Monte Carlo wave functions and nonlinear master equations

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The Monte Carlo wave-function method has recently proved to be an efficient tool in the analysis of linear dissipative quantum systems, i.e., systems with linear equations of motion for their density matrix. We generalize this method to systems with nonlinear master equations of a parametrized Lindblad form, which includes master equations obtained by Hartree-Fock approximations. Convergence properties of the algorithm are discussed in detail. The method is illustrated by a numerical analysis of the bosonic enhancement of laser cooling of trapped particles. [S1050-2947(96)08411-9]

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I. INTRODUCTION

In quantum mechanics we are used to dealing with linear equations of motion for wave functions or density matrices. In cases with a large number of interacting particles these equations may be difficult or even impossible to solve, and one may try to replace them by an approximate few particle equation. In such an equation the effect of the other particles is incorporated in a mean field term which is, in turn, derived from the current few-particle state itself. An example of such a self-consistent approach is the Hartree or Hartree-Fock treatment applied in many fields of physics. The resulting approximate equation of motion is a nonlinear one.

With the low temperatures and high densities available in laser cooling and trapping, samples of ultracold atoms have become promising new states of matter for the study of collective behavior. By laser cooling and evaporative cooling it has been possible [1–3] to produce samples in thermal equilibrium with a macroscopic number of atoms in a single quantum state — termed a Bose-Einstein condensate. Another interesting possibility is to produce a Bose-Einstein condensate directly with laser cooling [4–6]. Also, interesting phenomena occur in the propagation of multiply populated atomic wave packet states in laser fields where both quantum statistical effects and the actual interaction between particles come into play [7–9]. All these phenomena can approximately be described by nonlinear equations of motion.

In laser cooling, dissipation (by spontaneous emission of light) is an essential ingredient in the dynamics, making these problems very difficult to treat numerically. Already, the integration of the master equation for a single atom cooled in a laser field presents a formidable task, and in three dimensions numerical solutions have only been provided by use of the Monte Carlo wave-function technique [10]. It is therefore natural to consider the application of this technique also to the nonlinear master equations considered in the many-body situation.

It has been proven [11–14] that Monte Carlo wave functions apply to any linear master equation of the so-called Lindblad form. A brief review of the algorithm is presented in Sec. II. It has been speculated [7] that such a treatment cannot be generalized to nonlinear master equations, and, indeed, modifications are necessary as presented in Sec. III. The idea is to propagate in parallel a number of state vectors: at each time step in the calculation the whole ensemble is needed to determine the coefficients in the equation of motion of the individual state vectors. The resulting coupling among the state vectors in the simulation makes it difficult to assess the accuracy of the method. This is why in Sec. IV we shall discuss the convergence properties of the method proposed. Our conclusion, supported by an analytical and a numerical analysis, is that the statistical error follows the usual scaling law $1/\sqrt{n}$, where n is the number of state vectors, and that there exists a bias of the results relative to the exact density matrix solution, scaling only as $1/n$ and which is therefore negligible for large n. Nonlinear master equations derived from the coupled Maxwell-Bloch equations (Bloch-Hartree and Bloch-Hartree-Fock equations) are discussed in Sec. V. A simplified form of these equations, keeping only the bosonic enhancement of optical pumping in a laser cooling situation, is simulated with Monte Carlo wave functions in Sec. VI.

II. SIMULATION ALGORITHM FOR LINEAR MASTER EQUATIONS OF LINDBLAD TYPE

It has been proven [15] that to preserve the required properties of a density matrix (normalization, positivity) any linear master equation must be of the so-called Lindblad form:

$$\frac{d}{dt}\rho = \frac{1}{i\hbar}[H_{\rm eff}\rho - \rho H_{\rm eff}^{\dagger}] + \sum_m C_m \rho C_m^{\dagger}, \tag{1}$$

$$H_{\rm eff} = H - \frac{1}{2} i\hbar \sum_m C_m^{\dagger} C_m . \tag{2}$$

The effective Hamiltonian $H_{\rm eff}$ is a sum of a Hermitian Hamiltonian H and an anti-Hermitian part leading to a reduction of the norm of the density operator. This reduction,

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representing the decay of unstable states induced by a coupling to the environment, is exactly balanced by the last ''sandwich-terms'' in Eq. (1).

As discussed by several authors [11–14,16,17], it is possible to evolve wave functions in time, so that an average over a large number of independent realizations leads to the same predictions as the master equation for the system.

Assume the Monte Carlo wave function $|\psi(t)\rangle$ at time t. To propagate this function in time we first calculate the wave function $|\psi_0(t+dt)\rangle$ obtained by evolving $|\psi(t)\rangle$ with the non-Hermitian Hamiltonian $H_{\rm eff}$:

$$|\psi_0(t+dt)\rangle=\left(1+\frac{1}{i\hbar}H_{\rm eff}dt\right)|\psi(t)\rangle \tag{3}$$

for a ''small'' time step dt. The square of the norm of $|\psi_0(t+dt)\rangle$ is $1-\delta p$, where δp reads

$$\delta p=\sum_m \delta p_m=\sum_m dt\langle\psi(t)|C_m^\dagger C_m|\psi(t)\rangle. \tag{4}$$

At this stage we introduce a random element in the evolution. Either the wave function $|\psi_0(t+dt)\rangle$ replaces $|\psi(t)\rangle$, or with a probability δp we apply a quantum jump, i.e., the wave function is collapsed on a specific state $C_m|\psi(t)\rangle$ with a probability $\delta p_m/\delta p$. At time $t+dt$ we have one of the normalized wave functions:

$$\text{with probability } 1-\delta p,\quad |\psi(t+dt)\rangle=\frac{|\psi_0(t+dt)\rangle}{\sqrt{1-\delta p}};$$

$$\text{with probability } \delta p_m,\quad |\psi(t+dt)\rangle=\frac{C_m|\psi(t)\rangle}{\sqrt{\delta p_m/dt}}. \tag{5}$$

In this description of the Monte Carlo method we have introduced a ''small'' time step dt. In fact, the proper stochastic process for the wave function $|\psi(t)\rangle$ is obtained for an infinitesimally small dt. In a numerical calculation this mathematical limit $dt\to 0$ may be difficult to achieve in practice, and a direct implementation of the previously described random walk with a finite dt may lead to severe accuracy problems. The solution is to formulate the Monte Carlo wave function method in terms of the ''delay function'' [18]. The quantum jumps are then not decided from the expression (4), linear in the ''small'' time step dt, and the user may apply a more accurate numerical integration technique, e.g., higher order Runge-Kutta, suitable for the derivation of the delay function and the wave function in the problem; this point is particularly relevant for the nonlinear situations to be described, where an adaptive stepsize control for the integration scheme may be required.

For any Hermitian operator B, the expectation value $\langle\psi(t)|B|\psi(t)\rangle$ is now a stochastic variable, and the correspondence between the Monte Carlo simulation and the solution of the master equation implies that

$$\langle\langle\psi(t)|B|\psi(t)\rangle\rangle=\mathrm{Tr}[\rho(t)B], \tag{6}$$

where $\langle\cdots\rangle$ denotes the average over an infinite number of independent realizations, and $\rho(t)$ is the exact solution of Eq. (1).

In practice one deals with a finite number n of realizations. The finite sample estimate of the mean value of B, $b^{(n)}=(1/n)\Sigma_{i=1}^n\langle\psi_i(t)|B|\psi_i(t)\rangle$, is itself a stochastic variable. The precision with which $b^{(n)}$ approximates $\mathrm{Tr}[\rho(t)B]$ is thus related to the fluctuations in this stochastic variable. To determine these fluctuations one would in principle have to repeat the simulation with n wave functions a large number of times, and from this calculate the mean and the variance. This procedure is well known in the present case of linear master equations, because the various wave functions are statistically independent. It is useful, however, to give here a detailed discussion in order to facilitate the transposition to the case of nonlinear master equations. We therefore define the averages over repetitions of the simulation with n wave functions:

$$\langle b^{(n)}\rangle_{\rm rep}=\left\langle\frac{1}{n}\sum_{i=1}^n\langle\psi_i(t)|B|\psi_i(t)\rangle\right\rangle_{\rm rep}, \tag{7}$$

$$\mathrm{var}_{\rm rep}(b^{(n)})\equiv\langle(b^{(n)})^2\rangle_{\rm rep}-\langle b^{(n)}\rangle_{\rm rep}^2. \tag{8}$$

Inserting the expression for $b^{(n)}$ in this equation we obtain

$$\mathrm{var}_{\rm rep}(b^{(n)})=\frac{1}{n^2}\sum_{i,j=1}^n\langle\langle\psi_i(t)|B|\psi_i(t)\rangle\langle\psi_j(t)|B|\psi_j(t)\rangle\rangle_{\rm rep}-\langle b^{(n)}\rangle_{\rm rep}^2. \tag{9}$$

We now make use of the following identities, expressing the fact that the expectation values $\langle\psi_i(t)|B|\psi_i(t)\rangle$ are independent stochastic variables:

$$\langle\langle\psi_i(t)|B|\psi_i(t)\rangle\rangle_{\rm rep}=\langle\langle\psi(t)|B|\psi(t)\rangle\rangle, \tag{10}$$

$$\langle\langle\psi_i(t)|B|\psi_i(t)\rangle\langle\psi_j(t)|B|\psi_j(t)\rangle\rangle_{\rm rep}=\langle\langle\psi(t)|B|\psi(t)\rangle^2\rangle \quad \text{for } i=j \tag{11}$$

$$=\langle\langle\psi(t)|B|\psi(t)\rangle\rangle^2 \quad \text{for } i\neq j. \tag{12}$$

This leads to

$$\langle b^{(n)}\rangle_{\rm rep}=\langle\langle\psi(t)|B|\psi(t)\rangle\rangle, \tag{13}$$

$$\mathrm{var}_{\rm rep}(b^{(n)})=\frac{1}{n}\,\mathrm{var}(\langle\psi|B|\psi\rangle). \tag{14}$$

The variance scales as $1/n$, which implies that the error bars shrink as $1/\sqrt{n}$ as usual for sampling statistics. In explicit numerical implementations only one realization is made with n wave functions and the quantity $\mathrm{var}(\langle\psi|B|\psi\rangle)$ is estimated by the sample variance

$$\frac{1}{n-1}\sum_{i=1}^n[\langle\psi_i(t)|B|\psi_i(t)\rangle-b^{(n)}(t)]^2 \tag{15}$$

as discussed in more detail in [14].

III. SIMULATION ALGORITHM FOR NONLINEAR MASTER EQUATIONS OF PARAMETRIZED LINDBLAD TYPE

We assume a physical problem leading to the first order differential equation in time:

$$\frac{d}{dt}\rho = F[\rho]_{\mathrm{NL}}, \tag{16}$$

where ρ is a density matrix and F acts nonlinearly on ρ as indicated by the subscript ''NL.''

To make the following discussion less abstract we shall refer to the example of spontaneous emission of N two-level atoms (ground state g and excited state e) in the case where all atoms are assigned the same classical center-of-mass position. In the absence of a mean atomic dipole, the excited state population of the atoms may be described by the phenomenological equation for superradiance [19]:

$$\frac{d}{dt}\rho_{ee} = -\Gamma[1+(N-1)(1-\rho_{ee})]\rho_{ee}. \tag{17}$$

It is written here without a geometrical reduction factor and we have replaced N by $N-1$ to recover the usual one-atom case for $N=1$. The coefficient Γ denotes the single atom spontaneous emission rate. This equation will be derived as an example of the Bloch-Hartree-Fock equations in Sec. V.

In the nonlinear case we do not have an equivalent of Lindblad's theorem, giving a necessary form to F ensuring that the norm and positivity of ρ is conserved in Eq. (16). We propose a class of equations which we believe will embrace most of the relevant nonlinear master equations.

First, we write Eq. (16) in the suggestive parametrized form:

$$\frac{d}{dt}\rho = L(\sigma)[\rho], \tag{18}$$

$$\sigma = \rho, \tag{19}$$

where the Liouvillian operator $L(\sigma)$ acts linearly on the density matrix ρ, without necessarily being a linear function of its density matrix argument σ. It should be expected that the derivation of the nonlinear master equation would lead to such a parametric appearance of $F[\rho]_{\mathrm{NL}}$. For example, in a mean field treatment, σ represents the density matrix for the other atoms in the sample, and Eq. (19) represents the self-consistency in such a treatment. For the superradiance example, such a parametrization is clearly possible: Equation (17) is equivalent to the usual equation for the single atom decay problem but with an effective rate $\Gamma_{\mathrm{eff}}=\Gamma[1+(N-1)(1-\sigma_{ee})]$, where as in Eq. (19), $\sigma_{ee}=\rho_{ee}$. We note that the parametrized form (18) and (19) does not generally define $L(\sigma)$ in a unique way. For example, a product of two density matrix elements $\rho_{ij}\rho_{kl}$ appearing on the right-hand side (RHS) of Eq. (16) may both be represented by $\sigma_{ij}\rho_{kl}$ and by $\rho_{ij}\sigma_{kl}$. Similarly, a Hamiltonian $H(\sigma)$ may be replaced by $H(\sigma)+f(\sigma)$, where $f(\sigma)$ is any c-number function, without changing the pertaining commutator in the master equation Eq. (16).

Second, we suppose that $L(\sigma)[\rho]$ can be put in the Lindblad form Eq. (1) where the C_m operators and the Hamiltonian H may now depend on the density matrix σ. The existence of such a *parametrized Lindblad form* is crucial for our ability to simulate the master equation with Monte Carlo wave functions. Note that this will at the same time ensure that Eq. (16) preserves all the desired properties of a density matrix.

It is not evident that a nonlinear master equation will naturally appear in this form. Using the nonuniqueness of $L(\sigma)$, however, one may succeed in bringing Eq. (16) into the desired form. We treat here in detail the case of a nonlinear term of the form

$$\frac{d}{dt}\rho = -\frac{1}{2}\{W(\rho),\rho\} \equiv -\frac{1}{2}[W(\rho)\rho+\rho W(\rho)], \tag{20}$$

which will appear in the physical examples of Sec. V. We assume that in this equation the operator $W(\rho)$ is Hermitian for any Hermitian matrix ρ so that the density matrix ρ remains Hermitian. The trace of ρ has to be preserved by Eq. (20), which implies

$$\mathrm{Tr}[W(\rho)\rho]=0 \tag{21}$$

for any ρ. We want to bring Eq. (20) into the parametrized form (18) and (19) where the Liouvillian $L(\sigma)[\rho]$ is of the Lindblad form. Eq. (20) contains the equivalent of the first term on the RHS of Eq. (1), but the ''sandwich-term'' is missing. We use Eq. (21) to provide such a term vanishing for $\sigma=\rho$ [20]:

$$L(\sigma)[\rho] = -\frac{1}{2}\{W(\sigma),\rho\} + \mathrm{Tr}[W(\sigma)\rho]\sigma. \tag{22}$$

A second step is to ensure that the last term in Eq. (22) is positive. This is not immediately the case as shown by Eq. (21), but it can be made positive when $W(\sigma)$ is bounded from below, i.e., when one can find a real number $\gamma(\sigma)$ such that $W(\sigma)+\gamma(\sigma)$ is positive. This is the case in the physical discussion of Sec. V. Replacing $W(\sigma)$ by $W(\sigma)+\gamma(\sigma)$ we finally obtain instead of Eq. (20):

$$L(\sigma)[\rho] = -\frac{1}{2}\{W(\sigma)+\gamma(\sigma),\rho\} + \mathrm{Tr}[(W(\sigma)+\gamma(\sigma))\rho]\sigma. \tag{23}$$

One can then check that this expression reduces to the right-hand side of Eq. (20) for $\sigma=\rho$. It can furthermore be put in the parametrized Lindblad form, with jump operators $C_{m_1,m_2}=\sqrt{\pi_{m_1}}|m_1\rangle\langle m_2|[W(\sigma)+\gamma(\sigma)]^{1/2}$, where $\{|m\rangle\}$ is the set of eigenstates of $\sigma(t)$: $\sigma=\Sigma_m \pi_m |m\rangle\langle m|$. This discussion is also relevant when $\sigma\equiv\rho_0$ is a fixed density matrix and $W(\sigma)\equiv 0$. Equation (23) in this case reduces to the linear inhomogeneous master equation often used to describe open systems where particles enter at a certain rate γ with a given density matrix ρ_0 and leave the sample by some loss mechanism [21].

We now turn to the wave-function treatment of nonlinear master equations of parametrized Lindblad form. Clearly, for any fixed value of $\sigma(t)$ one is able to simulate Eq. (18) which is linear in ρ with the usual algorithm Eq. (5). The fact

that σ should be set equal to ρ at each time step [according to Eq. (19)] leads to the following suggestion: A large number n of wave functions are evolved in parallel, and we assume that at time t these wave functions produce a good approximation to the density matrix $\rho(t)$. In the subsequent time evolution of the wavefunctions, the nonlinearity is accounted for by constructing the current $\sigma(t)$ by the approximation

$$\sigma(t)=\rho^{(n)}\equiv\frac{1}{n}\sum_{i=1}^{n}|\psi_i^{(n)}(t)\rangle\langle\psi_i^{(n)}(t)|. \tag{24}$$

This $\sigma(t)$, treated as a parameter, now yields the linear master equation for $\rho(t)$, Eq. (18), which is simulated by the Monte Carlo wave functions in the usual way. It is important that the wave functions are propagated in parallel, so that $\sigma(t)$ can be updated with sufficient precision for the subsequent time evolution. This procedure yields the correct result for $n\to\infty$. For a finite n, however, one expects a systematic error (bias) due to the approximation in Eq. (24). That is, in addition to the statistical error, found also in the linear case, a discrepancy with the exact density matrix is due to the use of inaccurate terms in the Liouvillian $L(\sigma)$ inferred from Eq. (24). Also, the n wave functions in a given realization are no longer statistically independent, so that the statistical error cannot be estimated from a single realization as in Eq. (15), and the scaling law for the statistical error is not obvious. Section IV is devoted to a discussion of these aspects.

Our simple superradiance example illustrates these features. For this problem the simulation algorithm is particularly simple: we start with a number n of wave functions, all equal to the excited state vector at time $t=0$. This number of wave functions should not be confused with the number of atoms, N. At any time during the evolution, each wave function may experience a quantum jump, collapsing it to the ground state with a transition rate given by $\Gamma_{\rm eff}$, the previously collapsed wave functions remaining forever equal to the ground state vector. As the simulation proceeds, the value of $\Gamma_{\rm eff}$ increases according to the current number n_g of wave functions equal to the ground state vector, $\Gamma_{\rm eff}=\Gamma+\Gamma(N-1)n_g/n$. This causes the known deviation from the exponential decay law.

By taking a small number of wave functions we may readily explore the bias effects mentioned above. With only one wave function, the decay rate $\Gamma_{\rm eff}$ is seen to have the constant value Γ until the state is collapsed onto the ground state vector, i.e., irrespective of the value of N the simulation proceeds as a simulation of usual single atom decay. Already with two wave functions a difference appears: initially we have the single-atom decay rate Γ, but as soon as one of the states has been collapsed into the ground state, the decay rate for the remaining state vector attains the larger value $\Gamma_{\rm eff}=(N+1)\Gamma/2$. Averaged over a large number of realizations, this will produce a nonexponential behavior for the mean excited state population. With the notation of Sec. II, $(B=|e\rangle\langle e|)$, we get

$$\langle b^{(2)}(t)\rangle_{\rm rep}=\frac{N-1}{N-3}\exp(-2\Gamma t)-\frac{2}{N-3}\exp(-(N+1)\Gamma t/2). \tag{25}$$

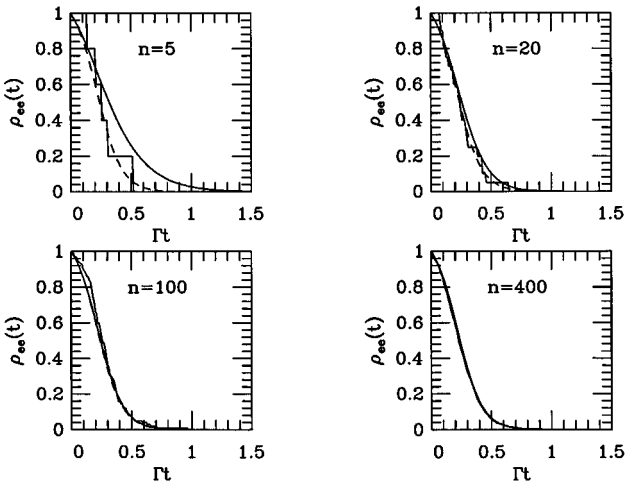

FIG. 1. Excited state population as function of time for a number of $N=10$ atoms in the superradiance model. Predictions of the Monte Carlo method are shown for various numbers n of wave functions: the curves with jumps correspond to a single realization with n wave functions, the solid curves are the averages over 64 000 realizations. Numerical errors are reduced by use of the ''delay function'' technique. The dashed line is the exact density matrix result.

The convergence of $b^{(n)}(t)$ towards the density matrix result

$$\rho_{ee}(t)=\frac{N}{N-1+\exp(N\Gamma t)} \tag{26}$$

for increasing values of the number of wave functions n can be followed in Fig. 1. For each value of n the n-step solid curve corresponds to $b^{(n)}(t)$ for a single realization, the smooth solid curve corresponds to the average $\langle b^{(n)}(t)\rangle_{\rm rep}$ of $b^{(n)}(t)$ over a large number of realizations, and the dashed line represents the exact solution Eq. (26). The number of atoms is $N=10$ in the figures. It will be shown in the next section that for this particular superradiance problem a number of wave functions $n\gg N$ is required in the simulation in order to produce accurate results. In the numerical calculation, as emphasized in the preceding section, we use the technique of the ''delay function'' [18] to avoid time discretization errors.

We end this section with a practical consideration on the simulation of the nonlinear master equation (20); this will be useful in Sec. VI. Our presentation of the jump operators C_{m_1,m_2} after Eq. (23) might indicate that a costly diagonalization of σ is required for each time step t where a quantum jump occurs. Fortunately this is not necessary. According to Eq. (24), $\sigma(t)$ is already obtained in the simulation as a statistical mixture of states $|\psi_i(t)\rangle$. Equation (23) can then also be represented by jump operators $C_{j,m}(t)=(1/\sqrt{n})|\psi_j(t)\rangle\langle e_m|[W(\sigma(t))+\gamma(\sigma(t))]^{1/2}$, where j ranges from 1 to n and where $\{|e_m\rangle\}$ is any orthonormal basis. $C_{j,m}|\psi_i(t)\rangle$ is proportional to $|\psi_j(t)\rangle$ for any m, and if the wave function $|\psi_i(t)\rangle$ experiences a quantum jump at time $t+dt$, which occurs with a probability $\delta p=\langle\psi_i(t)|W(\sigma(t))+\gamma(\sigma(t))|\psi_i(t)\rangle dt$, either nothing happens $(i=j)$ or it is simply replaced by another member $|\psi_j(t)\rangle$ of the current ensemble of Monte Carlo wave func-

tions. The relative probability of a collapse to a specific $|\psi_j(t)\rangle$ is $\Sigma_m||C_{j,m}|\psi_i(t)\rangle||^2/(\delta p/dt)=1/n$, and one simply has to choose j with uniform weights on the numbers between 1 and n.

IV. CONVERGENCE PROPERTIES OF THE SIMULATION IN THE NONLINEAR CASE

The aim of the calculation is to determine the mean value of some operator B, $b(t)\equiv \mathrm{Tr}[\rho(t)B]$, where ρ is the exact solution of Eq. (16). When the master equation (16) can be put in the parametrized Lindblad form, a simulation by n Monte Carlo wave functions is possible, where the maximal value of n in the numerical implementation is limited by both the calculation time and the required memory. The result of the simulation is a stochastic variable $b^{(n)}(t)$ $=\mathrm{Tr}[\rho^{(n)}(t)B]$, where the density matrix $\rho^{(n)}(t)$ is given by Eq. (24).

To estimate to which extent $b^{(n)}(t)$ is a good approximation of $b(t)$, we consider, as in Eqs. (7) and (8), the average and the variance of $b^{(n)}(t)$ over an infinite number of realizations of the n wave-function simulation. To ease our notation we will omit the subscript ''rep'' in what follows. We define a systematic error (a ''bias'') due to the finite size of the sample and a statistical uncertainty:

$$\mathrm{Bias}\equiv\langle b^{(n)}(t)\rangle-b(t), \tag{27}$$

$$(\mathrm{Uncertainty})^2\equiv \mathrm{var}(b^{(n)}(t)) \tag{28}$$

$$=\langle(\mathrm{Tr}(\rho^{(n)}B))^2\rangle-(\mathrm{Tr}(\langle\rho^{(n)}\rangle B))^2$$

$$=\mathrm{Tr}[(\langle\rho^{(n)}\otimes\rho^{(n)}\rangle-\langle\rho^{(n)}\rangle\otimes\langle\rho^{(n)}\rangle)(B\otimes B)]. \tag{29}$$

We have introduced the tensor products $B\otimes B$ and $\rho^{(n)}\otimes\rho^{(n)}$ and used the definition of the trace on the tensor product space which yields $\mathrm{Tr}[(\rho^{(n)}\otimes\rho^{(n)})(B\otimes B)]$ $=(\mathrm{Tr}[\rho^{(n)}B])^2$.

From Eq. (24) it appears that the expanded form of the tensor product $\rho^{(n)}\otimes\rho^{(n)}$ involves two types of terms. The first type is a product of dyadics $|\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|\otimes|\psi_j^{(n)}\rangle\langle\psi_j^{(n)}|$ with $i\neq j$ $[n(n-1)$ terms]; as discussed below, the mean of such a product is expected to decorrelate in the limit of $n\to\infty$. The second type of term has $i=j$ in the tensor product (n terms); the mean of such a product does not decorrelate even for $n\to\infty$. It is therefore necessary to consider the behavior of such individual terms, and we introduce the notation

$$O_i^{(n)}(t)\equiv|\psi_i^{(n)}(t)\rangle\langle\psi_i^{(n)}(t)|, \tag{30}$$

$$O_{i,j}^{(n)}(t)\equiv O_i^{(n)}(t)\otimes O_j^{(n)}(t)\cdots. \tag{31}$$

The expressions leading to the bias and the statistical uncertainty in Eqs. (27) and (29) now read:

$$\langle b^{(n)}(t)\rangle-b(t)=\mathrm{Tr}(\langle\delta O_1^{(n)}\rangle B), \tag{32}$$

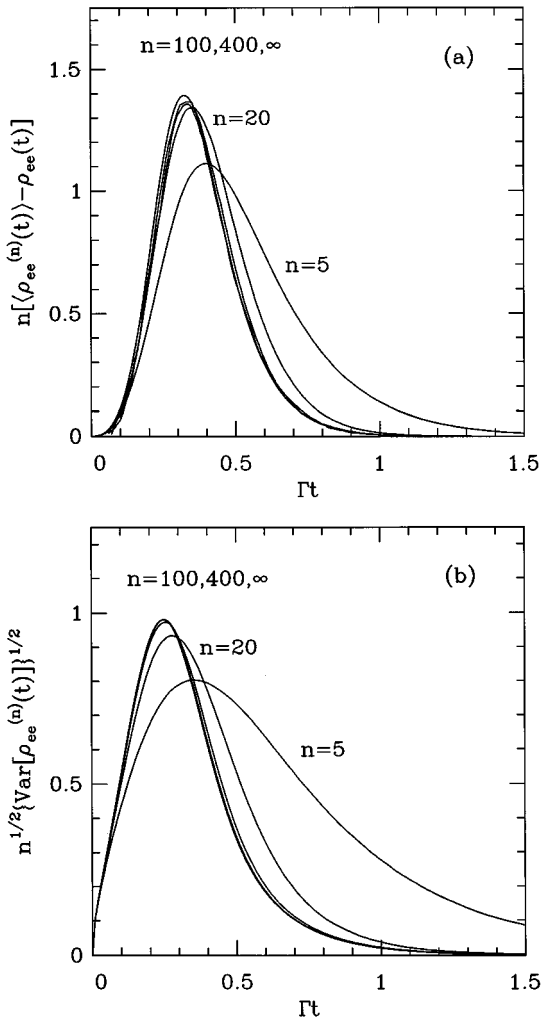

FIG. 2. Superradiance model for $N=10$ atoms; (a) systematic bias and (b) statistical uncertainty on the excited state population in the Monte Carlo wave-function results, for increasing numbers n of wave functions. To display the scaling with n we have multiplied the bias by n and the statistical uncertainty by $n^{1/2}$. The line $n=\infty$ is the analytical prediction. As in Fig. 1, the averages are performed over 64 000 realizations.

$$\mathrm{var}(b^{(n)}(t))=\frac{1}{n}\mathrm{Tr}[(\langle\delta O_{1,1}^{(n)}\rangle)(B\otimes B)]$$

$$+\frac{n-1}{n}\mathrm{Tr}[\langle\delta O_{1,2}^{(n)}(t)\rangle(B\otimes B)], \tag{33}$$

where the additional quantities have been introduced:

$$\langle\delta O_1^{(n)}\rangle\equiv\langle O_1^{(n)}\rangle-\langle O_1^{(\infty)}\rangle, \tag{34}$$

$$\langle\delta O_{1,1}^{(n)}(t)\rangle\equiv\langle O_{1,1}^{(n)}(t)\rangle-\langle O_1^{(n)}(t)\rangle\otimes\langle O_1^{(n)}(t)\rangle, \tag{35}$$

$$\langle\delta O_{1,2}^{(n)}(t)\rangle\equiv\langle O_{1,2}^{(n)}(t)\rangle-\langle O_1^{(n)}(t)\rangle\otimes\langle O_1^{(n)}(t)\rangle. \tag{36}$$

In the derivation of Eqs. (32) and (33) we have taken advantage of the interchangeability of the n wave functions which allows us to replace mean values $\langle O_{i,j}^{(n)}\rangle$ by $\langle O_{1,1}^{(n)}\rangle$ or $\langle O_{1,2}^{(n)}\rangle$ depending on whether $i=j$ or $i\neq j$.

The form of Eq. (33) is logically split into two terms. For a linear master equation problem, the first one scaling as $1/n$ is identical to the expression Eq. (14), and the second one, which explicitly involves the statistical correlation between the wave functions, exactly vanishes in this case. In the nonlinear case, the wave functions are coupled and the second term will in general not vanish for a finite n. We shall present arguments below showing that this contribution vanishes as $1/n$ for large n, which could not be simply inferred from the behavior of the $(n-1)/n$ prefactor. In this limit $n\to\infty$ the first term retains the usual interpretation of a sample variance for wave functions $|\psi_i^{(n)}(t)\rangle$ simulating the parametrized equation (18) with $\sigma(t)=\langle O_1^{(\infty)}\rangle$ being the exact solution of the master equation. An interesting feature due to the same $1/n$ scaling law of both terms in Eq. (33) is therefore that the sample variance estimate Eq. (15) does not give the correct statistical uncertainty for a simulation of a nonlinear master equation.

The average of the quantities defined in Eqs. (30) and (31) is required to estimate the convergence of the proposed simulation scheme towards the exact density matrix result. We shall now derive equations of motion for these averages.

Consider the Monte Carlo wave function $|\psi_1^{(n)}(t)\rangle$ at time t. Its time evolution from t to $t+dt$ proceeds as given by Eq. (5), but with the C_m operators and $H_{\rm eff}$ in Eq. (1) now depending on the n wave-function estimate of the density matrix Eq. (24) at time t. According to Eq. (5) the average of $O_1^{(n)}(t+dt)$ over all possible realizations [no jump with probability $1-\delta p$, jump to one of the $C_m|\psi_1^{(n)}(t)\rangle$ with probability δp_m] reads

$$\overline{O_1^{(n)}}(t+dt)=(1-\delta p)\frac{(1+(dt/i\hbar)H_{\rm eff}(\rho^{(n)}(t))]O_1^{(n)}(t)[1-(dt/i\hbar)H_{\rm eff}^{\dagger}(\rho^{(n)}(t))]}{\sqrt{1-\delta p}\sqrt{1-\delta p}}$$
$$+\sum_m \delta p_m \frac{C_m(\rho^{(n)}(t))O_1^{(n)}(t)C_m^{\dagger}(\rho^{(n)}(t))}{\sqrt{\delta p_m/dt}\sqrt{\delta p_m/dt}}. \tag{37}$$

After cancellation of $1-\delta p$ and of the δp_m's one recognizes the evolution during dt due to the Liouvillian of parametrized Lindblad form. With a further average over all possible realizations between the initial time of the evolution and the time t, we get

$$\frac{d}{dt}\langle O_1^{(n)}(t)\rangle=\langle L(\rho^{(n)}(t))[O_1^{(n)}(t)]\rangle. \tag{38}$$

In the linear case one directly obtains the agreement between the master equation and the Monte Carlo wave-function simulation. Due to the $\rho^{(n)}$ dependence of the Liouvillian in the nonlinear case the right-hand side of Eq. (38) may differ from the *a priori* required form $L(\langle\rho^{(n)}\rangle)[\langle O_1^{(n)}\rangle]$. We should expect, however, that in the limit of large n the stochastic $\rho^{(n)}$ fluctuates less and less so that $L(\rho^{(n)})$ may be considered as a constant in the mean value calculation.

Equation (38) is not closed in $\langle O_1^{(n)}\rangle$, and in the Appendix we shall expand the dependence of $L(\rho^{(n)})$ on $\rho^{(n)}$ in order to obtain a hierarchy of equations coupling $\langle O_1^{(n)}\rangle$, $\langle O_{1,2}^{(n)}\rangle$, ... The solution of this hierarchy ascertains the above expectation, when $L(\rho)$ depends polynomially on ρ: the proposed procedure converges to the exact density matrix results in the limit of large n. More precisely, simulations performed in the way proposed with n wave functions reproduce the mean values with a bias, Eq. (27),

$$\text{Bias}\propto\frac{1}{n}, \tag{39}$$

and within a statistical uncertainty, Eq. (29),

$$\text{Uncertainty}\propto\frac{1}{\sqrt{n}}. \tag{40}$$

The values of the time dependent coefficients in the proportionality relations (39) and (40) are also relevant in practice: as mentioned in the Appendix, they can be subject to amplification when the solution of the nonlinear master equation is unstable, a situation that is not forbidden by the parametrized Lindblad form and leads to convergence problems in the simulation for too long interaction times.

In the Appendix explicit equations are given in the limit $n\to\infty$ for the statistical uncertainty and for the bias in the case of an affine dependence Eq. (A1) of $L(\sigma)$ on σ [see Eqs. (A8), and (A10)]. For the simple model of superradiance discussed in Sec. III, we have found an analytical solution to these equations. The corresponding predictions for the bias and the statistical uncertainty in the excited state population ($B=|e\rangle\langle e|$) are shown as function of time in Fig. 2. To display the scaling of these quantities with n we have multiplied them by n and $\sqrt{n}$, respectively.

We have also plotted in Fig. 2 the exact bias (times n) and the exact statistical uncertainty (times $\sqrt{n}$) for the finite values of n considered in Fig. 1. Note that this bias is simply obtained as the difference between the smooth solid curves (average over a large number of realizations) and the dashed line (exact master equation result) in Fig. 1. The convergence of the numerical results to the asymptotic analytical ones is observed in Fig. 2, as n increases.

The analytical formulas for the bias and the statistical uncertainty in the excited state population are involved but can be simplified in the limit of a large number of atoms N:

$$\text{Bias} \equiv \langle \rho_{ee}^{(n)} \rangle - \rho_{ee} \simeq \rho_{ee}\rho_{gg}^2 N/n, \tag{41}$$

$$(\text{Uncertainty})^2 \equiv \text{var}(\rho_{ee}^{(n)}) \simeq \rho_{ee}^2 \rho_{gg}^2 N/n, \tag{42}$$

where $\rho_{ee}^{(n)}$ is the mean excited state population obtained by a single simulation with n wave functions, and ρ_{ee} is the exact excited state population Eq. (26).

V. PHYSICAL EXAMPLES OF NONLINEAR MASTER EQUATIONS

In this section, we consider a real physical system, a gas of N atoms coupled by the electric dipole interaction to the electromagnetic field. A nonlinear master equation for the one-atom density matrix ρ_1 has been derived by several authors [7,8]. In Ref. [7] the starting point is a master equation for the N-atom density matrix $\rho_{1,2,\ldots,N}$. From this equation a master equation for the one-atom density ρ_1 is derived, involving a coupling to the two-atom density matrix $\rho_{1,2}$; it is turned into an approximate closed equation for ρ_1 through Hartree or Hartree-Fock approximations to $\rho_{1,2}$.

A. General Bloch-Hartree-Fock equations

The nonlinear equation obtained by the Hartree approximation $\rho_{1,2} \equiv \rho(1,2) \simeq \rho_1(1) \otimes \rho_1(2)$ has a simple interpretation in terms of the coupled Maxwell-Bloch equations used to described the propagation of a classical field through an atomic medium [9]. In these equations the atom 1 is considered as a probe particle; it is driven by the field

$$\vec{E}_d = \vec{E} + \frac{1}{3\varepsilon_0}\vec{P}. \tag{43}$$

The first term $\vec{E}(\vec{r},t)$ is the sum of the incoming laser field, $\vec{E}_L(\vec{r},t)$ and of the mean field created by the $N-1$ other atoms. The second term containing the density of polarization $\vec{P}(\vec{r},t)$ created by the $N-1$ atoms is a local field correction [22]. In the case of a monochromatic laser field of angular frequency ω_L we introduce the positive frequency components $\vec{\mathcal{E}}_d$ of the driving field, $\vec{\mathcal{E}}_L$ of the laser field, and $\vec{\mathcal{P}}$ of the polarization of the medium. That is, the driving field is decomposed as

$$\vec{E}_d(\vec{r},t) = \vec{\mathcal{E}}_d(\vec{r}) e^{-i\omega_L t} + \text{ c.c.} \tag{44}$$

and similar relations hold for the laser field and the polarization. Equation (43) then reduces to

$$\vec{\mathcal{E}}_d(\vec{r}) = \vec{\mathcal{E}}_L(\vec{r}) + \frac{1}{\varepsilon_0}\int d^3\vec{r}\,'[\tilde{g}(\vec{r}-\vec{r}\,')]\vec{\mathcal{P}}(\vec{r}\,'), \tag{45}$$

with the expression for the 3×3 matrix $[\tilde{g}(\vec{r})]$ $(\alpha,\beta = x,y,z)$ giving the field radiated by a dipole for $\vec{r} \neq 0$:

$$\begin{aligned}\tilde{g}_{\alpha\beta}(\vec{r}) &= -\int \frac{d^3\vec{k}}{(2\pi)^3}\sum_{\vec{\varepsilon}\perp\vec{k}} ck\varepsilon_\alpha\varepsilon_\beta e^{i\vec{k}\cdot\vec{r}} \\ &\quad \times \frac{1}{2}\left(\frac{1}{\omega_L - ck + i0^+} - \frac{1}{\omega_L + ck + i0^+}\right) - \frac{2}{3}\delta_{\alpha\beta}\delta(\vec{r}) \\ &= -\frac{k_L^3}{4\pi}\frac{e^{ik_L r}}{k_L r}\left[\left(1 + \frac{3i}{k_L r} - \frac{3}{k_L^2 r^2}\right)\frac{r_\alpha r_\beta}{r^2}\right. \\ &\quad \left. - \left(1 + \frac{i}{k_L r} - \frac{1}{k_L^2 r^2}\right)\delta_{\alpha\beta}\right]. \end{aligned} \tag{46}$$

The expression Eq. (45) is inserted into the optical Bloch equation for the density matrix of atom 1,

$$\frac{d}{dt}\rho_1(t) = \mathcal{L}[\rho_1(t)] + \frac{1}{i\hbar}[-\vec{D}_1 \cdot \vec{E}_d(\vec{R}_1,t), \rho_1(t)], \tag{47}$$

where $\vec{R}_1$ is the atomic center-of-mass position operator and $\vec{D}_1$ is the atomic dipole operator. In Eq. (47) the Liouvillian $\mathcal{L}$ incorporates the atomic kinetic and internal energies and the effect of spontaneous emission. In a mean field treatment the same one-atom density matrix is used for all atoms and the driving electric field in Eq. (45) depends on ρ_1 through the mean polarization density $\vec{P}$:

$$\vec{P}(\vec{r},t) = (N-1)\text{Tr}(\rho_1(t)\,\delta(\vec{r}-\vec{R}_1)\vec{D}_1) \tag{48}$$

(with a trace Tr taken over both internal and external atomic degrees of freedom). Finally, one is left with a nonlinear master equation for ρ_1. This equation is clearly in the parametrized Lindblad form Eq. (18) with $L(\sigma)$ having an affine dependence on σ, and it can be simulated by Monte Carlo wave functions. We shall refer to this equation as the Bloch-Hartree master equation. A discussion of its validity can be found in [9].

A nonlinear equation with a further approximation is obtained if one assumes that the N-particle system is described by a pure state which factors into a product of N identical effective single particle state vectors (Hartree wave function). Dissipation of a kind that formally preserves this property has been studied by Goldstein *et al.*, and the application of Monte Carlo wave functions has been discussed [23].

When quantum statistical effects caused by the bosonic or fermionic nature of the atoms come into play, the Hartree approximation has to be supplemented by an exchange term, as it is done in the Hartree-Fock approximation for the two-atom density matrix:

$$\rho_{1,2}(1,2) \simeq (1 + \eta P_{1,2})[\rho_1(1) \otimes \rho_1(2)], \tag{49}$$

where $P_{1,2}$ exchanges the states of particles 1 and 2, and where $\eta = +1$ for bosons, $\eta = -1$ for fermions. This formula (49) may be applied only to weakly degenerate systems $[\text{Tr}(\rho_1^2) \ll 1]$, since otherwise the two-particle density matrix does not have unit trace (we shall come back to this point and an alternative symmetrization ansatz in Sec. V B).

The extra term in the master equation due to this exchange correction reads

$$\left(\frac{d}{dt}\rho_1\right)_{\text{exch}} = \frac{1}{i\hbar}[H_{\text{exch}}\rho_1 - \rho_1 H_{\text{exch}}^\dagger], \tag{50}$$

We have introduced the exchange Hamiltonian, depending on $\sigma=\rho_1$ and acting on ρ_1:

$$H_{\text{exch}}(\sigma)\rho_1 = \eta(N-1)\text{Tr}_2\left[\frac{-1}{\varepsilon_0}\left(\sum_{\alpha,\beta}\tilde{g}_{\alpha\beta}(\vec{R}_1-\vec{R}_2)D_{1,\alpha}^{(+)} \times D_{2,\beta}^{(-)} + \text{H.c.}\right)P_{1,2}[\rho_1(1)\otimes\sigma(2)]\right]. \tag{51}$$

The superscripts $(+/-)$ stand for the raising or lowering parts of the atomic dipole operators $\vec{D}_1$ and $\vec{D}_2$ for the atoms 1 and 2. A more transparent form can be obtained, without the permutation operator $P_{1,2}$, by performing explicitly the trace over atom 2. The result reads in the continuous basis of localized atomic states,

$$\begin{aligned}\langle\vec{r}|H_{\text{exch}}(\sigma)|\vec{r}'\rangle = &-\eta(N-1)/\varepsilon_0\sum_{\alpha,\beta}[\tilde{g}_{\alpha\beta}(\vec{r}-\vec{r}')D_\alpha^{(+)} \\ &\times\langle\vec{r}|\sigma|\vec{r}'\rangle D_\beta^{(-)} + \tilde{g}_{\alpha\beta}^*(\vec{r}-\vec{r}')D_\alpha^{(-)} \\ &\times\langle\vec{r}|\sigma|\vec{r}'\rangle D_\beta^{(+)}],\end{aligned} \tag{52}$$

where the asterisk stands for the complex conjugate.

It appears that $H_{\text{exch}}(\sigma)$ has no matrix element between the internal atomic ground state and the internal atomic excited state, it merely consists of a complex and spatially nonlocal modification of the energy of the atomic levels. The real part of $\tilde{g}_{\alpha\beta}(\vec{r})$ obviously gives rise to the Hermitian part of $H_{\text{exch}}(\sigma)$: it leads to a shift of the atomic energy levels, which will modify, e.g., the polarizability of the gas [24].

The imaginary part of $\tilde{g}_{\alpha\beta}(\vec{r})$ gives rise to the anti-Hermitian part of $H_{\text{exch}}(\sigma)$, which is as in Eq. (20) conveniently characterized by the operator

$$\hbar W(\sigma) \equiv i[H_{\text{exch}}(\sigma) - H_{\text{exch}}^\dagger(\sigma)] \tag{53}$$

so that a positive contribution to W is a departure rate, a negative one is a feeding rate. Transforming Eq. (52) with the help of the Fourier decomposition of the imaginary part of $\tilde{g}_{\alpha\beta}$ leads to the more explicit operatorial form for $W(\sigma)$:

$$W(\sigma) = \eta(N-1)\frac{3\Gamma}{8\pi}\int d^2\vec{n}\sum_{\vec{\varepsilon}\perp\vec{n}} e^{ik_L\vec{n}\cdot\vec{r}}[(\vec{\Delta}^{(+)}\cdot\vec{\varepsilon})\sigma(\vec{\Delta}^{(-)}\cdot\vec{\varepsilon}) - (\vec{\Delta}^{(-)}\cdot\vec{\varepsilon})\sigma(\vec{\Delta}^{(+)}\cdot\vec{\varepsilon})]e^{-ik_L\vec{n}\cdot\vec{r}}, \tag{54}$$

where $d^2\vec{n}$ stands for the usual invariant integration over the unit sphere ($|\vec{n}|=1$). We have introduced in Eq. (54) the dimensionless operator

$$\vec{\Delta} = \vec{D}/d, \tag{55}$$

where the constant d is the electric dipole moment of the atomic transition; the matrix elements of $\vec{\Delta}$ in the standard angular momentum basis are simply Clebsch-Gordan coefficients. $\Gamma = d^2k_L^3/3\pi\varepsilon_0\hbar$ is the rate of spontaneous emission. Equation (54) shows that for bosons ($\eta=1$), $W(\sigma)$ is negative in the internal atomic ground state and positive in the internal atomic excited state; the conclusion is reversed for fermions ($\eta=-1$). W therefore represents the expected enhancement or reduction of transition rates associated to Bose or Fermi statistics. Note that the effect of the positive and negative parts of W on the total population cancel: in the nonlinear master equation, the ρ_1 dependence of H_{exch} ensures that Eq. (50) preserves the trace of ρ_1.

The incorporation of Eq. (50) into the Bloch-Hartree Eqs. (47) leads to an equation of motion for ρ_1 which we refer to as the Bloch-Hartree-Fock equation. This equation is not of the parametrized Lindblad form: the Hermitian part of H_{exch} is treated in the usual way, but the non-Hermitian part is not compensated by a ''sandwich'' term. In order to provide a simulation scheme for the Bloch-Hartree-Fock equation we thus need a means to treat a master equation of the form

$$\frac{d}{dt}\rho = -\frac{1}{2}\{W(\rho),\rho\} + L_{\text{Lind}}(\rho)[\rho], \tag{56}$$

where the Liouvillian $L_{\text{Lind}}(\rho)$ is of the parametrized Lindblad type. We have shown already in Sec. III that the type of nonlinear term $\{W(\rho),\rho\}$ can be put in a parametrized Lindblad form also, with a Liouvillian given by Eq. (23). As explained in Sec. III, one has to bound $W(\sigma)$ from below with some (negative) number $-\gamma(\sigma)$, which is clearly possible here [see Eq. (54), $||W(\sigma)||$ is bounded by $3\Gamma(N-1)$].

Once this form (23) has been obtained it can be straightforwardly simulated: As above, see Eq. (24), the Monte Carlo wave functions are used to provide the value of σ. Each wave function $|\psi_i^{(n)}\rangle$ in a simulation with n wave functions is now propagated as follows. With a probability $1-\delta p$, where $\delta p = idt\langle\psi_i^{(n)}(t)|H_{\text{eff}} - H_{\text{eff}}^\dagger|\psi_i^{(n)}(t)\rangle/\hbar$, $|\psi_i^{(n)}(t)\rangle$ is evolved during dt according to the effective Hamiltonian

$$H_{\text{eff}} = H_{\text{eff}}^{\text{Lind}} - i\hbar[W(\sigma)+\gamma(\sigma)]/2, \tag{57}$$

where the first term is the regular contribution of L_{Lind}, and $|\psi_i^{(n)}\rangle$ is subsequently renormalized. With the probability δp, $|\psi_i^{(n)}\rangle$ experiences a quantum jump. This quantum jump can be of two types. Type 1 is generated by the sandwich terms of L_{Lind} in the usual way; it has the probability $\delta p_1 = idt\langle\psi_i^{(n)}(t)|H_{\text{eff}}^{\text{Lind}} - H_{\text{eff}}^{\text{Lind}\dagger}|\psi_i^{(n)}(t)\rangle/\hbar$. Type 2 corresponds to the exchange jumps discussed at the end of Sec. III: $|\psi_i^{(n)}\rangle$ is collapsed to one of the $|\psi_j^{(n)}(t)\rangle$ where j is chosen with uniform weights on the numbers between 1 and n.

B. Application to superradiance

The phenomenon of superradiance is often considered in the limiting case of atoms localized within a region much smaller than the optical wavelength. In principle this should lead to strong resonant dipole-dipole interaction between ground and excited state atoms, diverging as $1/r^3$ with the interatomic distance r. The effect of this interaction is

present in the real part of $\tilde{g}_{\alpha\beta}(\vec{r})$. It is generally neglected (see [25] for a discussion of this approximation) and one is left with the so-called Dicke model. The atoms are then all localized in $\vec{r}=0$:

$$\rho_{1,\ldots,N}(t)=|\vec{r_1}=0,\ldots,\vec{r_N}=0\rangle\langle\vec{r_1}=0,\ldots,\vec{r_N}=0| \otimes \sigma_{1,\ldots,N}(t), \tag{58}$$

$\sigma_{1,\ldots,N}(t)$ being a purely internal matrix, and the radiated field (46) is replaced by i times its imaginary part in $\vec{r}=0$:

$$-\frac{d^2}{\varepsilon_0}\tilde{g}_{\alpha\beta}(\vec{r})\to-\frac{i\hbar\Gamma}{2}\delta_{\alpha\beta}. \tag{59}$$

We want to emphasize here that the Hartree-Bloch-Fock equations simplified in the Dicke limit reduce, in the absence of laser light, to the standard phenomenological equation for superradiance (17), provided that Bose statistics ($\eta=1$) is considered. At this stage the consideration of quantum statistical properties of the atoms may seem surprising: superradiance can take place even if the atoms are distinguishable entities with identical resonance frequencies. The use of bosonic statistics (rather than fermionic or boltzonic statistics) is dictated by the internal symmetry of the initial atomic state: if all the atoms are prepared initially in the excited state, $\sigma_{1,\ldots,N}(t=0)$ has the bosonic symmetry (completely symmetric eigenstates) and keeps this symmetry by further evolution, because the atoms are coupled the same way to the electromagnetic field. Contrary to the derivation of Eq. (17) presented in [19], which intermediately assumes a nonvanishing mean dipole moment, the collective atomic behavior here appears as an exchange effect — like in the Dicke model no optical coherences are postulated.

As a side remark we wish to come back to the Hartree-Fock symmetrization ansatz (49). This expression has two problems, which are particularly severe close to pure state situations: it does not have unit trace

$$\mathrm{Tr}_{1,2}[(1+\eta P_{12})\rho_1(1)\otimes\rho_1(2)]=1+\eta\mathrm{Tr}_1(\rho_1^2(1))\neq 1,$$

and it does not yield the single atom density matrix $\rho_1(1)$ by a partial trace, $\rho_1(1)\neq\mathrm{Tr}_2\rho_{1,2}(1,2)$. If we want to deal with the natural initial state for superradiance, the pure state with all atoms excited at $t=0$, we may therefore worry that the ansatz (49) does not lead to an appropriate nonlinear master equation. However, a better Hartree-Fock ansatz can be obtained by diagonalizing σ_1:

$$\sigma_1=\pi_a|a\rangle\langle a|+\pi_b|b\rangle\langle b| \tag{60}$$

and by symmetrizing and normalizing the product states in each dyadic term in $\sigma_1\otimes\sigma_1$ independently:

$$|aa\rangle\to|aa\rangle,$$

$$|bb\rangle\to|bb\rangle,$$

$$|ab\rangle,|ba\rangle\to\frac{1}{\sqrt{2}}(|ab\rangle+|ba\rangle). \tag{61}$$

In the absence of laser light, σ_1 is diagonal in the $|e\rangle,|g\rangle$ basis ($a=e,b=g$) and contrary to Eq. (49) the resulting approximation for $\sigma_{1,2}$ for $\eta=1$,

$$\sigma_{1,2}\simeq\pi_e^2|ee\rangle\langle ee|+\pi_e\pi_g(|eg\rangle+|ge\rangle)(\langle eg|+\langle ge|) +\pi_g^2|gg\rangle\langle gg|, \tag{62}$$

has both $\mathrm{Tr}_2(\sigma_{1,2})=\sigma_1$ and it is correctly normalized.

Equation (49) differs from Eq. (62) by double counting of the first and the last terms in the latter equation, and according to Eq. (50) it provides an extra contribution

$$\mathrm{Tr}_2[(D_{1,\alpha}^{(+)}D_{2,\beta}^{(-)}+\text{ H.c.})(\pi_e^2|ee\rangle\langle ee|+\pi_g^2|gg\rangle\langle gg|)]=0 \tag{63}$$

to the master equation. The fact that this contribution vanishes implies that the questionable approximation (49) leads to the same master equation for σ_1 as the more correct ansatz (62).

The agreement between the master equations following from Eqs. (49) and (62) holds in the absence of a driving field only. When a laser is present, the eigenstates of σ_1 become time dependent and they no longer coincide with $|e\rangle,|g\rangle$. We have here checked numerically that the predictions of the Dicke model are more accurately reproduced by the application of the symmetrizations (61) in this case.

C. In the low saturation regime

The Bloch-Hartree-Fock master equation can be simplified when the atomic sample is subject to laser cooling. Indeed laser cooling routinely leads to a mean atomic kinetic energy on the order of a few recoil energies $\hbar^2k_L^2/2M$ or less ($k_L=\omega_L/c$ is the laser wave vector). In the usual regime of a broad linewidth ($\hbar\Gamma\gg\hbar^2k_L^2/2M$, where Γ is the spontaneous emission rate), this allows one to neglect the atomic motion in the internal excited state:

$$\left\langle\frac{p^2}{2M}\right\rangle\ll\hbar\Gamma. \tag{64}$$

Furthermore in laser cooling configurations the laser field is often sufficiently detuned from the atomic resonance that the fraction of atoms in the internal excited state remains small. In this low saturation regime the coupling from the internal ground state to the internal excited state by the driving field in the medium (45) can be treated perturbatively:

$$|V_{\mathrm{ad}}|^2\ll\hbar^2(\delta^2+\Gamma^2/4). \tag{65}$$

$\delta=\omega_L-\omega_A$ is the detuning between the laser frequency and the resonance frequency of the atom. The symbol V_{ad} stands for the atom-driving field coupling operator:

$$V_{\mathrm{ad}}=V_{\mathrm{ad}}^{(+)}+V_{\mathrm{ad}}^{(-)}=V_{\mathrm{ad}}^{(+)}+\text{ H.c.} \tag{66}$$

$$V_{\mathrm{ad}}^{(+)}=-\vec{D}^{(+)}\cdot\vec{\mathcal{E}}_d(\vec{r}), \tag{67}$$

where $\vec{D}^{(+)}$ is the raising part of the atomic dipole operator. Note that the time dependence of the atom-driving field coupling at the angular frequency ω_L has been suppressed by use of a ''rotating frame'' at the same frequency.

In the absence of collective effects ($N=1$) it is known that the internal atomic excited state can be eliminated adiabatically [26] when both conditions (64) and (65) are satisfied. One is left with a master equation on the restriction of the density matrix to the internal ground state, $(\rho_{1,gg})$. It is possible to generalize this calculation to the Bloch-Hartree-Fock equations for $N\neq 1$ and we briefly give the main steps of the derivation.

First, we write explicitly the equations of motion for matrix elements between states from either the same or different internal energy manifolds:

$$\frac{d}{dt}\rho_{1,eg}=\frac{1}{i\hbar}[-\hbar\delta-i\hbar\Gamma/2+(H_{\rm exch})_{ee}]\rho_{1,eg}+\frac{1}{i\hbar}V_{\rm ad}^{(+)}\rho_{1,gg}, \tag{68}$$

$$\frac{d}{dt}\rho_{1,ee}=-\Gamma\rho_{1,ee}+\frac{1}{i\hbar}[(H_{\rm exch})_{ee}\rho_{1,ee}-\rho_{1,ee}(H_{\rm exch})_{ee}^{\dagger}] + \frac{1}{i\hbar}(V_{\rm ad}^{(+)}\rho_{1,ge}-\rho_{1,eg}V_{\rm ad}^{(-)}), \tag{69}$$

$$\frac{d}{dt}\rho_{1,gg}=\frac{1}{i\hbar}\left[\left(\frac{p^2}{2M}+(H_{\rm exch})_{gg}\right)\rho_{1,gg}+V_{\rm ad}^{(-)}\rho_{1,eg} -\rho_{1,gg}\left(\frac{p^2}{2M}+(H_{\rm exch})_{gg}^{\dagger}\right)-\rho_{1,ge}V_{\rm ad}^{(+)}\right] + \frac{3\Gamma}{8\pi}\int d^2\vec{n}\sum_{\vec{\varepsilon}\perp\vec{n}}\vec{\Delta}^{(-)}\cdot\vec{\varepsilon}\,\exp(ik_L\vec{n}\cdot\vec{r})\rho_{1,ee} \times\exp(-ik_L\vec{n}\cdot\vec{r})\vec{\Delta}^{(+)}\cdot\vec{\varepsilon}. \tag{70}$$

$\vec{\Delta}$ is given by Eq. (55). Taking advantage of Eq. (64) we have kept the contribution of the atomic kinetic energy in the evolution of $\rho_{1,gg}$ only. According to condition (65) we have neglected in Eq. (68) the coupling to $\rho_{1,ee}$ by $V_{\rm ad}$ which would account for saturation effects. In this equation we have also disregarded the contribution of $(H_{\rm exch})_{gg}$: it is proportional to the excited state population [see Eq. (52)] and it becomes much smaller than $\hbar\Gamma$ in the limit (65).

The last term in Eq. (70) involves a sum over the direction $\vec{n}$ ($\vec{n}^2=1$) and the polarization $\vec{\varepsilon}$ of the spontaneously emitted photon.

From Eq. (69) one first expresses in the adiabatic approximation the optical coherences of ρ_1 in the rotating frame as a function of the ground state elements $\rho_{1,gg}$:

$$\rho_{1,eg}=\frac{1}{\hbar\delta+i\hbar\Gamma/2-(H_{\rm exch})_{ee}}V_{\rm ad}^{(+)}\rho_{1,gg}, \tag{71}$$

where $(H_{\rm exch})_{ee}$ stands for the restriction of the exchange Hamiltonian (51) to the internal excited state. In this expression the effect of the exchange Hamiltonian readily appears as a modification of the atomic line. This modification indicates that the optical response of the medium to a light field is sensitive to quantum statistics. For example, Eq. (71) can be used to derive the polarizability of a homogeneous Bose gas ($\eta=1$) for an atomic transition from a $j_g=0$ angular momentum ground state to a $j_e=1$ angular momentum excited state. To second order in the atomic density, the resulting expression for the polarizability differs from the Lorentz-Lorenz formula for a classical gas by the contribution of $(H_{\rm exch})_{ee}$. A rigorous derivation of the polarizability [24] confirms the existence of this term; it also gives another quadratic correction in the atomic density sensitive to the Bose statistics, involving the effect of the resonant dipole-dipole interaction between the atoms, which is left out in the Hartree-Fock mean field treatment.

The next step is to obtain the excited state matrix elements. A slightly less straightforward derivation than the one of the optical coherences leads to

$$\rho_{1,ee}=\frac{1}{\hbar\delta+i\hbar\Gamma/2-(H_{\rm exch})_{ee}}V_{\rm ad}^{(+)}\rho_{1,gg}V_{\rm ad}^{(-)} \times\frac{1}{\hbar\delta-i\hbar\Gamma/2-(H_{\rm exch})_{ee}^{\dagger}}. \tag{72}$$

The last step is to use the expressions (71) and (72) to eliminate all the excited state matrix elements from the time derivative of the ground state density matrix in Eq. (70). The substitution of $\rho_{1,ee}$ by Eq. (72) gives rise to feeding terms of the sandwich form $C_m\rho_{1,gg}C_m^{\dagger}$, where the index m represents all possible directions $\vec{n}$ and polarizations $\vec{\varepsilon}$. Departure terms $-\frac{1}{2}\{C_m^{\dagger}C_m,\rho_{1,gg}\}$ counterbalancing these sandwich-terms in the Lindblad form (1) appear when we transform the contributions of $\rho_{1,eg}$ and $\rho_{1,ge}$ to Eq. (70) according to identities of the type $A^{-1}=(A^{\dagger})^{-1}A^{\dagger}A^{-1}$. This leads to the following nonlinear master equation for the ground state one-atom density matrix:

$$\frac{d}{dt}\rho_{1,gg}=\frac{1}{i\hbar}[\mathcal{H}\rho_{1,gg}-\rho_{1,gg}\mathcal{H}^{\dagger}] + \frac{3\Gamma}{8\pi}\int d^2\vec{n}\sum_{\vec{\varepsilon}\perp\vec{n}}[C(\vec{n},\vec{\varepsilon})\rho_{1,gg}C(\vec{n},\vec{\varepsilon})^{\dagger} -\tfrac{1}{2}\{C(\vec{n},\vec{\varepsilon})^{\dagger}C(\vec{n},\vec{\varepsilon}),\rho_{1,gg}\}]. \tag{73}$$

All the operators $\mathcal{H}$ and $C(\vec{n},\vec{\varepsilon}),C(\vec{n},\vec{\varepsilon})^{\dagger}$ entering as coefficients in this master equation depend on the density matrix $\rho_{1,gg}$ itself. The non-Hermitian Hamiltonian $\mathcal{H}$ includes the lightshift of the ground state internal sublevels by the driving field plus the contribution of the ground state exchange Hamiltonian $(H_{\rm exch})_{gg}$:

$$\mathcal{H}=\frac{p^2}{2M}+(H_{\rm exch})_{gg}+V_{\rm ad}^{(-)}\frac{1}{\hbar\delta-i\hbar\Gamma/2-(H_{\rm exch})_{ee}^{\dagger}} \times[\hbar\delta-(H_{\rm exch})_{ee}^{\dagger}]\frac{1}{\hbar\delta+i\hbar\Gamma/2-(H_{\rm exch})_{ee}}V_{\rm ad}^{(+)}. \tag{74}$$

The jump operators $C(\vec{n},\vec{\varepsilon})$ contain the quantum statistical corrections to the atomic line:

$$C(\vec{n},\vec{\varepsilon})=\vec{\Delta}^{(-)}\cdot\vec{\varepsilon}\,\exp(-ik_L\vec{n}\cdot\vec{r}) \times\frac{1}{\hbar\delta+i\hbar\Gamma/2-(H_{\rm exch})_{ee}}V_{\rm ad}^{(+)}. \tag{75}$$

Equation (73) has the same structure as the Bloch-Hartree-Fock master equation without elimination of the excited state. It can therefore also be simulated by Monte Carlo wave functions, as illustrated in Sec. VI.

D. Rate equations with quantum statistical effects

It is possible to obtain physically suggestive equations from the master equation (73). The idea is to introduce the time dependent orthonormal atomic basis diagonalizing the density matrix $\rho_{1,gg}(t)$ at each time t:

$$\rho_{1,gg}(t)=\sum_n \Pi_{g,n}(t)|g,n(t)\rangle\langle g,n(t)|, \tag{76}$$

$$\langle g,n(t)|g,n'(t)\rangle=\delta_{n,n'}. \tag{77}$$

In this basis the time evolution of the populations $\Pi_{g,n}(t)$ is given by

$$\begin{aligned}\frac{d}{dt}\Pi_{g,n}(t)&=\frac{d}{dt}[\langle g,n(t)|\rho_{1,gg}|g,n(t)\rangle]\\&=\langle g,n(t)|\left(\frac{d}{dt}\rho_{1,gg}\right)|g,n(t)\rangle+\Pi_{g,n}(t)\left[\left(\frac{d}{dt}\langle g,n(t)|\right)|g,n(t)\rangle+\langle g,n(t)|\left(\frac{d}{dt}|g,n(t)\rangle\right)\right]\\&=\langle g,n(t)|\left(\frac{d}{dt}\rho_{1,gg}\right)|g,n(t)\rangle+\Pi_{g,n}(t)\frac{d}{dt}[\langle g,n(t)|g,n(t)\rangle].\end{aligned} \tag{78}$$

Since the state vectors $|g,n(t)\rangle$ are normalized to unity, the last term in Eq. (78) vanishes and the time derivative of the populations reduces to

$$\frac{d}{dt}\Pi_{g,n}(t)=\langle g,n(t)|\left(\frac{d}{dt}\rho_{1,gg}\right)|g,n(t)\rangle \tag{79}$$

A first type of contribution to Eq. (79) comes from the Lindblad part of Eq. (73), i.e., the part containing the C and $C^\dagger$ operators:

$$\left(\frac{d}{dt}\Pi_{g,n}(t)\right)_{\text{Lind}}=\sum_{n'}(\gamma_{g,n'\to g,n}\Pi_{g,n'}-\gamma_{g,n\to g,n'}\Pi_{g,n}). \tag{80}$$

The transition rates appearing in this system differ from the transition rates in the single atom case because of the quantum statistical corrections to the atomic line:

$$\gamma_{g,n\to g,n'}=\frac{3\Gamma}{8\pi}\int d^2\vec{n}\sum_{\vec{\varepsilon}\perp\vec{n}}|\langle g,n'|C(\vec{n},\vec{\varepsilon})|g,n\rangle|^2. \tag{81}$$

A second type of contribution to Eq. (79) comes from the anti-Hermitian part of $\mathcal{H}$. The first exchange term in Eq. (74) is simply $(H_{\text{exch}})_{gg}$; it leads to a modification of the feeding term of $\Pi_{g,n}$ due to quantum statistics:

$$\left(\frac{d}{dt}\Pi_{g,n}(t)\right)_{\text{exch,gg}}=\eta(N-1)\sum_{n'}\Pi_{g,n'}\gamma_{g,n'\to g,n}\Pi_{g,n}. \tag{82}$$

The second exchange term in Eq. (74) involves $(H_{\text{exch}})_{ee}$ and leads to a quantum statistical correction of the departure rate from $|g,n\rangle$:

$$\left(\frac{d}{dt}\Pi_{g,n}(t)\right)_{\text{exch,ee}}=-\eta(N-1)\sum_{n'}\Pi_{g,n'}\gamma_{g,n\to g,n'}\Pi_{g,n}. \tag{83}$$

When both quantum statistical corrections to Eq. (79) are included, one gets transition rates between states depending on the occupation number of the final state in the intuitively expected manner:

$$\begin{aligned}\left(\frac{d}{dt}\Pi_{g,n}(t)\right)_{\text{HF}}=\sum_{n'}\{&\gamma_{g,n'\to g,n}\Pi_{g,n'}[1+\eta(N-1)\Pi_{g,n}]\\&-\gamma_{g,n\to g,n'}\Pi_{g,n}[1+\eta(N-1)\Pi_{g,n'}]\}.\end{aligned} \tag{84}$$

Finally the difference between the Bloch-Hartree-Fock master equation and simple rate equations including quantum statistics lies in the fact that (i) the jump operators contain quantum statistical corrections to the atomic line, and (ii) the eigenbasis $|g,n(t)\rangle$ is not known *a priori* but is determined by the time evolution and for the nonlinear problem this has to be done in a complicated self-consistent manner [27].

VI. A NUMERICAL EXAMPLE: LASER COOLING OF BOSONIC ATOMS IN A WEAK HARMONIC TRAP

We now illustrate the Monte Carlo wave-function technique with the solution of a nonlinear master equation of the form (73) for laser cooling of trapped bosons ($\eta=1$). The laser field is detuned on the blue side ($\delta>0$) of a $j_g=1\to j_e=1$ atomic transition. It is obtained as a superposition of linearly polarized running waves with wave vectors $\pm k_L\vec{e}_z$ ($\vec{e}_z$ is the unit vector along z axis) and with linear polarizations making a relative angle of $\pi/4$. Its positive frequency part is therefore given by

$$\vec{\mathcal{E}}=\mathcal{E}_0\{[\cos(\theta/2)\vec{e}_x+\sin(\theta/2)\vec{e}_y]e^{ik_Lz} +[\cos(\theta/2)\vec{e}_x-\sin(\theta/2)\vec{e}_y]e^{-ik_Lz}\}, \tag{85}$$

where θ is equal to $\pi/4$.

It is known that this configuration leads to subrecoil laser cooling [29] for free atoms. There exists indeed in this case an atomic (internal+external) state $|\psi_D\rangle$ (the ''dark'' state) which is not coupled to the laser and which is stationary with respect to the kinetic energy operator [30]. The atoms are confined in momentum space by a Sisyphus effect [31], within an interval of a few $\hbar k_L$, and pile up in long-lived atomic states close to the dark state. When time proceeds, two peaks emerge in the momentum distribution around $\pm\hbar k_L$.

Extensions of dark state cooling of atoms in a trap have been proposed in [32]. They rely either on flat bottom potentials or harmonic traps in the Lamb-Dicke regime (energy level separation $\hbar\Omega_{\rm osc}$ much larger than the recoil energy $\hbar^2k_L^2/2M$); in both cases an almost dark state exists. We consider here a harmonic trap with an oscillation frequency smaller than the recoil energy. This is more easily achieved experimentally, but it does not provide as good a dark state.

As we shall discuss later, the Hartree-Fock ansatz does not give a complete account of the collective effects involved in laser cooling of atoms. We simply want here to illustrate the positive effect of the bosonic enhancement factors in Eq. (84) on the efficiency of the cooling process, which has been described by simple rate equations in [4–6]. We therefore simplify Eq. (73) by the following approximations.

(i) We neglect the renormalization of the jump operators C_m by the bosonic line shift and broadening. The resulting master equation is nonlinear only because of the dependence of the effective Hamiltonian $\mathcal{H}$ with ρ_1. We neglect the difference between the mean electric field and the incoming laser field (the atoms are pumped by the cooling process into states weakly coupled to the laser light).

(ii) We construct a one-dimensional model by assuming that some additional cooling mechanism (not included in the master equation) keeps the atoms in the ground state $|0,0\rangle$ of a harmonic trap in the x,y plane. Only the atomic motion along z is left as a dynamical variable. At each time t, $\rho_{1,gg}$ is assumed to factorize as $|0,0\rangle\langle 0,0|\otimes\sigma(t)$. The corresponding master equation for $\sigma(t)$ is obtained by taking the trace of Eq. (73) over the transverse motion. The effect of this trace is to suppress the x,y dependent terms from the effective Hamiltonian $\mathcal{H}$ (transverse kinetic energy and potential), to contract to unity the translation operators $\exp(\pm ik_L(n_xx+n_yy))$ in the sandwich-terms, and to replace the function $\tilde{g}_{\alpha\beta}(\vec{r})$ in $\mathcal{H}$ by its transverse average $\overline{g_{\alpha\beta}}(z)$ over the distribution $(M\Omega_{\rm osc}^{\perp}/h)\exp(-M\Omega_{\rm osc}^{\perp}(x^2+y^2)/2\hbar)$, where $\Omega_{\rm osc}^{\perp}$ is the transverse oscillation frequency.

(iii) We neglect the real part of $\overline{g_{\alpha\beta}}(z)$, i.e., the Hermitian part of $\mathcal{H}$ depending on the Bose statistics. The transverse trap is supposed for simplicity to be in the Lamb-Dicke regime ($\Omega_{\rm osc}^{\perp}\gg\hbar k_L^2/m$), so that the resulting $\overline{g_{\alpha\beta}}(z)$ is easy to calculate. The only nonvanishing components included are then given by

$$\overline{g_{xx}}(z)=\overline{g_{yy}}(z)=i\frac{k_L^3}{8\pi}\int_{-1}^{1}du\,\frac{1+u^2}{2}e^{ik_Luz}, \tag{86}$$

$$\overline{g_{zz}}(z)=i\frac{k_L^3}{8\pi}\int_{-1}^{1}du(1-u^2)e^{ik_Luz}. \tag{87}$$

More explicit expressions can be deduced from the identity

$$\frac{1}{2}\int_{-1}^{1}du\;u^2e^{i\kappa u}=\frac{\sin\kappa}{\kappa}+2\frac{\cos\kappa}{\kappa^2}-2\frac{\sin\kappa}{\kappa^3}. \tag{88}$$

Numerically the Monte Carlo wave functions are discretized in position space. The evolution due to the σ-independent part of $\mathcal{H}$,

$$\mathcal{H}_0=\frac{p_z^2}{2M}+\frac{1}{2}M\Omega_{\rm osc}^2z^2+V_{AL}^{(-)}\frac{\hbar\delta}{\hbar^2(\delta^2+\Gamma^2/4)}V_{AL}^{(+)}, \tag{89}$$

is obtained by a splitting between the kinetic energy term and the potential energy terms. A Fast Fourier transform is used to calculate the effect of the kinetic energy operator. The contribution of the σ-dependent part of $\mathcal{H}$ is treated by a first order Euler's scheme with an adaptive stepsize control; it is represented by a dense matrix both in position and momentum representation so that costly matrix multiplications are required at each time step. The additive term $\gamma(\sigma)$ imposed by the simulation scheme is optimally obtained by a numerical diagonalization of the anti-Hermitian part W defined in Eq. (53); $-\gamma(\sigma)$ is then the smallest (negative) eigenvalue of W. The contribution of the last term of Eq. (74) to $\gamma(\sigma)$ is a small (negative) quantity, since the atoms are mainly in states noncoupled to the laser, and it suffices to diagonalize $(H_{\rm exch})_{gg}$ only.

As done in [32], we introduce as a convenient basis the eigenstates $|l\rangle, l\geqslant 1$ of $\mathcal{H}_0$. These states differ from the one of the bare harmonic oscillator because of the coupling to the laser field. The energy spectrum as a function of l has now an irregular distribution of energy levels around a straight line reminiscent of the purely harmonic case. The time evolution of the populations $\pi_l\equiv\langle l|\sigma|l\rangle$ of the first energy levels $|l\rangle$ for $N=20$ atoms is shown in Fig. 3(a). The initial state is a thermal distribution of the harmonic oscillator at a temperature of 10 times the recoil temperature $T_R=\hbar^2k_L^2/Mk_B$. It evolves into a steady state after a time on the order of 100 times the recoil time $\tau_R=M/\hbar k_L^2$. The average over time of the π_l's for $250\tau_R<t<500\tau_R$ is shown in Fig. 3(b). As compared to the one-atom case ($N=1$), the populations of the first two energy levels are strongly increased by the bosonic effect; the more populated level is now $|l=2\rangle$ instead of $|l=1\rangle$ in the one-atom case. The position distribution $\Pi(z)=\langle z|\sigma|z\rangle$ [see Fig. 3(c)] and the momentum distribution $\Pi(p)=\langle p|\sigma|p\rangle$ [see Fig. 3(d)] are also clearly different.

To see the influence of the number of Monte Carlo wave functions on the results of the simulation we have done a calculation with a smaller number of wave functions than in Fig. 3, $n=250$ rather than $n=1000$. The steady state Π_l's for $n=250$ and $n=1000$ (averaged over $250\tau_R<t<500\tau_R$) are very close (the difference for the most populated level $l=2$

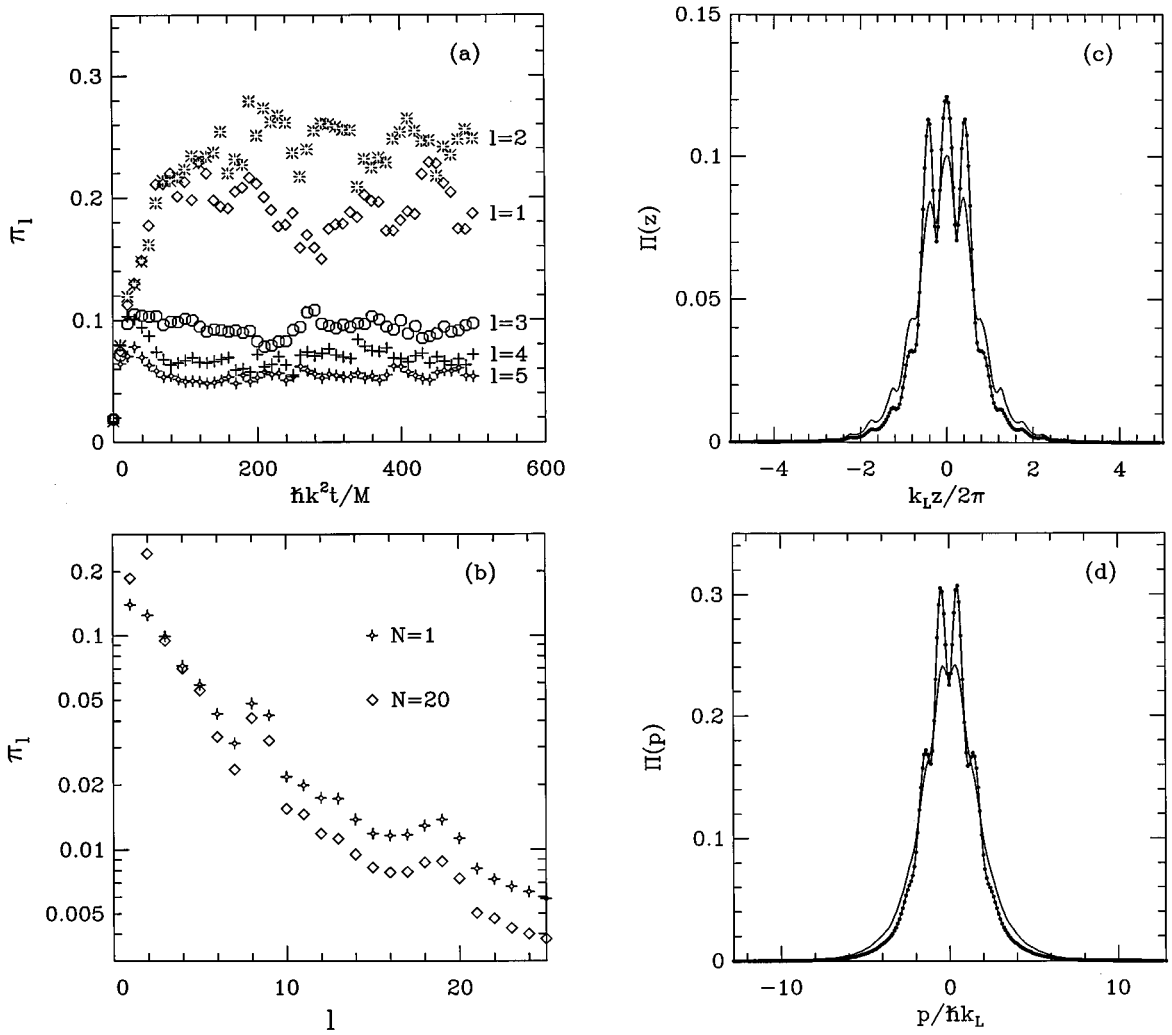

FIG. 3. Laser cooling of N bosons in the lin(π/4)lin laser configuration. The oscillation frequency in the harmonic trap is given by $\Omega_{\rm osc}=0.4\hbar k^2/M$. The atom-laser detuning $\delta=2\Gamma$ and the Rabi frequency $\Omega=-d\mathcal{E}_0/2\hbar=(5/2)17^{1/2}(\hbar k^2\Gamma/M)^{1/2}$ lead to a modulation depth of the lightshift of the $g,m_z\neq 0$ coupled state of $25\cos(\pi/4)\hbar^2k^2/M$. The calculations are performed with $n=1000$ Monte Carlo wave functions in the case $N=20$ and $n=250$ in the case $N=1$. (a) Populations of the energy levels of $\mathcal{H}_0$ as function of time for $N=20$ atoms. (b) Populations averaged over times $t>250M/\hbar k^2$ for $N=1$ and $N=20$. (c) Time averaged position distribution and (d) time averaged momentum distribution for $N=1$ (solid lines) and for $N=20$ (solid lines with symbols).

is 3% only). The time averaged position and momentum distributions are also similar, but are asymmetric for $n=250$. We have checked that this asymmetry is decreased by an average over a longer interaction time, so that it corresponds to statistical uncertainty, not to a systematic error.

VII. CONCLUSION

In summary we have generalized in this paper the application of Monte Carlo wave functions to the solution of nonlinear master equations. We have focused on a special class of nonlinear equations, termed ''of parametrized Lindblad form,'' for which we have discussed in detail the convergence properties of the method. In particular, we identified a systematic error inversely proportional to the number of applied wave functions and a statistical uncertainty of the method having the usual $1/\sqrt{n}$ dependence on the number of wave functions, but with a numerical factor that cannot simply be estimated from a single run with n wave functions. We have shown how to bring certain nonlinear terms in a master equation into a form such that our simulation scheme applies.

Monte Carlo wave functions may now be applied in simulations of nonlinear master equations. Such equations may be purely phenomenological, containing nonlinear terms as effective physical corrections, or they may be derived in more systematic ways, e.g., by application of a Hartree or a Hartree-Fock ansatz to the BBGKY hierarchy of equations for an N-body system. We focused on examples of the latter kind, for which we both pointed out how to arrive at equations of the parametrized Lindblad form and performed simulations to test the feasibility of the method. Quantum statistical enhancement of spontaneous emission in velocity-selective coherent population trapping has recently been studied by a direct numerical solution of the Fock-Bloch master equation; the calculation, however, was restricted to periodic boundary conditions and relatively short interaction times [28]. We have shown that with the Monte Carlo wave-

function technique the effect of a realistic trapping potential could be included and the long time limit (i.e., the steady state) of laser cooling could be investigated.

The study of cold and dense samples of atoms is an interesting field in its own right. The nonlinear equations studied have been put forward as a foundation of nonlinear atom optics, and they bear on the interesting problems associated with propagation of light through quantized media. Most recently the role of quantum statistical effects has become prominent in connection with Bose-Einstein condensation and the prospects of atom-lasers. Our major example was exactly one where the effects of quantum statistics on the center-of-mass motion of atoms in a laser cooling situation was studied. However, simple models have suggested that the possibility of obtaining a Bose-Einstein condensate with laser cooling only is hampered by the reabsorption of fluorescence photons by the atoms [4] and by the exchange of virtual photons (resonant dipole-dipole interaction) [33]. Neither of these phenomena are incorporated by the Hartree-Fock ansatz (49) and by the resulting master equation (73). Phenomenological or more elaborate modifications to Eq. (73) would have to take these effects into account, if the method suggested in this paper is applied to the study of laser cooling of bosons. The dynamics of formation of a Bose-Einstein condensate with evaporative cooling is also an important problem, directly connected to the recent experimental achievements of Bose-Einstein condensation. Its theoretical study leads to nonlinear master equations (with Hartree-Fock and quantum Boltzmann terms), and Monte Carlo wave-function methods could be useful in this case as well.

An aspect of Monte Carlo wave functions is their ability to shed more light on the role of different mechanisms in the density matrix evolution, and we anticipate that the wave-function approach may be helpful at the present stage, where we still have much to learn about the structure and the validity of the nonlinear master equations.

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APPENDIX HIERARCHY OF EQUATIONS FOR $\langle O_1^{(n)}\rangle$, $\langle O_{1,2}^{(n)}\rangle$, ...

As emphasized in Sec. IV, Eq. (38) for the time evolution of the mean value of $O_1^{(n)}$ is not a closed equation. To show this more explicitly let us consider an affine dependence of $L(\sigma)$ on σ:

$$L(\sigma)[\rho]=L_0[\rho]+L_1[\rho\otimes\sigma], \tag{A1}$$

where the L_1 is a linear operator from the two-particle Liouville space into the one-particle Liouville space. After the substitution of Eq. (24) for $\rho^{(n)}$, Eq. (38) now involves mean values of operators $[1/n]O_{i,1}^{(n)}(t)$, $i=1,\ldots,n$ in addition to $O_1^{(n)}$ After average over realizations, the $n-1$ terms with $i\neq 1$ lead to a contribution $[(n-1)/n]\langle O_{1,2}^{(n)}\rangle$, and the single $i=1$ term leads to $[1/n]\langle O_{1,1}^{(n)}\rangle$:

$$\frac{d}{dt}\langle O_1^{(n)}\rangle=L_0[\langle O_1^{(n)}\rangle]+\frac{n-1}{n}L_1[\langle O_{1,2}^{(n)}\rangle]+\frac{1}{n}L_1[\langle O_{1,1}^{(n)}\rangle]. \tag{A2}$$

At this point we observe the need for equations of motion for $\langle O_{1,1}^{(n)}\rangle$ and $\langle O_{1,2}^{(n)}\rangle$, and more generally for the mean value of quantities $\langle O_{\ldots}^{(n)}\rangle$ with $1+p$ indices when $L(\sigma)$ has a polynomial dependence of order p in σ.

The equation of motion for the mean value of the $O_{1,1}^{(n)}$ operator, obtained with the same reasoning as the one leading to Eq. (37), is quite involved. This is due to the fact that the probabilities of the various evolution branches (5), e.g., $1-\delta p$, are not canceled by the normalization factors, $1/(1-\delta p)^2$, of the product state vector. Actually, due to the factor $1/n$ in Eq. (A2), we just need to know that $\langle O_{1,1}^{(n)}\rangle$ converges to a finite value in order to derive the asymptotic behavior of $\langle O_1^{(n)}\rangle$ for large n. Furthermore the factor $1/n$ in the first term in Eq. (33) shows that $\langle O_{1,1}^{(n)}\rangle$ contributes as $1/\sqrt{n}$ to the scaling of the statistical uncertainty of the simulation.

To derive the equation for the mean value of the $O_{1,2}^{(n)}$ operator, we consider simultaneously the evolution of the Monte Carlo wave functions $|\psi_1^{(n)}\rangle$ and $|\psi_2^{(n)}\rangle$. From time t to time $t+dt$, the wave function $|\psi_2^{(n)}\rangle$ has a continuous evolution with a probability $1-\delta q$ or it jumps under the action of the operator $C_m(\rho^{(n)}(t))$ with probability δq_m. At each time step the stochastic evolution applied to each wave function is decided in the numerical simulation with the help of independent random numbers so that the considered pair of wave functions experiences (1) no jump at all, with a probability $(1-\delta p)(1-\delta q)$, (2) jump of the wave function $|\psi_1^{(n)}\rangle$ only, with a probability $\delta p(1-\delta q)$, (3) jump of the wave function $|\psi_2^{(n)}\rangle$ only, with a probability $\delta q(1-\delta p)$, (4) both wave functions jump, with a probability $\delta p\,\delta q$. To first order in dt and after averaging over all realizations from the initial time of the simulation, we get

$$\begin{aligned}\frac{d}{dt}\langle O_{1,2}^{(n)}\rangle&=\langle L(\rho^{(n)})[O_1^{(n)}]\otimes O_2^{(n)}+O_1^{(n)}\otimes L(\rho^{(n)})[O_2^{(n)}]\rangle\\&=\langle[L(\rho^{(n)})\otimes 1+1\otimes L(\rho^{(n)})][O_{1,2}^{(n)}]\rangle.\end{aligned} \tag{A3}$$

In the affine case (A1) this equation takes the explicit form

$$\begin{aligned}\frac{d}{dt}\langle O_{1,2}^{(n)}\rangle&=(L_0\otimes 1+1\otimes L_0)[\langle O_{1,2}^{(n)}\rangle]\\&\quad+\frac{n-2}{n}(L_1\otimes 1+1\otimes L_1)[\langle O_{1,2,3}^{(n)}\rangle]\\&\quad+\frac{1}{n}(L_1\otimes 1)[\langle O_{1,1,2}^{(n)}\rangle+\langle O_{1,2,2}^{(n)}\rangle]\\&\quad+\frac{1}{n}(1\otimes L_1)[\langle O_{1,2,1}^{(n)}\rangle+\langle O_{1,2,2}^{(n)}\rangle].\end{aligned} \tag{A4}$$

Again terms with two identical indices lead to a contribution scaling as $1/n$, whereas the terms with three different indices have to be determined by the successive equation in the hierarchy.

We are now able to anticipate the general form of the hierarchy. The unknowns $\langle O^{(n)}_{1,2,\ldots,k}\rangle$ can be grouped as elements in a vector obeying the equation

$$\frac{d}{dt}\begin{Bmatrix}\langle O_1^{(n)}\rangle\\ \langle O_{1,2}^{(n)}\rangle\\ \langle O_{1,2,3}^{(n)}\rangle\\ \vdots\end{Bmatrix}=[M]\begin{Bmatrix}\langle O_1^{(n)}\rangle\\ \langle O_{1,2}^{(n)}\rangle\\ \langle O_{1,2,3}^{(n)}\rangle\\ \vdots\end{Bmatrix}+\frac{1}{n}\begin{Bmatrix}S_1^{(n)}\\ S_{1,2}^{(n)}\\ S_{1,2,3}^{(n)}\\ \vdots\end{Bmatrix}. \quad \text{(A5)}$$

In the affine case $[M]$ is a matrix coupling given $\langle O^{(n)}_{1,2,\ldots,k}\rangle$ to itself and to $\langle O^{(n)}_{1,2,\ldots,k+1}\rangle$ so that $[M]$ is upper block triangular with one single block off-diagonal. In a more general polynomial dependence of $L[\sigma]$ on σ of order p $[M]$ is also upper block triangular but with p block off-diagonals. We have put in the inhomogeneous right-hand side of Eq. (A5), e.g., $S^{(n)}_{1,\ldots,k}/n$, terms dominated by a scaling as $1/n$ in $(d/dt)\langle O^{(n)}_{1,2\ldots,k}\rangle$: first, the $\langle O^{(n)}_{\ldots}\rangle$ quantities with at least two coinciding indices; second, the correction coming from the departure from unity of the coefficients of the $\langle O^{(n)}_{1,2,\ldots,k+q}\rangle$'s, $q=1,\ldots,p$ [cf. the factor $(n-1)/n$ in Eq. (A2) and the factor $(n-2)/n$ in Eq. (A4)]. In this way the coefficients of the matrix $[M]$ do not depend on n.

To zeroth order in $1/n$ the inhomogeneous part of Eq. (A5) is negligible, and the solution of this equation leads to

$$\langle O^{(\infty)}_{1,2,\ldots,k}\rangle=\langle O_1^{(\infty)}\rangle\otimes\langle O_1^{(\infty)}\rangle\otimes\cdots\otimes\langle O_1^{(\infty)}\rangle, \quad \text{(A6)}$$

where $\langle O_1^{(\infty)}\rangle$ is the solution of the nonlinear master equation, Eqs. (18) and (19). This result holds for any polynomial dependence of $L(\sigma)$ on σ. It can be checked easily in the affine case Eq. (A1), see the explicit equations (A2) and (A4) simplified in the limit $n\to\infty$.

To obtain the result to first order in $1/n$, we keep the inhomogeneous part in Eq. (A5) and replace each $S^{(n)}_{1,2\ldots,k}$ term by its asymptotic value for $n\to\infty$. The deviations of the $\langle O^{(n)}_{1,2,..,k}\rangle$'s from the previous asymptotic solution Eq. (A6) now solve an equation of motion with a linear part given by the matrix $[M]$ and with a source term scaling as $1/n$. Since these deviations are vanishing at the starting time of the simulation they scale as $1/n$ at future times. From this we conclude that the quantities in Eqs. (34) and (36) scale as $1/n$ for large n, which leads according to Eqs. (32) and (33) to the announced scaling laws Eq. (39) and Eq. (40).

In the case of an affine dependence Eq. (A1) it is possible to extract from Eq. (A5) more explicit equations valid to order $1/n$. The idea is to use a Hartree-ansatz to break the hierarchy in Eq. (A4):

$$\begin{aligned}\langle O^{(n)}_{1,2,3}\rangle\simeq&\langle O_1^{(n)}\rangle\otimes\langle O^{(n)}_{1,2}\rangle+P_{1,2}\langle O_1^{(n)}\rangle\otimes\langle O^{(n)}_{1,2}\rangle P_{1,2}\\&+\langle O^{(n)}_{1,2}\rangle\otimes\langle O_1^{(n)}\rangle-2\langle O_1^{(n)}\rangle\otimes\langle O_1^{(n)}\rangle\otimes\langle O_1^{(n)}\rangle,\end{aligned} \quad \text{(A7)}$$

where $P_{1,2}$ exchanges the first and second components in a tensorial product. Note that this goes one step further than the usual decorrelation prescription. We substitute this expression into Eq. (A4). We linearize the resulting equation in terms of the variables Eqs. (34) and (36), which vanish in the limit $n\to\infty$. We keep only the leading terms in the equation, i.e., a term like $\langle O_1^{(n)}\rangle\otimes\langle\delta O^{(n)}_{1,2}\rangle$ is replaced by $\langle O_1^{(\infty)}\rangle\otimes\langle\delta O^{(n)}_{1,2}\rangle$. We get finally

$$\begin{aligned}\frac{d}{dt}\langle\delta O^{(n)}_{1,2}\rangle\simeq&\frac{1}{n}\delta S^{(\infty)}_{1,2}+(L_0\otimes 1+1\otimes L_0)[\langle\delta O^{(n)}_{1,2}\rangle]\\&+(L_1\otimes 1)[\langle O_1^{(\infty)}\rangle\otimes\langle\delta O^{(n)}_{1,2}\rangle]\\&+(1\otimes L_1)[\langle\delta O^{(n)}_{1,2}\rangle\otimes\langle O_1^{(\infty)}\rangle]\\&+(L_1\otimes 1+1\otimes L_1)[P_{1,2}\langle O_1^{(\infty)}\rangle\otimes\langle\delta O^{(n)}_{1,2}\rangle P_{1,2}]\end{aligned} \quad \text{(A8)}$$

with the source term given by

$$\begin{aligned}\delta S^{(\infty)}_{1,2}=&(L_1\otimes 1)[\langle O_1^{(\infty)}\rangle\otimes\langle\delta O^{(\infty)}_{1,1}\rangle]\\&+(1\otimes L_1)[P_{1,2}\langle O_1^{(\infty)}\rangle\otimes\langle\delta O^{(\infty)}_{1,1}\rangle P_{1,2}].\end{aligned} \quad \text{(A9)}$$

This equation predicting a $1/n$ scaling for $\langle\delta O^{(n)}_{1,2}\rangle$ confirms the n dependence in Eq. (40).

The same procedure leads to the corresponding equation for the bias:

$$\begin{aligned}\frac{d}{dt}\langle\delta O_1^{(n)}\rangle\simeq&L_0[\langle\delta O_1^{(n)}\rangle]+L_1\Big[\langle\delta O_1^{(n)}\rangle\otimes\langle O_1^{(\infty)}\rangle+\langle O_1^{(\infty)}\rangle\\&\otimes\langle\delta O_1^{(n)}\rangle+\langle\delta O^{(n)}_{1,2}\rangle+\frac{1}{n}\langle\delta O^{(\infty)}_{1,1}\rangle\Big].\end{aligned} \quad \text{(A10)}$$

The term $L_0[\langle\delta O_1^{(n)}\rangle]$ and the first two terms inside the brackets acted upon by L_1 come from the linearization of the nonlinear master equation around the exact solution $\langle O_1^{(\infty)}\rangle$; they are homogeneous in $\langle\delta O_1^{(n)}\rangle$. The last two terms are inhomogeneous and contribute as a source term scaling as $1/n$. Note that the source terms can be amplified or damped during the time evolution, depending on the stability of the solution $\langle O_1^{(\infty)}\rangle$ to the nonlinear master equation.

To test these results we went to the next order in the Hartree prescription:

$$\begin{aligned}\langle O^{(n)}_{1,2,3,4}\rangle\simeq&\langle O_1^{(n)}\rangle\otimes\langle\delta O^{(n)}_{1,2,3}\rangle+P_{1,2}\langle O_1^{(n)}\rangle\otimes\langle\delta O^{(n)}_{1,2,3}\rangle P_{1,2}\\&+P_{1,3}\langle O_1^{(n)}\rangle\otimes\langle\delta O^{(n)}_{1,2,3}\rangle P_{1,3}+\langle\delta O^{(n)}_{1,2,3}\rangle\otimes\langle O_1^{(n)}\rangle\\&+\langle O^{(n)}_{1,2}\rangle\otimes\langle O^{(n)}_{1,2}\rangle+C_3\langle O^{(n)}_{1,2}\rangle\otimes\langle O^{(n)}_{1,2}\rangle C_3^{\dagger}\\&+C_3^{\dagger}\langle O^{(n)}_{1,2}\rangle\otimes\langle O^{(n)}_{1,2}\rangle C_3-2\langle O_1^{(n)}\rangle\otimes\langle O_1^{(n)}\rangle\\&\otimes\langle O_1^{(n)}\rangle\otimes\langle O_1^{(n)}\rangle,\end{aligned} \quad \text{(A11)}$$

where C_3 performs a cyclic permutation of the first three

components in a tensorial product, and where $\langle \delta O^{(n)}_{1,2,3} \rangle$ denotes the deviation of $\langle O^{(n)}_{1,2,3} \rangle$ from the Hartree approximation Eq. (A7). After lengthy calculations we have checked that in the limit of large n $\langle \delta O^{(n)}_{1,2,3} \rangle$ obeys a linear equation with a source term vanishing faster than $1/n$. This proves the consistency of the results Eq. (A8) and Eq. (A10).

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[27] It sometimes happens that the eigenbasis $|g,n(t)\rangle$ is completely or partially determined by symmetry reasons. This is the case, for example, for laser cooling in a square well potential with periodic boundary conditions compatible with the periodicity of the laser field: when the initial distribution is also periodic and when the Hartree term describing the absorption of the field in the medium (which would break the periodicity) is furthermore *neglected*, the $|g,n(t)\rangle$ are linear combinations of plane waves. Such a situation already considered in [4,28] leads to a great simplification of the problem.

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