}(t)\rangle$ is an element of the product space of the atomic space $\mathcal{H}_A=\{|g\rangle,|e\rangle\}$ and the Fock space $\mathcal{H}_F$, $|\Psi_{\rm AF}(t)\rangle\in\mathcal{H}_A\otimes H_F$. The atomic vectors $|\Psi(t)\rangle$ ($\in\mathcal{H}_A$) are the so-called atomic vacuum amplitudes; $|\Psi_{\mathbf{k},\lambda}\rangle$ are the atomic amplitudes in the presence of a scattered photon in the mode $\mathbf{k},\lambda$, etc. The atomic vacuum amplitudes obey the Schrödinger equation

$$i\frac{d}{dt}|\Psi(t)\rangle=H_{\rm eff}|\Psi(t)\rangle \tag{5}$$

with

$$H_{\rm eff}=(\omega_{eg}-i\tfrac{1}{2}\kappa)a^\dagger a-[\boldsymbol{\mu}_{eg}\cdot\mathcal{E}(\mathbf{x}=0,t)a^\dagger+{\rm H.c.}] \tag{6}$$

an effective atomic Hamiltonian, where κ is the spontaneous decay rate of the TLS. Note that the norm of $|\Psi(t)\rangle$ will decay due to the non-Hermiticity of $H_{\rm eff}$. This is re-

lated to the probability of spontaneous emission of the next photon as will be shown below.

The reduced atomic density matrix, which is obtained by tracing over the modes of the radiation field,

$$\rho_A(t)=\mathrm{Tr}_F[|\Psi_{AF}(t)\rangle\langle\Psi_{AF}(t)|] , \tag{7}$$

obeys the OBE's

$$\frac{d}{dt}\rho_A=-i(H_{\mathrm{eff}}\rho_A-\rho_A H_{\mathrm{eff}}^{\dagger})+\kappa a\rho_A a^{\dagger} . \tag{8}$$

A reduced atomic density operator in the subspace of $n=0,1,2,\ldots$ scattered photons is defined as

$$\rho_A^{(n)}(t)=\mathrm{Tr}_F[\underline{P}^{(n)}|\Psi_{\mathrm{AF}}(t)\rangle\langle\Psi_{\mathrm{AF}}(t)|] . \tag{9}$$

$\underline{P}^{(n)}$ is a projection operator onto the n-photon subspace, and Tr_F indicates the trace over the modes of the radiation field. As has been shown by Mollow, $\rho_A^{(n)}(t)$ obeys the equation of motion

$$\frac{d}{dt}\rho_A^{(n)}=-i(H_{\mathrm{eff}}\rho_A^{(n)}-\rho_A^{(n)}H_{\mathrm{eff}}^{\dagger}) +\kappa a\rho_A^{(n-1)}a^{\dagger}(1-\delta_{n0}) , \tag{10}$$

where the source terms $\kappa|g\rangle\langle g|\rho_{ee}^{(n-1)}$ correspond to the rate at which atoms are created in the ground state with the emission of the nth photon. Obviously, we have

$$\rho_A(t)=\sum_{n=0}^{\infty}\rho_A^{(n)}(t) . \tag{11}$$

A solution of Eq. (10) can be written in the form

$$\rho_A^{(0)}(t)=S_{t,0}\rho_A(0) , \qquad \rho_A^{(n)}(t)=\int_0^t dt' S_{t,t'}J\rho_A^{(n-1)}(t') , \tag{12}$$

with the notation for the source term

$$J\rho_A^{(n-1)}(t)=\kappa a\rho_A^{(n-1)}(t)a^{\dagger} . \tag{13}$$

The Green function of the homogeneous part of Eq. (10) is

$$S_{t,t'}\rho_A^{(n)}(t')=U_{t,t'}\rho_A^{(n)}(t')U_{t,t'}^{\dagger} , \tag{14}$$

with $U_{t,t'}$ the time evolution operator of the Schrödinger equation (5). By iterating (12) we get the n-photon contribution to the density matrix

$$\rho_A^{(n)}(t)=\int_0^t dt_n\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1 S_{t,t_n}JS_{t_n,t_{n-1}}\cdots JS_{t_1,0}\rho_A(0) \quad (n\geq 1) . \tag{15}$$

For the n-photon probabilities we obtain

$$P^{(0)}(t)=\mathrm{Tr}_A[S_{t,0}\rho_A(0)] , \qquad P^{(n)}(t)=\int_0^t dt_n\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1\mathrm{Tr}_A[S_{t,t_n}JS_{t_n,t_{n-1}}\cdots JS_{t_1,0}\rho_A(0)] . \tag{16}$$

The picture suggested by Eqs. (16) is the time evolution of an atom in a time interval $(0,t)$ which emits *exactly* n photons at times $t_n\geq\cdots\geq t_1$. Each photon emission is accompanied by the reduction of the atomic density operator to the ground state $|g\rangle$, as described by the operator J. The time evolution between emissions, given by $S_{t,t'}$, is governed by the non-Hermitian Hamiltonian H_{eff}. Equation (16) suggest the interpretation of

$$p_{[0,t)}(t_1,\ldots,t_n)=\mathrm{Tr}_A[S_{t,t_n}JS_{t_n,t_{n-1}}\cdots JS_{t_1,0}\rho_A(0)] \tag{17}$$

as an elementary probability density that the atom emits exactly n photons at times $t_1\leq\cdots\leq t_n$ during the time interval $[0,t)$. Furthermore,

$$\tilde{c}(t|t_n,\ldots,t_1)=\frac{\mathrm{Tr}_A[JS_{t,t_n}JS_{t_n,t_{n-1}}\cdots JS_{t_1,0}\rho_A(0)]}{\mathrm{Tr}_A[JS_{t_n,t_{n-1}}\cdots JS_{t_1,0}\rho_A(0)]} =\frac{p_{[0,t)}(t_1,\ldots,t_n,t)}{p_{[0,t_n)}(t_1,\ldots,t_n)} \quad (n\geq 1) \tag{18}$$

and

$$\tilde{c}(t)=\mathrm{Tr}_A[JS_{t,0}\rho_A(0)](n=0) \tag{19}$$

are the conditional probabilities that given $n=1,2,\ldots$ photons were emitted at times $t_1,\ldots,t_n$, the next photon is emitted at time t. Note that J is a non-negative definite operator which guarantees $\tilde{c}\geq 0$. The above interpretation is supported by the Srinivas-Davies theory of continuous measurement applied to photon counting.

In terms of the conditional probabilities we have

$$p_{[0,t)}(t_1,\ldots,t_n)=\left[1-\int_{t_n}^t dt'\tilde{c}(t'|t_n,\ldots,t_1)\right]\times\prod_{k=1}^{n}\tilde{c}(t_k|t_{k-1},\ldots,t_1) . \tag{20}$$

According to Eq. (20) the elementary n-photon probabilities are products of the conditional probabilities for the next photon being emitted at time t_k $(k=1,\ldots,n)$ times the probability that no photon is emitted in $[t_n,t)$.

B. Mollow's pure-state analysis of resonant light scattering

For an initial pure state $\rho_A(0)=|\Psi(0)\rangle\langle\Psi(0)|$, the atomic n-photon density operator (9) can be written in terms of atomic wave functions

$$|\Psi(t_n|t_{n-1},\ldots,t_1)\rangle\in\mathcal{H}_A . \tag{21}$$

These wave functions are defined recursively by the hierarchy of Schrödinger equations

$$i\frac{d}{dt}|\Psi(t|t_n,\ldots,t_1)\rangle = H_{\text{eff}}|\Psi(t|t_n,\ldots,t_1)\rangle \qquad (t \geq t_n) \quad (22)$$

and initial conditions

$$|\Psi(t_n|t_n,\ldots,t_1)\rangle = a|\Psi(t_n|t_{n-1},\ldots,t_1)\rangle \ . \quad (23)$$

Note that the phase of the $|e\rangle$ component of the wave function survives the projection to the ground state. For $n=0$ the wave functions (21) are identical to the atomic vacuum amplitudes defined in Eq. (5). Thus we have for $n=0$

$$\rho_A^{(0)}(t) = |\Psi(t)\rangle\langle\Psi(t)| \ , \quad (24)$$

and for $n \geq 1$

$$\rho_A^{(n)}(t) = \int_0^t \kappa\, dt_n \int_0^{t_n} \kappa\, dt_{n-1} \cdots \int_0^{t_2} \kappa\, dt_1 |\Psi(t|t_n,\ldots,t_1)\rangle\langle\Psi(t|t_n,\ldots,t_1)| \ . \quad (25)$$

The probability density (17) for n-photon emission is related to the norm of the corresponding wave function by

$$p_{[0,t)}(t_1,\ldots,t_n) = \kappa^n \| |\Psi(t|t_n,\ldots,t_1)\rangle \|^2 \ . \quad (26)$$

We therefore interpret $t_n \geq \cdots \geq t_1$ as the decay times at which a photon is spontaneously emitted, and the initial condition (23) as the reduction of the wave packet associated with this quantum jump. It is easy to verify that

$$\int_{t_n}^t dt' \bar{c}(t'|t_n,\ldots,t_1) = 1 - \frac{\| |\Psi(t|t_n,\ldots,t_1)\rangle \|^2}{\| |\Psi(t_n|t_n,\ldots,t_1)\rangle \|^2} \ , \quad (27)$$

i.e, the probability that a photon is emitted during $[t_n,t)$ is equal to the decay of the norm of the Mollow wave function, which has been normalized at time t_n of the last quantum jump.

For a TLS the conditional probability densities depend only on the *last* decay time t_n,

$$\bar{c}(t|t_n,\ldots,t_1) = \bar{c}(t|t_n) = \kappa|\Psi_e(t|t_n)|^2 \ , \quad (28)$$

so that the probability density factorizes,

$$p_{[0,t)} = [|\Psi_g(t|t_n)|^2 + |\Psi_e(t|t_n)|^2] \times \kappa|\Psi_e(t_n|t_{n-1})|^2 \cdots \kappa|\Psi_e(t_1)|^2 \ . \quad (29)$$

We emphasize that Eqs. (28) and (29) are true for a pure TLS only, not for the more general cases considered in the following sections.

For an initial mixed state the density matrix ρ_A can always be diagonalized,

$$\rho_A(0) = \sum_\alpha \rho_\alpha |\Psi_\alpha(0)\rangle\langle\Psi_\alpha(0)| \quad (30)$$

with probabilities p_α satisfying $0 \leq p_\alpha \leq 1$ and $\sum_\alpha p_\alpha = 1$.

C. Simulations

The pure-state representation (25) suggests simulating the reduced atomic density matrix $\rho_A(t)$ in terms of atomic wave functions. We rewrite Eq. (25), using Eq. (26),

$$\rho_A(t) = \sum_{n=0}^\infty \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 p_{[0,t)}(t_1,\ldots,t_n) |\tilde{\Psi}(t|t_n,\ldots,t_1)\rangle\langle\tilde{\Psi}(t|t_n,\ldots,t_1)| \ , \quad (31)$$

with normalized wave functions

$$|\tilde{\Psi}(t|t_n,\ldots,t_1)\rangle = |\Psi(t|t_n,\ldots,t_1)\rangle / \| |\Psi(t|t_n,\ldots,t_1)\rangle \| \ . \quad (32)$$

A MC integration can now be performed by drawing decay times $t_1,\ldots,t_n$ according to the probability density $p_{[0,t)}(t_1,\ldots,t_n)$. Such a MC integration for MC wave functions $|\chi(t)\rangle$ in a given time interval $[0,T)$ is implemented as follows.

(i) *Initial condition.* We choose an initial state, typically $|\chi(t_0=0)\rangle = |g\rangle$. To count the number of spontaneous emissions we introduce a photon counter n, which we initially set to zero.

(ii) *Time propagation.* We integrate the Schrödinger equation (5) up to the time of the next photon emission, determined by

$$\int_{t_n}^t d\tau \bar{c}(\tau|t_n,..,t_1) = 1 - \| |\chi(t)\rangle \|^2 = x \quad (33)$$

with $x \in [0,1]$ a random number drawn from a uniform distribution. We increase the photon counter by one $(n \to n+1)$ and set $t_n = t$ which we identify as the emission time of the nth photon. The quantum jump at t_n reduces the atomic wave function to the ground state [18],

$$|\chi(t_n)\rangle \leftarrow a|\chi(t_n)\rangle / \|a|\chi(t_n)\rangle\| \ . \quad (34)$$

We then proceed by integrating the Schrödinger equation (5) for $|\chi(t)\rangle$ until we reach the next decay time. We stop upon reaching the end of the chosen time interval.

(iii) *Average over realization.* Repeating the above simulation N times, we obtain an approximation for the atomic density matrix

$$\rho_A(t) \approx \frac{1}{N} \sum_{i=1}^N |\tilde{\chi}_i(t)\rangle\langle\tilde{\chi}_i(t)| \quad (35)$$

with $|\tilde{\chi}_i(t)\rangle = |\chi_i(t)\rangle / \| |\chi_i(t)\rangle \|$ and $i = 1,\ldots,N$ num-

bering the realizations. An estimate of the expectation value of an arbitrary atomic operator $\hat{\mathcal{O}}$ is

$$\langle\hat{\mathcal{O}}\rangle=\mathrm{Tr}_A[\hat{\mathcal{O}}\rho_A(t)]\approx\frac{1}{N}\sum_{i=1}^{N}\langle\tilde{\chi}_i(t)|\hat{\mathcal{O}}|\hat{\chi}_i(t)\rangle\ . \tag{36}$$

Stationary solutions of the OBE's can be simulated very efficiently by following one realization of the wave function $|\chi(t)\rangle$ over times much longer than the time scale of the damping of the atom, replacing the ensemble average by a time average to calculate an approximation of the stationary density matrix.

So far we have assumed a pure state for the initial condition. A mixed state (30) can be simulated by starting the simulations with pure states $|\Psi_\alpha(0)\rangle$ drawn according to the probabilities p_α.

Recently, Dalibard and Mølmer [16] have suggested a MC integration of the master equation based on propagating a Wigner-Weisskopf wave function. They simulate a sequence of photon-count–no-photon-count measurements (see also Cook [14], Sec. 4.2) on a grid with fixed time steps, much smaller than the time scale given by the spontaneous-emission lifetime, the inverse Rabi frequency, and the inverse detuning. Our simulation technique is more naturally formulated as a variable (global) time step integration where the non-Hermitian Schrödinger equation is integrated to the next decay time in typically a few steps using the propagator $U_{t,t'}$ of Eq. (5) [19].

As an illustration we plot in Figs. 1(a) and 1(b) a MC wave function $|\chi(t)\rangle$ as a function of time for $\Omega=\kappa$ and $\Delta=-\kappa$. Figure 1(a) shows the excited-state probability $|\langle e|\tilde{\chi}(t)\rangle|^2$, while in Fig. 1(b) we plot the corresponding norm $\||\chi(t)\rangle\|^2$. The decay times $t_1,\ldots,t_6$ are indicated by arrows; $x_1,\ldots,x_6$ are the corresponding random numbers [compare (33)]. Figure 2 shows a comparison of the exact solutions of the OBE's for the excited-state population $p_{ee}(t)$ for $\Omega=6\kappa$ and $\Delta=0$ with the simulation results for 100 and 1000 realization (stars and dashed line, respectively). For 10 000 realizations, the simulation result is indistinguishable from the exact solution.

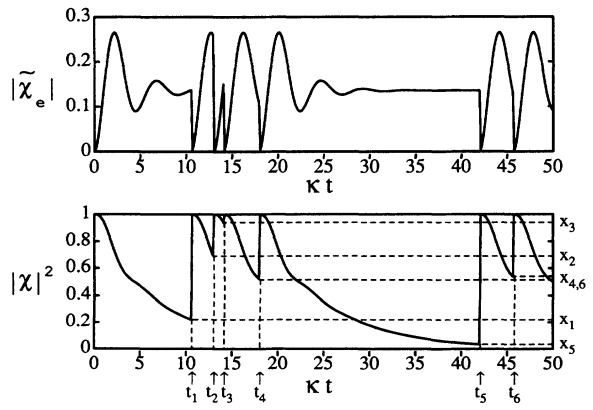

FIG. 1. Plot of a realization of the Monte Carlo wave function as a function of time: (a) excited-state probability $|\langle e|\tilde{\chi}(t)\rangle|^2$, (b) the corresponding norm $\||\chi(t)\rangle\|^2$. The parameters are $\Omega=\kappa$ and $\Delta=-\kappa$.

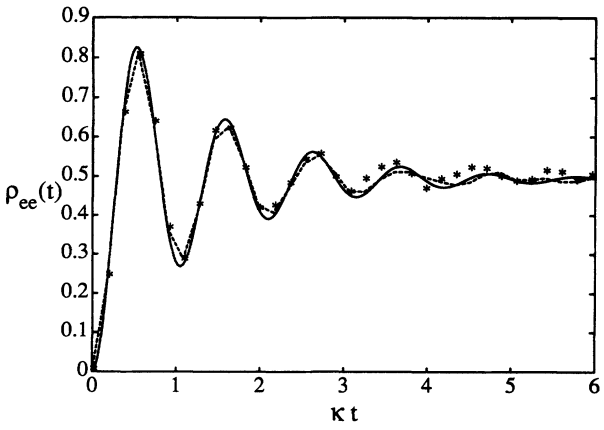

FIG. 2. Simulation predictions for the excited-state population $\rho_{ee}(t)$ are compared with the exact result derived from the optical Bloch equations. The stars correspond to 100 realizations. The dashed line has been computed with 1000 trajectories. For 10 000 realizations the simulation result is indistinguishable from the exact solution. The parameters are $\Omega=6\kappa$ and $\Delta=0$.

III. MECHANICAL LIGHT EFFECTS IN A TWO-LEVEL SYSTEM

In this section we generalize the approach of Sec. II to include the center-of-mass motion for the atom. We develop the master equation and its wave-function simulation for laser cooling of a TLS and illustrate the application of the simulation procedure to one-dimensional laser cooling of trapped ions [6,17]. Essential elements of this formalism were developed in our previous work [15].

A. Master equation and its simulation

We consider again a TLS driven by a laser and coupled to a reservoir of vacuum modes of the radiation field. The atomic part of the Hamiltonian (2) in the Schrödinger equation (1) now includes the kinetic energy $\hat{\mathbf{p}}^2/2M$, and possibly a potential $V(\mathbf{x})$. Analogous to Eq. (7) we define a reduced atomic density matrix $\rho_A(t)$ which can be shown [20] to obey the master equation

$$\frac{d}{dt}\rho_A=-i(H_{\mathrm{eff}}\rho_A-\rho_A H_{\mathrm{eff}}^\dagger)+\int d\Omega_{\hat{\mathbf{k}}}J_{\hat{\mathbf{k}}}\rho_A\ . \tag{37}$$

The non-Hermitian effective Hamiltonian

$$H_{\mathrm{eff}}=\frac{\hat{\mathbf{p}}^2}{2M}+V(\hat{\mathbf{x}})+(\omega_{eg}-i\tfrac{1}{2}\kappa)a^\dagger a -[\boldsymbol{\mu}_{eg}\cdot\mathcal{E}(\hat{\mathbf{x}},t)a^\dagger+\mathrm{H.c.}] \tag{38}$$

acts in the atomic Hilbert space $\mathcal{H}_A=L(R^3)\otimes\{|g\rangle,|e\rangle\}$, which is the product space of square-integrable center-of-mass wave packets and internal atomic states. In the interaction Hamiltonian the electric field of the laser is now evaluated at the atomic position operator $\hat{\mathbf{x}}$. Furthermore, we have defined

$$J_{\hat{\mathbf{k}}}\rho_A=\Phi(\hat{\mathbf{k}})e^{ik_{eg}\hat{\mathbf{k}}\cdot\hat{\mathbf{x}}}a\rho_A a^\dagger e^{-ik_{eg}\hat{\mathbf{k}}\cdot\hat{\mathbf{x}}}\ , \tag{39}$$

with $\Phi(\hat{\mathbf{k}})$ as the angular distribution of the spontaneously emitted photons which describes the mechanical momentum transfer $k_{eg}\hat{\mathbf{k}}$ with $k_{eg}=\omega_{eg}/c$ in Eq. (37) when the electrons return to the ground state by spontaneous emission.

Repeating the steps leading to Eq. (17) in Sec. II we identify

$$p_{[0,t)}(t_1,\hat{\mathbf{k}}_1;\ldots;t_n,\hat{\mathbf{k}}_n) = \mathrm{Tr}_A[S_{t,t_n}J_{\hat{\mathbf{k}}_n}S_{t_n,t_{n-1}}\cdots J_{\hat{\mathbf{k}}_1}S_{t_1,0}\rho_A(0)] \quad (40)$$

as the probability density that in the time interval $[0,t)$ exactly n photons are emitted at times $t_1,\ldots,t_n$ in directions $\hat{\mathbf{k}}_1,\ldots,\hat{\mathbf{k}}_n$. Furthermore, the conditional densities are

$$\tilde{c}(t,\hat{\mathbf{k}}|t_n,\hat{\mathbf{k}}_n;\ldots;t_1,\hat{\mathbf{k}}_1) = \frac{\mathrm{Tr}_A[J_{\hat{\mathbf{k}}}S_{t,t_n}J_{\hat{\mathbf{k}}_n}S_{t_n,t_{n-1}}\cdots J_{\hat{\mathbf{k}}_1}S_{t_1,0}\rho_A(0)]}{\mathrm{Tr}_A[J_{\hat{\mathbf{k}}_n}S_{t_n,t_{n-1}}\cdots J_{\hat{\mathbf{k}}_1}S_{t_1,0}\rho_A(0)]} . \quad (41)$$

In particular, the pure-state representation of the normalized atomic wave function takes on the form [15]

$$\rho_A(t)=\sum_{n=0}^{\infty}\int_0^t dt_n\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1\int d\Omega_{\hat{\mathbf{k}}_n}\cdots\int d\Omega_{\hat{\mathbf{k}}_1}p_{[0,t)}(t_1,\hat{\mathbf{k}}_1;\ldots;t_n,\hat{\mathbf{k}}_n) \times|\tilde{\Psi}(t|t_n,\hat{\mathbf{k}}_n;\ldots;t_1,\hat{\mathbf{k}}_1)\rangle\langle\tilde{\Psi}(t|t_n,\hat{\mathbf{k}}_n;\ldots;t_1,\hat{\mathbf{k}}_1)| . \quad (42)$$

Here $|\tilde{\Psi}(t|t_n,\hat{\mathbf{k}}_n;\ldots;t_1,\hat{\mathbf{k}}_1)\rangle$ is the normalized atomic wave function obtained by integrating the hierarchy of Schrödinger equations in (22) with H_{eff} given in (38) with initial conditions

$$|\Psi(t_n|t_n,\hat{\mathbf{k}}_n;\ldots;t_1,\hat{\mathbf{k}}_1)\rangle = ae^{ik_{eg}\hat{\mathbf{k}}_n\cdot\hat{\mathbf{x}}}|\Psi(t_n|t_{n-1},\hat{\mathbf{k}}_{n-1};\ldots;t_1,\hat{\mathbf{k}}_1)\rangle . \quad (43)$$

The factor involving the exponential function in Eq. (43) describes the kick the photon provides to the center-of-mass motion of the atom in spontaneous emission. We emphasize that in view of Eq. (43) the coherence of the center-of-mass packet of the atom as well as the phase of the excited-state component of the wave function is preserved in the quantum jump of the electron.

In this way it is straightforward to generalize the simulation prescription of Sec. II for the MC wave function $|\chi(t)\rangle\in\mathcal{H}_A$.

(i) *Initial condition.* We choose an initial state. Typically this will be of the form $|\chi(t_0=0)\rangle=|g\rangle\otimes|\phi\rangle$ with center-of-mass wave packet $|\phi\rangle$. We introduce a photon emission counter n which initially is set to zero, $n=0$.

(ii) *Integration loop.* For times $t<T$ we integrate the Schrödinger equation (5) until the emission time t given by

$$\int_{t_n}^{t}dt'\int d\Omega_{\hat{\mathbf{k}}}\tilde{c}(t',\hat{\mathbf{k}}|t_n,\hat{\mathbf{k}}_n;\ldots;t_1,\hat{\mathbf{k}}_1) = 1-\||\chi(t)\rangle\|^2=x , \quad (44)$$

with $x\in[0,1]$ a uniformly distributed random number. We increase the photon emission counter by one $(n\to n+1)$ and identify $t_n=t$ with the emission time. Next we choose a direction of the spontaneously emitted photon $\hat{\mathbf{k}}$ according to the angular distribution $\Phi(\hat{\mathbf{k}})$. The wave function after the quantum jump at time t_n is

$$|\chi(t_n)\rangle\leftarrow ae^{ik_{eg}\hat{\mathbf{k}}\cdot\hat{\mathbf{x}}}|\chi(t_n)\rangle/\|ae^{ik_{eg}\hat{\mathbf{k}}\cdot\hat{\mathbf{x}}}|\chi(t_n)\rangle\| . \quad (45)$$

We proceed by integrating the atomic Schrödinger equation (5) for $|\chi(t)\rangle$ until the next the decay time, etc.

(iii) *Averaging.* We repeat these simulations N times to get an approximation for the atomic density matrix according to (35). This reduced atomic density matrix contains all information on the internal atomic dynamics and the center-of-mass distribution.

B. Laser cooling in ion traps

To illustrate the simulation technique of Sec. III A we study here in some detail laser cooling of a two-level atom in a one-dimensional harmonic trap described by a trapping potential $V(x)=\frac{1}{2}M\nu^2x^2$ with oscillator frequency ν. The theory of laser cooling of trapped ions is well developed. We refer to reviews by Stenholm [17], Wineland and co-workers [21], and Blatt [22].

Below we choose to compare our MC results with analytical predictions of the theory developed by Javanainen, Lindberg, and Stenholm [17,23] for the Lamb-Dicke limit (LDL). In the LDL the particle is assumed to be confined within a spatial region much smaller than an optical wavelength, i.e., the parameter $\eta=a_0/\lambda\ll1$ with a_0 the size the harmonic-oscillator ground state and λ the wavelength of the laser [24]. In this limit the cooling time becomes slow compared with the internal time scale of the TLS and the harmonic-oscillator frequency. This allows an adiabatic elimination of the internal atomic degrees of freedom and leads to the master equation for the harmonic-oscillator populations $P_n(t)$,

$$\frac{d}{dt}P_n(t)=-\eta^2[(n+1)A_+ + nA_-]P_n(t) + \eta^2(n+1)A_-P_{n+1}(t)+\eta^2nA_+P_{n-1}(t) , \quad (46)$$

with $n=0,1,2,\ldots$. The coefficients $A_\pm$ are identified as

cooling and heating rates $n \rightarrow n \pm 1$. Explicit expression for $A_{\pm}$ in terms of the TLS parameters Ω, Δ, κ, and oscillator frequency ν have been given by Lindberg and Stenholm [20,25]. In terms of these rates the final energy for $t \rightarrow \infty$ is $E_f = \hbar\nu(n_f + \frac{1}{2})$ with mean population

$$n_f = A_+ / (A_- - A_+)(A_- > A_+) . \quad (47)$$

The stationary solution is a Bose-Einstein distribution

$$P_n^{\mathrm{st}} = (1 - A_+ / A_-)(A_+ / A_-)^n . \quad (48)$$

Time-dependent solutions have been given by Stenholm [25]. In particular, the mean occupation is

$$\langle n \rangle_t = n_0 e^{-Wt} + n_f (1 - e^{-Wt}) , \quad (49)$$

where $W = \eta^2 (A_- - A_+) \geq 0$ is the cooling rate. Cooling is found for detunings of the laser below resonance, $\Delta < 0$.

MC simulations results are not limited to the LDL and are not based on an adiabatic elimination assumption as Eq. (46). In contrast, the approximation inherent in a simulation procedure is that it is restricted to a finite number of trials N, and that the integration of the Schrödinger equation (5) requires representation of the center-of-mass wave function in a finite basis: In the present case we have chosen a truncated basis set of harmonic-oscillator states $|n\rangle$ with $0 \leq n \leq n_{\max}$. In Figs. 3 and 4 we compare our MC predictions with the above analytical results for the parameters $\Omega = \nu = \kappa$, $\Delta = -\kappa$, and Lamb-Dicke parameter $\eta = 0.1$. Initially, the atoms are prepared in the harmonic-oscillator state $|n = 8\rangle$, and $n_{\max} = 16$. An average over 1500 MC wave functions was taken. The angular distribution was assumed to be isotropic. Figure 3 is a plot of the distribution function $P_n(t)$ as a function of n for times $\kappa t = 15, 150, 500$ and $t \rightarrow \infty$ (stationary solution). The dashed lines are the analytical Lamb-Dicke formulas [17], while the symbols indicate the MC results. Figure 4 shows the distribution function $P_n(t)$ as a function of time κt for $n = 0, 2, 4, 6, 8$.

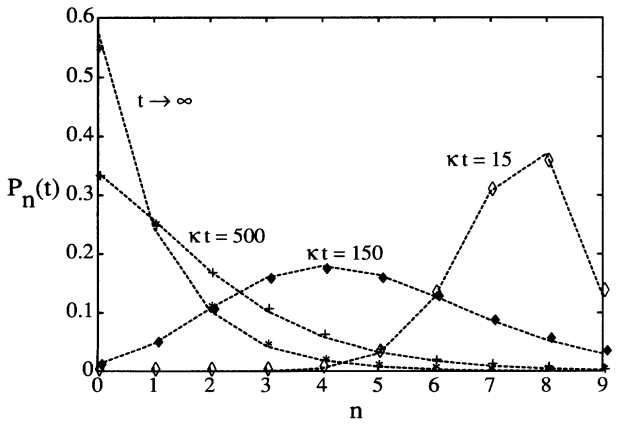

FIG. 3. Laser cooling of trapped ions. The distribution function $P_n(t)$ of the population of trap levels is plotted as a function of n for times $\kappa t = 15, 150, 500, \infty$. The dashed lines are the analytical results [17]. The symbols correspond to the simulations. The parameters are $\nu = 1, \Omega = 2, \Delta = 1$ in units of κ.

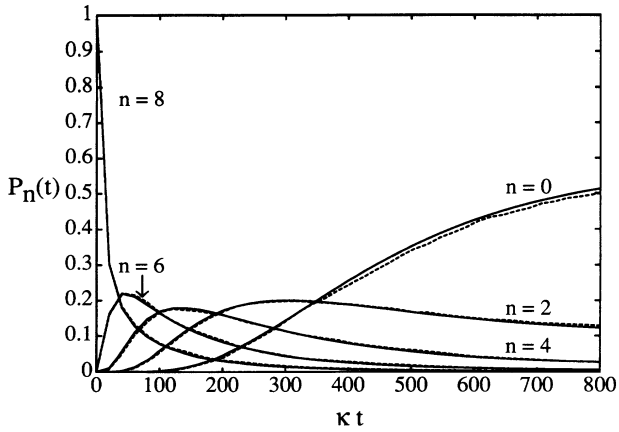

FIG. 4. Laser cooling of trapped ions. The distribution function $P_n(t)$ of the population of trap levels is plotted as a function of time κt for $n = 0, 2, 4, 6, 8$. The solid lines are the analytical results [17], while the dashed lines correspond to simulations. The parameters are the same as in Fig. 3.

The solid lines are the analytical results [17], while the dashed lines correspond to simulations. Agreement of simulation with the analytical results tends to be quite good.

IV. TWO-LEVEL SYSTEM WITH ZEEMAN SUBSTRUCTURE

In this section we generalize the treatment of Sec. II to include the Zeeman substructure. The angular momenta of the atomic ground- and excited-state levels are J_g and J_e, respectively. We choose as a basis the eigenstates of $J_{e,g}^z$, which we write as $|gm_g\rangle$ and $|em_e\rangle$. The master equation for the TLS driven by a laser field [26]

$$\mathcal{E}_{\mathrm{cl}}(\mathbf{x}=0,t) = \mathcal{E}_{\mathrm{cl}} \sum_{q=0,\pm 1} (-1)^q \epsilon_{-q} \mathbf{e}_q e^{-i\omega t} + \mathrm{c.c.} \quad (\sum_q |\epsilon|^2 = 1) \quad (50)$$

is

$$\frac{d}{dt}\rho_A = -i(H_{\mathrm{eff}}\rho_A - \rho_A H_{\mathrm{eff}}^{\dagger}) + \sum_{q=0,\pm 1} J_q \rho_A \quad (51)$$

with

$$H_{\mathrm{eff}} = (\omega_{eg} - i\tfrac{1}{2}\kappa) \sum_{m_e} |em_e\rangle\langle em_e| - \left[\tfrac{1}{2}\Omega_{eg} \sum_q (-1)^q \epsilon_{-q} \mathcal{A}_q e^{-i\omega t} + \mathrm{H.c.} \right] . \quad (52)$$

The $\mathbf{e}_q$ with $q = 0, \pm$ forms a spherical vector basis. κ is the radiative decay rate and Ω_{eg} is the average Rabi frequency as given by Shore [27]. Here we have introduced atomic lowering operators

$$\mathcal{A}_q = \sum_{m_e, m_g} \langle J_g m_g 1q | J_e m_e \rangle |gm_g\rangle\langle em_e| , \quad (53)$$

where $\langle J_e m_e | J_g m_g 1 q \rangle$ is a Clebsch-Gordan coefficient and

$$J_q \rho_A = \kappa \mathcal{A}_q \rho_A \mathcal{A}_q^\dagger \ . \tag{54}$$

As in Secs. II and III we introduce the probability densities

$$p_{[0,t)}(t_1,q_1;\ldots;t_n,q_n) = \mathrm{Tr}_A[S_{t,t_n} J_{qn} S_{t_n,t_{n-1}} \cdots J_{q1} S_{t_1,0} \rho_A(0)] \tag{55}$$

and conditional probability densities

$$\tilde{c}(t,q|t_n,q_n,\ldots,t_1,q_1) = \frac{\mathrm{Tr}_A[J_q S_{t,t_n} J_{qn} S_{t_n,t_{n-1}} \cdots J_{q1} S_{t_1,0} \rho_A(0)]}{\mathrm{Tr}_A[J_{qn} S_{t_n,t_{n-1}} \cdots J_{q1} S_{t_1,0} \rho_A(0)]} \tag{56}$$

for spontaneous emissions at times $t_n,\ldots,t_1$ with polarizations $q_n,\ldots,q_1$. In a similar way we introduce wave functions $|\Psi(t|t_n,q_n,\ldots,t_1,q_1)\rangle$, so that

$$\sum_q \int_{t_n}^t d\tau\, \tilde{c}(\tau,q|t_n,q_n,\ldots,t_1,q_1) = 1 - \frac{\||\Psi(t|t_n q_n,\ldots,t_1,q_1)\rangle\|^2}{\||\Psi(t_n|t_n,q_n,\ldots,t_1,q_1)\rangle\|^2} \ . \tag{57}$$

In terms of the Mollow wave functions the density matrix is

$$\rho_A(t) = \sum_{n=0}^{\infty} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \sum_{q_1,\ldots,q_n} p_{[0,t)}(t_1,q_1;\ldots;t_n,q_n) |\tilde{\Psi}(t|t_n,q_n;\ldots;t_1,q_1)\rangle\langle\tilde{\Psi}(t|t_n,q_n;\ldots;t_1,q_1)| \tag{58}$$

where the tilde again indicates normalization.

The resulting simulation procedure for the MC wave functions $|\chi(t)\rangle$ is the same as in the preceding sections. The polarization of the emitted photons is chosen according to the probability distribution $P_q(t)/\sum_q P_q(t)$ with

$$P_q(t) = \mathrm{Tr}_A[J_q S_{t,0} \rho_A(0)] / \mathrm{Tr}_A[S_{t,0} \rho_A(0)] \ .$$

The wave function after the quantum jump with emission of a photon of polarization q is

$$|\chi(t_n)\rangle \leftarrow \mathcal{A}_q |\chi(t_n)\rangle / \|\mathcal{A}_q |\chi(t_n)\rangle\| \ . \tag{59}$$

An interesting question is the manifestation of trapping states [28] in the simulation procedure. Trapping states (or dark states) correspond to linear combinations of atomic ground states which are not coupled by the atomic dipole matrix element to the excited atomic state. These trapping states appear as eigenstates of H_{eff} with purely real (nondecaying) eigenvalues. Thus these dark states will lead to

$$\sum_q \int_{t_{n-1}}^{\infty} d\tau\, \tilde{c}(\tau,q|t_{n-1},q_n,\ldots,t_1,q_1) < 1 \ , \tag{60}$$

so that there is a finite probability for the emission time t_n of the next photon to be $t_n \to \infty$.

V. CONCLUSIONS

In this paper we have developed a MC simulation of the atomic master equation for spontaneous emission in terms of atomic wave functions. The starting point of our theory has been Mollow's pure-state analysis of resonant light scattering and its interpretation in the context of the Srinivas-Davies theory of continuous measurements in photodetection. We have shown that realizations of the time evolution of atomic wave functions can be constructed which correspond to an ensemble of laser-driven atoms undergoing a sequence of spontaneous emissions. The atomic decay times are drawn according to the photon-counting distributions. Each of these spontaneous-emission events (quantum jumps) is associated with a projection of the atomic wave function to the ground state of the atom. In addition to developing the formalism for a TLS, we have presented an extension of the theory to include mechanical light effects, and a generalization to atomic systems with Zeeman substructure.

Potential areas of application for the present technique as a calculational tool are laser cooling of atoms, where the center-of-mass motion of the atom must be described quantum mechanically, in particular in situations with complicated atomic level structure, and two- and three-dimensional models. In addition, the present method is ideally suited to model spontaneous emission in atomic beam deflections from running, standing, or evanescent light waves [5].

A wave-function simulation can also be developed for damped harmonic oscillators (damped modes of the radiation fields) and can be generalized to include a thermal or squeezed bath. This opens the prospect of applying this simulation procedure to solve cavity QED problems [29] where one or a few atoms interact strongly with a cavity mode of the radiation field.

Note added in proof. In the meantime we have become aware of the work of H. Carmichael (unpublished) and C. Cohen-Tannoudji, F. Bardou, and A. Aspect [in *Laser Spectroscopy X*, edited by M. Ducloy, E. Giacobino, and G. Camy (World Scientific, Singapore, in press)]. Carmichael discusses a simulation algorithm similar to Ref. [16]. Cohen-Tannoudji, Bardou, and Aspect simulate wave functions for velocity-selective coherent population trapping.

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[18] By normalizing $|\chi\rangle$ at time t_n we ensure that the probability for the next photon emission is given by Eq. (33). Note that the simulation procedure to determine the decay time $t=t_n$ guarantees a nonzero norm $\|a|\chi(t_n)\rangle\|>0$.

[19] For a TLS $\{|g\rangle,|e\rangle\}$ (without external degrees of freedom, etc.) the decay time t_n depends only on the time interval t_n-t_{n-1} with t_{n-1} the last emission time, and is independent of earlier times $t_{n-2},\ldots,t_1$ [compare Eq. (28)]. Thus, to determine t_n for a given random number x_n we can set up a table for the inverse of (28) at the beginning of the calculation. These decay times also provide very good first estimates for the determination of $t_n(x_n)$ according to (33) in the case of mechanical light effects.

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