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To cite this article: Klaus Mølmer and Yvan Castin 1996 *Quantum Semiclass. Opt.* **8** 49

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Monte Carlo wavefunctions in quantum optics

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Abstract. In this paper we present a review of the Monte Carlo wavefunction method. We discuss some aspects of its application in numerical simulations, and we comment on some of its relations to the foundations of quantum physics. Finally, we investigate the generalization to problems that have so far not been considered tractable by this method—in particular, nonlinear master equations may become relevant, and we discuss the application of Monte Carlo wavefunctions to such problems.

1. Introduction

A quantum system which is not isolated from its surroundings must be described by quantities which are more general than a wavefunction, and its dynamics shows features beyond those contained in the usual solutions of Schrödinger's equation. An atom decaying by spontaneous emission due to the coupling to the surrounding quantized electromagnetic field, or a field mode which is damped due to absorption or leakage of photons through mirrors, are examples of such 'open systems' in quantum optics. Unlike in other fields of physics, damping in quantum optics problems often occurs on the same time-scale as coherent processes (e.g. laser excitation). Thus, it neither restricts the system dynamics to the final state of the decay process, nor can it be accounted for by a simple perturbative correction to the results of the coherent evolution.

The conventional treatment of such systems involves the introduction of the *system density matrix* ρ , where a partial trace has formally eliminated the degrees of freedom of the surroundings. Under conditions often fulfilled in quantum optics problems the Schrödinger equation of motion for the total system + surroundings wavefunction leads to a good approximation to a linear equation of motion, the so-called master equation, for $\rho(t)$.

Recently, a novel treatment of such systems was introduced. Provided a stochastic element is included in the evolution, it is possible to apply wavefunctions rather than density matrices. These wavefunctions may be useful both in numerical calculations, because a wavefunction is a smaller object to propagate in time than a density matrix, and in studies of the dynamics of simple quantum systems, because a wavefunction simulation provides a possible 'route' for a quantum system to take, i.e. possible interpretations of various phenomena. This very recent insight was obtained more or less simultaneously in a number of groups albeit with different motivations and reasoning, and now there are various examples of stochastic wavefunctions applied to quantum optics problems in the ways mentioned.

In section 2, a brief review of the method and its interpretation is presented. Aspects concerning the application in numerical calculations are discussed in section 3. Section 4

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is devoted to a discussion of the ‘meaning’ of the simulated wavefunctions; as it turns out, this issue stimulates a discussion of the foundations of quantum mechanics. Finally, in section 5 we shall outline some generalizations of the Monte Carlo wavefunction technique to master equations different from the forms considered so far.

2. System–reservoir coupling, density matrices and Monte Carlo wavefunctions

In this section we shall outline the common origin of the density matrix and Monte Carlo wavefunctions. We use the Wigner–Weisskopf treatment of spontaneous decay in a parallel derivation of the damping terms in the master equation and an explicit presentation of how to describe the spontaneous decay of a superposition of atomic states by wavefunctions. The generalization to arbitrary master equations is presented.

2.1. The two-level atom coupled to the quantized radiation field

Due to the usual $\vec{A} \cdot \vec{p}$ or $\vec{E} \cdot \vec{d}$ coupling between an atom and the quantized radiation field, excited atomic states are not stable. We consider an atom with only one excited state $|e\rangle$ with an energy E_A above the ground state $|g\rangle$ with energy $E_g \equiv 0$. An initial state of the atom + quantized field with no photons present, will evolve into a state populating also different one-photon states, $|1_\lambda\rangle$ with a field energy of E_λ .

The treatment by Weisskopf and Wigner is a second-order perturbation theory calculation. Let W_λ denote the coupling matrix element between the discrete level $|e\rangle \otimes |0\rangle$ and the continuum states $|g\rangle \otimes |1_\lambda\rangle$. We expand the atom + field wavefunction at time t as $|\Psi(t)\rangle = a(t)|g\rangle \otimes |0\rangle + b(t)e^{-iE_A t/\hbar}|e\rangle \otimes |0\rangle + \sum_\lambda b_\lambda(t)e^{-iE_\lambda t/\hbar}|g\rangle \otimes |1_\lambda\rangle$. (1)

The ground-state atom with no photons in the radiation field is not coupled to any other state, hence $a(t)$ is a constant, whereas the Schrödinger equation for the amplitudes b_λ yields

$$i\hbar \frac{d}{dt} b_\lambda(t) = e^{i(E_\lambda - E_A)t/\hbar} W_\lambda b(t). \quad (2)$$

This equation is integrated, and the result is inserted in the equation for $b(t)$:

$$\frac{d}{dt} b(t) = \frac{-1}{\hbar^2} \sum_\lambda \int_0^t dt' e^{i(E_\lambda - E_A)(t' - t)/\hbar} |W_\lambda|^2 b(t'). \quad (3)$$

Now, if $|W_\lambda|^2$ is essentially constant over a broad energy range $\hbar\Delta$, and if $b(t)$ can be assumed to vary on a long time-scale τ , so that we can choose $\Delta^{-1} \ll t \ll \tau$, we may take $b(t')$ out of the t' -integral above. The integral of the remaining exponential, extended to $t = \infty$, yields $\hbar[\pi\delta(E_\lambda - E_A) + i\mathcal{P}(\frac{1}{E_\lambda - E_A})]$. The subsequent sum (integral) over the energies E_λ (with the appropriate density of states) then gives the factors in the closed equation for $b(t)$,

$$\frac{d}{dt} b(t) = \left(-\frac{\Gamma}{2} + i\frac{\delta E}{\hbar}\right) b(t) \quad (4)$$

where $\Gamma \propto |W_\lambda|_{(E_\lambda=E_A)}^2$. The energy shift δE (the principal value part of the integral) is included in the energy E_A in practical applications, so that we have at time $t + dt$ ($\Gamma dt \ll 1$),

$$|\Psi(t + dt)\rangle = a(t)|g\rangle \otimes |0\rangle + b(t) \left(1 - \frac{\Gamma}{2} dt\right) e^{-iE_A(t+dt)/\hbar} |e\rangle \otimes |0\rangle + \sum_\lambda b_\lambda(t + dt) e^{-iE_\lambda(t+dt)/\hbar} |g\rangle \otimes |1_\lambda\rangle. \quad (5)$$

We shall not need an expression for the value of $b_\lambda(t + dt)$ here; we just note that since the total wavefunction (5) is normalized, the total population of the one-photon component is readily determined from the values of the two zero-photon amplitudes.

2.1.1. Density matrix and master equation. Our theory should be capable of predicting the outcome of experiments measuring any physical property of the system (the atom). Physical quantities are represented by linear operators, A , and may be specified completely by their action on states within a basis $\{|i\rangle\}$, e.g. $\{|g\rangle, |e\rangle\}$,

$$A|j\rangle = \sum_i A_{ij}|i\rangle \quad \text{i.e.} \quad A = \sum_{ij} A_{ij}|i\rangle\langle j|. \quad (6)$$

Any operator can be written in the form (6), hence all information about the system is contained in the set of expectation values $\langle\langle|i\rangle\langle j|\rangle\rangle$. The *density matrix* is a *catalogue* containing these numbers

$$\rho_{ij} = \langle\langle|i\rangle\langle j|\rangle\rangle \quad (7)$$

a definition which agrees with the one introduced to describe a large *ensemble* of K different state vectors $|\psi^{(k)}\rangle = \sum_i c_i^{(k)}|i\rangle$, for which the ensemble mean of operator expectation values precisely involve

$$\rho_{ij} = \frac{1}{K} \sum_k c_i^{(k)} c_j^{(k)*} \equiv \overline{c_i c_j^*}. \quad (8)$$

In the case of the two-level atom, we obtain a 2 by 2 density matrix with elements ρ_{ij} , $i, j = e$ or g . The interaction between the atom and the quantized field causes the evolution obtained in (5), and from this we readily obtain the rate of change of expectation values of operators $|g\rangle\langle e|$, $|e\rangle\langle e|$, etc. Under the assumption that emitted photons do not change the future evolution, i.e. that the above calculation with initially no photons present is applicable at all times, we obtain damping terms to be inserted into the equation of motion for the density matrix,

$$\dot{\rho}_{ee} = -\Gamma\rho_{ee} \quad \dot{\rho}_{eg} = -\frac{\Gamma}{2}\rho_{eg} \quad \dot{\rho}_{ge} = -\frac{\Gamma}{2}\rho_{ge} \quad \dot{\rho}_{gg} = \Gamma\rho_{ee}. \quad (9)$$

The evolution of the density matrix is given by the *master equation*, and incorporating a Hamiltonian H acting only on the system, the master equation has the form

$$\frac{d}{dt}\rho = \frac{1}{i\hbar}[H, \rho] + \mathcal{L}_{\text{relax}}[\rho] \quad (10)$$

where $\mathcal{L}_{\text{relax}}[\rho]$ represents the terms in (9). In particular, H may contain the coupling to a laser field.

2.1.2. Monte Carlo wavefunction treatment. If we are allowed to neglect interference terms between the zero- and one-photon components of $|\Psi(t + dt)\rangle$ in (5), we lose no information by treating these two components independently as far as one-time averages are concerned. At each time step dt with a probability equal to the norm $|a(t + dt)|^2 + |b(t + dt)|^2 = (1 - |b(t)|^2\Gamma dt)$ we simply replace $|\Psi(t + dt)\rangle$ by its (normalized) zero-photon component, or with the remaining probability $|b(t)|^2\Gamma dt$ by the one-photon component.

This is done statistically in the density matrix treatment, but it may also be done by simulation: at each time step, dt , we make a choice: *either* the wavefunction is evolved during dt according to Schrödinger's equation, including the decay term (non-Hermitian component) for the excited state amplitude (4), and the wavefunction is renormalized, *or*

the system performs a *quantum jump*, and the wavefunction is put equal to the ground-state wavefunction, $|g\rangle$ (atomic part of the one-photon component in (5)). The jump occurs with probability $\delta p = \Gamma |b(t)|^2 dt$. This evolution is then repeated over and over again [1].

Like the density matrix approach, this procedure removes the variables of the radiation field from our calculation, and it has an appealing interpretation: the random element corresponds exactly to the consequence of an ideal detection of the number of photons present in the field at time $t+dt$. According to the quantum theory of measurements, the only possible detector readouts are the integer eigenvalues of the photon number operator, and subsequent to detection the wavefunction must collapse on the corresponding eigenstates. In the most common photodetection process, the detection of a photon actually removes it from the field, so that both detection events have an atomic state times the vacuum state of the quantized field as a final state. This fits perfectly with our subsequent evolution of the state vectors. A more detailed account of the connection to existing photodetection theory may be found in [2]. The quantum jump event occurs with a probability which is just the probability that a photon is detected during the time interval, and the ensuing state vector is the final state of this process: the atomic ground state. Having no photons present at time t the most likely event is that no photon is detected, and then a slight rotation of the wavefunction occurs: after a reduction of the excited state amplitude and a renormalization the probability amplitude for being in the ground state has increased, and the one for being in the excited state has decreased.

The continuous part is *a priori* less intuitive, but is necessary to incorporate in the evolution, and, indeed, it provides a non-trivial insight into the dynamics of simple quantum systems. For example, it explains how n atoms, all initially in a coherent superposition of the ground and excited states, can relax towards the ground state without emitting n fluorescence photons (which would result in a macroscopic violation of energy conservation). In a simulation with a large number of wavefunctions a fraction of the atoms end up in the ground state as consequence of quantum jumps, and a remaining fraction ‘get rid of’ their excited state components without leading to detection of light, simply by following the continuous rotation towards the ground state, gradually increasing the $|g\rangle \otimes |0\rangle$ amplitude $a(t)$ in (1). The fraction of atoms choosing either of these paths turns out to be just $|b(t=0)|^2$ and $|a(t=0)|^2$, as expected.

2.2. General system–reservoir interaction

There are many examples of quantum systems coupled to their surroundings in a way that allows the above type of elimination. The system Hilbert space may have any number of dimensions (also infinite) and not just two as in the example, and the surrounding reservoir may consist of separate components leading to different decay channels for the system.

Based on a few mathematical and physical criteria, it is possible to prove that the master equation for the density matrix can always be put on the so-called Lindblad form [3]. (In section 5 we shall come back to a discussion of physically motivated deviations from this form and their possible treatment by means of Monte Carlo wavefunctions.)

In the general case, one has to derive the master equation directly from the system–reservoir coupling, or to derive the explicit stochastic procedures to apply in a Monte Carlo wavefunction treatment, and to this end the existence of a universal form is of only little help. However, the existence of a specified form of the master equation leads to an important conclusion concerning the generality of the Monte Carlo wavefunction method: all physical problems describable by a density matrix obeying a master equation of Lindblad form can also be treated by Monte Carlo wavefunctions!

2.2.1. The Lindblad form of the master equation. A quantum system with a Hamiltonian H , coupled in addition to a large and broad-band reservoir (the necessary criteria for the elimination of the degrees of freedom of the reservoir in our treatment) may experience damping and energy changes, not accounted for by H . We can account for the system–reservoir coupling by absorbing energy changes in a redefinition of H and by applying damping terms in the master equation for the density matrix of the system. This master equation has the appearance,

$$\frac{d}{dt}\rho = \frac{1}{i\hbar}[H, \rho] + \mathcal{L}_{\text{relax}}[\rho] \quad (11)$$

with $\mathcal{L}_{\text{relax}}[\rho]$ being of the general Lindblad form [3]:

$$\mathcal{L}_{\text{relax}}[\rho] = -\frac{1}{2} \sum_m (C_m^\dagger C_m \rho + \rho C_m^\dagger C_m) + \sum_m C_m \rho C_m^\dagger \quad (12)$$

where C_m^\dagger is the adjoint of C_m , and both C_m and C_m^\dagger have dimensions of $\sqrt{1/\text{time}}$. This specific form is required in order to preserve the interpretation of ρ as a density matrix, i.e. $\text{Tr}(\rho) = 1$ must be conserved, and the probability $\langle \psi | \rho | \psi \rangle$ of being in any state $|\psi\rangle$ must be larger than or equal to zero for all times and for any choice of $\rho(t=0)$. Note that (12) does not determine the C_m 's in a unique way.

In equation (12) the first sum is an anticommutator; it contains decay terms decreasing the total population $\text{Tr}(\rho)$ of ρ . The ‘sandwich’ terms of the second sum are feeding terms and have a positive contribution to $(d/dt)\text{Tr}(\rho)$.

In the case of the two-level atom coupled to the radiation field initially in the vacuum state, there is only one operator $C_m = \sqrt{\Gamma}|g\rangle\langle e|$. The anticommutator in (12) originates in the derivation of the master equation from the evolution of the component of the atom + field wavefunction in the initial state of the field, i.e. the zero-photon subspace. It describes the decay of the excited state population and of the e – g coherences. The sandwich term originates from the trace of the total wavefunction of the atom + field over the field involving field states different from the initial vacuum state, i.e. reservoir states with one fluorescence photon. This term represents the feeding of the ground state by spontaneous emission.

This connection of the decay terms to the initial state of the reservoir, and of the ‘sandwich’ terms to perturbed reservoir states, is not specific to the two-level atom. Furthermore, in the general case, an arbitrary number of C_m operators can be involved, describing the possible branching of decay in different channels, see examples presented in [4].

2.2.2. MCWF treatment of general master equation of Lindblad form. We shall now present a scheme for evolving Monte Carlo wavefunctions in time, so that, on average, they will lead to the same predictions as the master equation (11) for the system. As in the simple two-state analysis, the evolution contains two elements: continuous reduction of amplitudes followed by renormalization of the whole wavefunction, and quantum jumps occurring at random according to specified probabilities.

Assume the wavefunction $|\phi(t)\rangle$. To propagate this function in time we first calculate the wavefunction $|\phi^{(1)}(t+\delta t)\rangle$ obtained by evolving $|\phi(t)\rangle$ with the non-Hermitian Hamiltonian to first order in dt :

$$\tilde{H} = H - \frac{i\hbar}{2} \sum_m C_m^\dagger C_m \quad (13)$$

$$|\phi^{(1)}(t+dt)\rangle = \left(1 + \frac{1}{i\hbar} \tilde{H} dt\right) |\phi(t)\rangle. \quad (14)$$

Since \tilde{H} is not Hermitian, this new wavefunction is not normalized. The square of its norm is $\langle \phi^{(1)}(t + dt) | \phi^{(1)}(t + dt) \rangle = 1 - \delta p$ where δp reads

$$\delta p = \sum_m \delta p_m = dt \sum_m \langle \phi(t) | C_m^\dagger C_m | \phi(t) \rangle. \quad (15)$$

The magnitude of the step dt is adjusted so that this calculation to first order is valid; in particular it requires $\delta p \ll 1$.

The probability of having no jump is $1 - \delta p$ in which event we simply renormalize the function $|\phi^{(1)}(t + dt)\rangle$ to get the new wavefunction $|\phi(t + dt)\rangle$. Alternatively, a quantum jump may take place, with a probability δp , and it collapses the wavefunction on a specific state $C_m |\phi(t)\rangle$ with a relative probability $\delta p_m / \delta p$. So, at time $t + dt$ we have one of the normalized wavefunctions

$$\begin{aligned} \text{with probability } 1 - \delta p: \text{ no jump } \quad |\phi(t + \delta t)\rangle &= \frac{|\phi^{(1)}(t + \delta t)\rangle}{\sqrt{1 - \delta p}} \\ \text{with probability } \delta p_m: \text{ jump } \quad |\phi(t + \delta t)\rangle &= \frac{C_m |\phi(t)\rangle}{\sqrt{\delta p_m / \delta p}}. \end{aligned} \quad (16)$$

The jumps may be decided by taking random numbers ε at each time step dt and comparing them to the probability δp : if ε is uniformly distributed between zero and unity, the probability that $\varepsilon < \delta p$ equals δp , and hence this event may be used as a criterion for performing one of the jumps in (16). Which one of the jumps in (16) to perform on the wavefunction may be determined subsequently by taking a new random number ε and comparing it to the relative probabilities $\delta p_m / \delta p$.

Another implementation of the procedure [5,6] accumulates the probability that no jump has occurred (the most likely event during each dt) in a delay function $P(t)$. Setting $P(t) = 1$ immediately after a jump at time t_0 , and multiplying it by $1 - \delta p$ in each subsequent time-step, it is easy to show that the resulting function $P(t)$ is the probability that the state vector makes no jump in the interval between t_0 and t . In simple problems the delay function may be determined analytically. In numerical applications the delay function approach has the advantage of using fewer random numbers, the next jump may be decided as the instant t when the value of $P(t)$ reaches a certain random number $\tilde{\varepsilon}$ chosen right after the previous jump event, and in being less sensitive to the uniformity and correlations of the random number generator in the vicinity of $\varepsilon = 0$. Furthermore, it may form a basis for optimizing the integration routine of the Schrödinger equation for each wavefunction: the continuous evolution may be performed by higher-order routines, e.g. a Runge–Kutta scheme, and when the delay function approaches the value ε the step size may be adapted, so as to get the jump at just the right moment.

It is easy to prove [2,4] that the Monte Carlo simulation scheme reproduces, on the average, the results of the master equation (11). Performed in practice, such an average involves only a finite number of wavefunctions and hence an error due to sampling statistics appears. We discuss this in the following section.

In conclusion, we have two alternative means for treating dissipative quantum systems, Monte Carlo wavefunctions and the density matrix. They lead to equivalent results but in different ways, each having its virtues and disadvantages. Their connection is analogous to the one between the Langevin and the Fokker–Planck equation for, e.g. Brownian motion. For some problems it may be useful to adopt the Monte Carlo wavefunctions as a means to *simulate* the result of a given master equation, for others the density matrix may be preferred for its deterministic calculation of mean values of the stochastic evolution (16).

3. Numerical applications

In this section we discuss various aspects of the application of Monte Carlo wavefunctions as a numerical tool. The motivation for such an application is that for a system with N basis states, the density matrix has N^2 elements obeying a set of linear equations, where each Monte Carlo wavefunction has only N components. The wavefunctions provide results that are correct only on average, hence a number n of wavefunctions is required to provide such average results with sufficient precision. In particular, problems with very large N , so that n wavefunctions with $n \ll N$ are sufficient, may benefit from a MCWF treatment.

We discuss in this section a few general properties of the simulations, and we give a numerical example for a problem where the Monte Carlo wavefunction method seems to be the only feasible and reliable method to actually produce results: 3D laser cooling.

3.1. Sample mean and variance

Suppose that n independent wavefunctions $|\psi_i(t)\rangle$ have been evolved in time, and that the expectation values $a_i(t) = \langle \psi_i | A | \psi_i \rangle$ of an operator A have been calculated for the n wavefunctions. We then obtain the sample mean

$$a_{(n)}(t) = \frac{1}{n} \sum_{i=1}^n a_i(t) \quad (17)$$

which provides an approximation to the exact mean value $\text{Tr}(\rho(t)A)$. As usual when numbers are sampled from some distribution the statistical error on the determination of the mean value is estimated by $\delta a_{(n)}/\sqrt{n}$, where $(\delta a)_{(n)}^2$ is the sample variance of the a_i 's

$$(\delta a)_{(n)}^2(t) = \frac{1}{n} \sum_{i=1}^n a_i(t)^2 - a_{(n)}^2(t). \quad (18)$$

The analysis and the presentation of numerical data obtained by this method is thus clear: the method provides both expectation values and accompanying error bars with a half width $\delta a_{(n)}/\sqrt{n}$.

It is difficult to make quantitative predictions about the size of the error bars without performing the simulations, but a few observations may be useful.

(i) Adding, and subtracting, in (18) the sample mean of the operator A^2 , and assuming that sample means are good approximations to the exact mean of the operators A and A^2 (large- n limit), we can estimate

$$\begin{aligned} (\delta a)_{(n)}^2(t) &\simeq \text{Tr}(\rho A^2) - (\text{Tr}(\rho A))^2 \\ &\quad - \frac{1}{n} \sum_{i=1}^n (\langle \phi^{(i)}(t) | A^2 | \phi^{(i)}(t) \rangle - \langle \phi^{(i)}(t) | A | \phi^{(i)}(t) \rangle^2). \end{aligned} \quad (19)$$

This expression shows that our sample variance will be smaller than the quantum uncertainty of the operator determined by the density matrix in the first line of (19). As seen from the second line, the sample variance depends on the character of the Monte Carlo wavefunctions in the intuitive way that wavefunctions with large uncertainties lead to mean values which are bound to be less scattered than those of spectrally narrow wavefunctions. In section 4 we discuss the existence of multiple simulation schemes for the same problem. This may have implications in numerical treatments, as they may lead to different size error bars, and hence be different from the point of view of efficiency.

(ii) In [4] we distinguished between 'local' and 'global' operators, such as, for example, the population of a single state and quantities involving a large group of states. Operators of

the first kind have larger fluctuations relative to their mean than the ones of the second kind and hence it may be more difficult to determine their expectation values by a simulation. As it was already shown in [4], however, the finite ‘widths’ of the Monte Carlo wavefunctions may substantially improve the quality of predictions as compared to the most simple estimates. Again, we recall, that the calculations themselves provide error bars, hence we may estimate the quality of the simulation empirically.

(iii) In some problems the density matrix $\rho(t)$ converges to a steady state ρ^{st} . Even in this case the Monte Carlo wavefunctions have, in general, no steady state and each expectation value $a_i(t)$ keeps fluctuating with time. If we are only interested in steady-state mean values we may, however, replace the variables $a_i(t)$ by their time average \bar{a}_i on a time interval of arbitrary duration, after the system is assumed to be in the steady state. An approximation of $\text{Tr}(\rho^{\text{st}}A)$ can then be derived from the sample mean of the \bar{a}_i ’s. Indeed, when averaged over a sufficiently long time, a single $a_i(t)$ is sufficient to predict the correct steady-state expectation value, but by applying a number n of wavefunctions, we get both the improvement of averaging the individual $a_i(t)$ ’s, and thereby approaching the exact mean, and we still have a measure of the statistical error $\delta\bar{a}/\sqrt{n}$, where $(\delta\bar{a})^2$ is now the sample variance of the \bar{a}_i ’s. This procedure represents an improvement of the numerical technique as the continuation of the simulation over even a short time interval, after we have arrived at the assumed steady-state conditions, requires a relatively small increase in computing time but it may lead to a significant reduction of the error bars.

Finally, it is of relevance for numerical applications that:

(iv) It is often easier to write a routine that propagates wavefunctions than density matrices because the equations are fewer and simpler. In particular, one readily generalizes coherent evolution problems to include dissipative effects: one only needs to make minor corrections in the Hamiltonian in the coherent evolution routine and then to add the jumps. With just a few wavefunctions one gets a ‘quick and dirty’ estimate of the evolution of a dissipative system.

(v) Many density matrix problems benefit from selection rules that make certain coherences $\rho_{i_0j_0}$ vanish at all times, or from symmetries that lead to similar reductions in the number of quantities to be considered. These reductions apply to the Monte Carlo wavefunctions as well, so that, for example, no wavefunction contains non-vanishing amplitudes c_{i_0} and c_{j_0} simultaneously. They are, in fact, even easier to identify and certainly easier to implement in the wavefunction formalism. Also, approximations such as the adiabatic elimination of excited states of atoms in weak laser fields are more easily carried out in the wavefunction formalism of the problem.

3.2. Numerical example: 3D laser cooling

Recently, we have applied the MCWF method in a full quantum treatment of laser cooling in three dimensions [7].

By laser cooling it is possible to obtain samples of atoms with kinetic energies in the microkelvin range [8, 9]. For recent reviews of the experimental achievements and theoretical methods, see [10, 11]. A quantum formulation of the problem leads [12], in the limit of large detunings, to a universal law for the mean kinetic energy of the atoms,

$$E_K/E_{\text{Rec}} = f(\hbar|\delta|s/(2E_{\text{Rec}})) \quad (20)$$

where the recoil energy, $E_{\text{Rec}} = (\hbar k)^2/2M$, has been introduced, with k being the laser wavenumber and M the atomic mass. The (negative) detuning of the laser frequency with respect to the atomic transition frequency is denoted by δ , and we have introduced the

saturation parameter $s = 2|\Omega|^2/(4\delta^2 + \Gamma^2)$, where Γ is the decay rate of the excited state and where Ω is the Rabi frequency (atom–laser coupling amplitude).

The number of elements of the atomic density matrix ρ is proportional to the square of the number of points in a grid covering the centre-of-mass momentum range, e.g. for $|p_i| \leq 20\hbar k$, $i = x, y, z$, and a discretization of $\hbar k$ we get $(2 \times 20 + 1)^3 \simeq 5 \times 10^9$ elements, a number which should be multiplied by the number of matrix elements relative to the atomic electronic states. Monte Carlo wavefunctions are likely to be the only realistic means for a quantitative study of this problem.

The calculation is reasonably straightforward: we introduce the ground- and excited-state components of the atomic state vector $|\psi_g\rangle$ and $|\psi_e\rangle$, obeying the coupled linear equations where \vec{p} denotes the atomic momentum operator,

$$i\hbar \frac{d}{dt} |\psi_e\rangle = \left(\frac{\vec{p}^2}{2M} - \hbar\delta - i\hbar\Gamma/2 \right) |\psi_e\rangle + V^{(+)} |\psi_g\rangle \quad (21)$$

$$i\hbar \frac{d}{dt} |\psi_g\rangle = \frac{\vec{p}^2}{2M} |\psi_g\rangle + V^{(-)} |\psi_e\rangle. \quad (22)$$

A non-Hermitian part $\propto \Gamma$ enters explicitly as a damping term in the evolution of $|\psi_e\rangle$. Equations (21), (22) are obtained in a rotating frame and $V^{(\pm)}$ denote the raising and lowering part of the atom–laser interaction Hamiltonian.

Quantum jumps occur according to the current spontaneous emission rate, $\delta p = \Gamma dt \langle \psi_e | \psi_e \rangle$. There is a branching corresponding to an infinitely large number of C_m operators in (12) representing emission of a photon with a polarization \vec{e}_S and a wavevector \vec{k}_S , and the state vector after ‘detection’ of such a photon is

$$|\psi\rangle \rightarrow |\psi\rangle_{\vec{k}_S, \vec{e}_S} = (\vec{e}_S^* \cdot \vec{D}^{(-)}) e^{-i\vec{k}_S \cdot \vec{R}} |\psi_e\rangle \quad (23)$$

where the exponential factor containing the position operator \vec{R} of the atom translates the atomic momentum by the photon recoil $-\hbar\vec{k}_S$, the operator $\vec{e}_S^* \cdot \vec{D}^{(-)}$ contains the lowering part of the atomic dipole operator, and it projects the atom into the ground state. Justified by the widths of the calculated distributions being several $\hbar k$, we have simplified to emission of photons along the coordinate directions \vec{e}_x, \vec{e}_y and \vec{e}_z , only.

Polarization gradient cooling is most efficient at low saturation $s \ll 1$, and we eliminate the excited state from the calculation: neglecting $\vec{p}^2/2M$ as compared to $\hbar\Gamma/2$ and putting $d|\psi_e\rangle/dt = 0$ in (21) we obtain $|\psi_e\rangle = (\hbar\delta + i\hbar\Gamma/2)^{-1} V^{(+)} |\psi_g\rangle$. When inserted in (22), this introduces the effective ground-state potential operator $(\hbar\delta + i\hbar\Gamma/2)^{-1} V^{(-)} V^{(+)}$, and in (23) it yields quantum jumps among ground-state wavefunctions.

The laser configuration is a superposition of fields propagating along the coordinate axes. We expand the centre-of-mass components of the wavefunction on a set of states with momenta $\vec{p} = \vec{p}_0(t) + \hbar k(n_x, n_y, n_z)$, where n_x, n_y and n_z are integers. Indeed, an initial momentum eigenstate will, at any later times, have an exact expansion on these states, and with the simplified emission pattern described above, $\vec{p}_0(t)$ can be set to 0 at all times. For calculations of momentum distributions with $p_{i,\text{rms}} \leq 7\hbar k$, $i = x, y, z$, it is sufficient to take $-20 \leq n_x, n_y, n_z \leq 20$.

Measurements of mean kinetic energies in 3D optical molasses have been performed on $j_g \rightarrow j_e = j_g + 1$ atomic transition, with $j_g = 2$ and $j_g = 3$ in two isotopes of Rb [9] and with $j_g = 4$ in Cs [8]. We have investigated these three types of transition, and $j_g = 1$. The mean steady-state kinetic energy of the atoms E_K is obtained as a function of the parameter $\hbar|\delta|s/2$ for a detuning of $\delta = -5\Gamma$ and for one closely investigated laser configuration defined by three pairs of beams of counterpropagating orthogonal linear polarizations, the

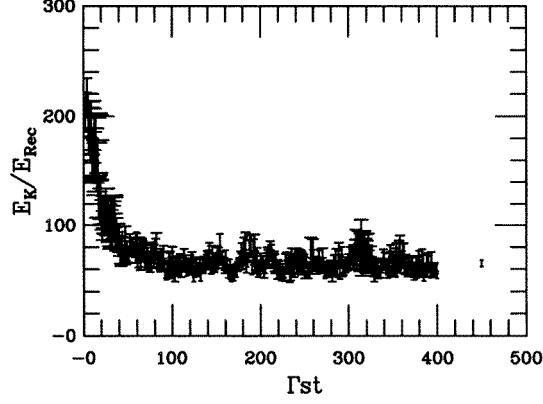


Figure 1. Mean kinetic energy as a function of time for the atomic transition $j_g = 3 \rightarrow j_e = 4$. The results, with error bars, are shown for a simulation with nine wavefunctions, the laser-atom detuning is $\delta = -5\Gamma$ and the lightshift reads $\hbar|\delta|s/2 = 25E_{\text{Rec}}$. To the right in the figure is shown the mean value and error bar obtained after a time averaging of the individual contributions over the second half of the time evolution. The laser-field configuration is the one commonly referred to as $\text{lin}\perp\text{lin}$.

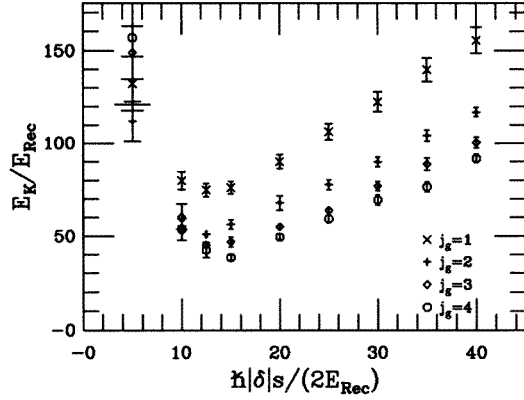


Figure 2. Mean kinetic energy as a function of lightshift for the atomic transitions $j_g \rightarrow j_e = j_g + 1$, $j_g = 1, 2, 3$ and 4 . The laser field configuration is the one commonly referred to as $\text{lin}\perp\text{lin}$, and the atom-laser detuning is $\delta = -5\Gamma$. Colder initial atomic distributions than in figure 1 are considered so that relaxation times are shorter and the error bars are smaller.

so-called $\text{lin}\perp\text{lin}$ configuration. The field amplitude E_0 in each beam is included in the Rabi frequency $\Omega = dE_0/\hbar$, where d is the atomic dipole moment.

After an interaction time of a few hundred $(\Gamma s)^{-1}$ the mean expectation values $a_i(t) = \langle \phi_i(t) | \vec{p}^2 / 2M | \phi(t) \rangle$ fluctuate around a constant level, but the fluctuations are large compared to the value of the sample mean, see figure 1. This implies that $n \simeq 100$ wavefunctions would be needed to yield results with, say, 10% precision. We apply the time-averaging procedure described above over a subsequent time interval which we take to be of the same duration as the one needed to achieve a steady state. This leads to a reduction in the scattering of expectation values, i.e. of our error bars by a factor of $\simeq 3$, so at the expense of a factor of two in integration time we get an improvement corresponding to a factor $\simeq 10$ in number of wavefunctions, and simulations *with only six to twelve wavefunctions* suffice to yield the results with the error bars summarized in figure 2. The mean kinetic energies shown are in good agreement with the experimental values [7].

The low level of statistical uncertainty on our results, shown in figure 2 and in [7], was beyond our expectations, and it brings promise for further applications within this field.

4. The meaning of Monte Carlo wavefunctions

4.1. The physics in a single-wavefunction realization

The Monte Carlo wavefunction method may be applied to simple systems for which density matrix solutions are readily obtained. By following the time evolution of a single wavefunction one may then get an insight into the mechanisms leading to certain phenomena. There are two reasons for this: it is easier to keep track of, say, two or three amplitudes, than of four or nine density matrix elements, and in the wavefunction evolution the change with time can be explicitly linked with the physical mechanism coupling the relevant amplitudes. In particular, the continuous ‘no-jump’ evolution may be responsible for transitions that are difficult to identify in the master equation. In section 2 we gave the decay of a superposition state in a two-level atom as a particularly simple example. Other examples where physical pictures have been obtained successfully by this approach are: dark states and velocity selective coherent population trapping [6], lasing without inversion [13], etc.

It is quite general that the Monte Carlo evolution represents a possible history of the system wavefunction in the presence of a suitable continuous detection process [1, 2]. Simulations of systems which are actually being monitored are therefore particularly interesting, and as emphasized by Carmichael, we are then propagating, *in parallel* a conditioned wavefunction *and* a classical detection signal. The statistics of jumps in the simulations are therefore directly comparable with the statistics in photocounts in a photodetection experiments. Anti-bunching, sub-Poissonian statistics, and other aspects of the random character of photocount signals can therefore be studied directly in such simulations. This approach may be compared to the, often cumbersome, treatments involving correlation functions and the quantum regression theorem. As for numerical applications, it is a question of the specific needs of a certain problem as to whether Monte Carlo wavefunctions present a useful approach to a problem or not.

Since the density matrix is Hermitian it may always be diagonalized providing a probabilistic interpretation in terms of its eigenstates and eigenvalues. Only in very few cases, however, will this represent a physically motivated disentangling of the density matrix as the eigenstates of the matrix ρ usually play no natural role in the dynamics of the system or in relation to any reasonable detection scheme. The Monte Carlo method, in contrast, produces an ensemble of wavefunctions that have such a physical motivation, e.g. the treatment of the decay of a superposition state of the two-level atom, mentioned in section 2, provides two populations, a fraction of the atoms in the ground state, and another fraction in a superposition state eventually approaching the ground atomic state. Unlike the eigenstates of ρ (or of any Hermitian system operator), these states are not even orthogonal; their physical significance is associated with measurements on the surroundings and not on the system itself. The wavefunctions also illustrate the ‘dynamics’ in a steady state obtained as an ensemble average of constantly evolving state vectors, see, for example, the discussion of damped Rabi oscillations or of Doppler cooling in [4].

In section 4.2 we show that several simulation schemes may be applied to the same physical problem. One class of simulations is related by a unitary transform among the C_m operators. Another class replaces the evolution involving quantum jumps by a stochastic differential equation for the Monte Carlo wavefunctions. This has a number of consequences, in particular, for the interpretation of the method. Recently, stochastic wavefunctions have appeared in the theory of the measurement process in quantum mechanics, and in section 4.3 we indicate in which way our derivation of such an equation may contribute to this discussion.

4.2. Non-uniqueness of the simulation scheme

4.2.1. *Unitary transform among C_m operators.* Suppose that the relaxation operator can both be written as in (12) and as

$$\mathcal{L}_{\text{relax}}(\rho) = -\frac{1}{2} \sum_m (D_m^\dagger D_m \rho + \rho D_m^\dagger D_m) + \sum_m D_m \rho D_m^\dagger. \quad (24)$$

Physically this duality naturally appears when the evolution of the system is invariant for a unitary transformation T :

$$T \mathcal{L}_{\text{relax}}(\rho) T^\dagger = \mathcal{L}_{\text{relax}}(T \rho T^\dagger). \quad (25)$$

In this case one has simply

$$D_m = T^\dagger C_m T. \quad (26)$$

Mathematically it is always possible to define such a set of operators by

$$D_m = \sum_k U_{mk} C_k \quad (27)$$

where U_{km} is any unitary matrix.

Although predictions concerning operator averages are the same—the master equation is unchanged—the physical pictures given by Monte Carlo simulations following either of the two forms may be very different. The continuous ‘no-jump’ evolution is given by the same non-Hermitian Hamiltonian, but jumps occur with different branching channels and probabilities: instead of following the dynamics in (16), the system may jump to one of the states $D_m|\phi(t)\rangle$ with a probability $\delta p_m^{(D)} = \langle \phi(t) | D_m^\dagger D_m | \phi(t) \rangle dt$.

A physical example, discussed in detail in [4], is the one of spontaneous emission of an atom with a Zeeman sublevel structure in the ground state. The master equation then shows a branching of the decay into a sum of three terms (corresponding to sums in (1) over photon states with three different polarizations). This branching then becomes manifest in the simulations through the C_m , $m = 0, \pm 1$ operators associated with the detection of a photon of polarization m along, for example, the z -axis. For this problem, the operator T may be a simple rotation, so that the D_m ’s correspond to decay by emission of a photon of definite polarization m along a different direction \hat{e} . Or, it may represent the change from a basis of circular polarizations to one of linear or elliptic polarizations, or to rotations among these.

4.2.2. *Continuous stochastic differential equations.* In addition to the different stochastic jump approaches it is possible to apply stochastic differential equations, leading to continuously, but still randomly, evolving Schrödinger wavefunctions. Such equations, representing ‘quantum state diffusion’, have a longer history, considered by some researchers as a possible means to formally describe quantum state evolution during measurements. Indeed, within the theory of quantum measurements, several authors [14–18] have pointed out that the effects of the master equation on ρ could be simulated by stochastic wavefunctions, the meaning of which is still a matter of dispute. The numerical applications of the stochastic differential equations on equal footing with the jump approach was realized immediately when the latter was used in dissipative quantum optics problems, see, for example, [19].

In fact, Carmichael considered not only the case of direct photoelectron counting but also homodyne detection of the signal from a photoemissive source [2]. In such a detection the field emitted from the source is mixed with a strong local oscillator field, and the combined signal intensity is recorded. As most photons emanate from the local oscillator, the state of the system, e.g. an atom, conditioned on the detection of a photon in the combined field, deviates only weakly from the state given that no photon has been detected. On the other hand

the combined signal is very intense, hence changes occur very often to the system wavefunction in such a simulation: the state vector obeys a continuous stochastic differential equation.

Inspired by the work of Carmichael, we showed in [20], that from the jump approach, applicable to any master equation of Lindblad type, one can, in a systematic way, obtain continuous stochastic equations, coinciding with the ones already derived by Gisin and others. These equations can therefore, in general, be attributed an interpretation in terms of a detection on a mixed ‘system + local oscillator’ signal. This connection is demonstrated below.

A detailed account of the application to actual homodyne and heterodyne detection of the signal from a laser excited two-level atom with numerical examples has been given by Wiseman and Milburn [21], and, by now, a large amount of work exists on the use of the different approaches. An interesting distinction, worth mentioning in this context and reviewed, e.g. in [22], is between regarding the noise in the stochastic equations as being due to input noise (vacuum fluctuations in the reservoir coupled to the system) or output noise (monitored signal from the system). The two are, of course, connected, but the latter view seems to be the one capable of assigning an element of reality to the stochastic wavefunctions.

We apply an extension of the ideas in the above subsection to show the connection between the quantum jump method described in (16), and stochastic differential equations [20]. First, we may add to the Lindblad form a new C_m operator proportional to the identity operator $\mathbb{1}$ which gives a vanishing contribution to the master equation. Next, we perform a transformation among the C_m operators of the form (27), so that we rewrite the relaxation terms in the master equation:

$$\mathcal{L}_{\text{relax}}(\rho_S) = -\frac{1}{2} \sum_{m,\varepsilon} (D_{m,\varepsilon}^\dagger D_{m,\varepsilon} \rho_S + \rho_S D_{m,\varepsilon}^\dagger D_{m,\varepsilon}) + \sum_{m,\varepsilon} D_{m,\varepsilon} \rho_S D_{m,\varepsilon}^\dagger \quad (28)$$

where $\varepsilon = \pm 1$ and where the $D_{m,\varepsilon}$ are defined as

$$D_{m,\varepsilon} = \frac{\mu \mathbb{1} + \varepsilon C_m}{\sqrt{2}}. \quad (29)$$

This expression is fully equivalent to (12). We now perform a Monte Carlo evolution of the wavefunctions, using the set of operators $D_{m,\varepsilon}$. If we assume that μ^2 is large compared to other rates in the system, the simulation with $D_{m,\varepsilon}$ operators involves a much larger number of quantum jumps in a given time interval Δt than a simulation with the C_m ’s. But the change of the wavefunction in a given quantum jump, $|\phi\rangle \rightarrow D_{m,\varepsilon}|\phi\rangle/\|D_{m,\varepsilon}|\phi\rangle\|$, is correspondingly much smaller since $D_{m,\varepsilon}$ is nearly proportional to the identity operator $\mathbb{1}$.

In the homodyne detection scheme considered by Carmichael, the $D_{m,\varepsilon}$ jump operators correspond precisely to the detection of a photon after one has mixed the light emitted by the system with the local oscillator field. The component $\mu \mathbb{1}$ represents an annihilation operator acting on the state of the local oscillator. If the oscillator is initially in a coherent state with a large mean photon number, this is equivalent to the multiplication by a c -number.

Assume values of μ and Δt such that the number of jumps $N_{m,\varepsilon}$ occurring with a given operator $D_{m,\varepsilon}$ during Δt is large compared to 1, and the evolution due to the other parts of the system dynamics is small. The operator \mathcal{O} describing the combined action of all jumps occurring during Δt is a product of the $D_{m,\varepsilon}$ and it can be approximated by

$$\mathcal{O} \simeq \left(\frac{\mu}{\sqrt{2}}\right)^N \left(\mathbb{1} + \frac{1}{\mu} \sum_m (N_{m,+} - N_{m,-}) C_m\right) \quad (30)$$

where $N = \sum_{m,\varepsilon} N_{m,\varepsilon}$ is the total number of jumps occurring during Δt . The wavefunction

at time $t + \Delta t$ can now be written before normalization:

$$|\phi(t + \Delta t)\rangle = \left(\mathbb{1} + \frac{1}{i\hbar} H \Delta t - \frac{1}{2} \Delta t \sum_m C_m^\dagger C_m + \sum_m \frac{N_{m,+} - N_{m,-}}{\mu} C_m \right) |\phi(t)\rangle \quad (31)$$

where we have taken into account both the non-Hermitian evolution during Δt and the effect of multiple quantum jumps. The numbers $N_{m,\varepsilon}$ are Poissonian random variables, and based on expressions analogous to (15), we obtain for the average values and standard deviations:

$$\overline{N_{m,\varepsilon}} \simeq \frac{\mu^2 \Delta t}{2} \left(1 + \frac{\varepsilon}{\mu} \langle C_m + C_m^\dagger \rangle \right) \quad \Delta N_{m,\varepsilon} \simeq \frac{\mu}{\sqrt{2}} \sqrt{\Delta t} \quad (32)$$

where the average value $\langle C_m + C_m^\dagger \rangle$ is taken in $|\phi(t)\rangle$. In the limit of large $N_{m,\varepsilon}$, we can then approximate the random variable $N_{m,+} - N_{m,-}$ appearing in (31) by

$$\frac{N_{m,+} - N_{m,-}}{\mu} = \Delta t \langle C_m + C_m^\dagger \rangle + \Delta \zeta_m \quad (33)$$

where $\Delta \zeta_m$ is a real Gaussian random variable with zero mean and a standard deviation equal to $\sqrt{\Delta t}$. Finally we normalize the wavefunction (31) and we obtain:

$$\begin{aligned} |\Delta \phi\rangle = & \frac{1}{i\hbar} H |\phi(t)\rangle \Delta t + \frac{1}{2} \sum_m (\langle C_m + C_m^\dagger \rangle C_m - C_m^\dagger C_m - \frac{1}{4} \langle C_m + C_m^\dagger \rangle^2) |\phi(t)\rangle \Delta t \\ & + \frac{1}{2} \sum_m (2C_m - \langle C_m + C_m^\dagger \rangle) |\phi(t)\rangle \Delta \zeta_m. \end{aligned} \quad (34)$$

In equation (34), we have kept terms linear in $\Delta \zeta_m$ and Δt , and we have replaced all the quadratic terms $\Delta \zeta_m \Delta \zeta_{m'}$ by their mean $\Delta t \delta_{m,m'}$. In the limit $\mu \rightarrow +\infty$, $\Delta t \rightarrow 0$, this equation can be interpreted as an Itô stochastic equation.

The phase of the local oscillator field may be controlled to experimentally extract the phase or the quadrature components of the radiated field; this amounts to changing μ into a complex number in the above treatment. Averaging over different settings of the phase of μ (corresponding for example to a heterodyne detection where the local oscillator has a frequency very different from the one of the source) we obtain yet another stochastic equation [20, 21]:

$$\begin{aligned} |\Delta \phi\rangle = & \frac{1}{i\hbar} H_S |\phi\rangle \Delta t + \sum_m (\langle C_m^\dagger \rangle C_m - \frac{1}{2} C_m^\dagger C_m - \frac{1}{2} \langle C_m^\dagger \rangle \langle C_m \rangle) |\phi\rangle \Delta t \\ & + \sum_m (C_m - \langle C_m \rangle) |\phi\rangle \frac{\Delta \xi_m}{\sqrt{2}} \end{aligned} \quad (35)$$

where $\langle C_m \rangle = \langle \phi | C_m | \phi \rangle$, and where the $\Delta \xi_m$ are independent complex Wiener processes [23].

In [21] the laser-excited two-level atom, decaying by spontaneous emission, is treated by different homodyne and heterodyne detection simulations, and very different distributions of wavefunctions in state space appear.

4.3. Quantum theory of measurements

The co-existence of various different stochastic treatments for the same master equation emphasizes that in a simulation we are not only simulating the system wavefunction, but the system wavefunction plus a classical detection record. If the system is not observed, the true wavefunction is the one of the system plus surroundings, as in (1), and neither of our simulations can be preferred over the others.

4.3.1. Monte Carlo wavefunctions and the EPR paradox. A particularly interesting case is when the non-uniqueness of the C_m -operator (e.g. in (26)) corresponds to the possibility of choosing among a set of different observables in the simulated measurement of the surroundings of the system. The effects of this choice of the observer reflects the non-local character of quantum mechanics which has, since the early days of quantum physics, challenged our understanding of reality in physics. It was formulated in the Einstein–Podolsky–Rosen paradox, and it has been verified by measurements, e.g. in experiments by Aspect [24] showing that the abundance of different polarization coincidences within pairs of photons were in disagreement with Bell’s inequality.

In [1, 4] we considered a simple example with two C_m -operators. An atom with ground and excited states, with angular momenta $J_g = J_e = 1$, is irradiated by a laser field composed of two waves with σ^+ and σ^- -polarization with respect to the z -axis. The excited $m_e = 0$ state may decay into either of the two $m_g = \pm 1$ states with equal probability but not into the $m_g = 0$ state because of a vanishing dipole matrix element (Clebsch–Gordan coefficient). The alternative detection of different polarization components of a fluorescence photon, leading to different final ground states of light emitting atoms, reveals an entanglement between the atomic state and the field state analogous to the EPR-type correlations in the polarization components of photon pairs.

The derivation of the master equation does not involve an analysis of the role of measurements in quantum physics and, in particular, no quantum jumps appear. As the quantized field is eliminated in the density matrix treatment, one may expect that measurements on this field should not alter our conclusions about the system (atom) dynamics. And, indeed, the typical evolution of wavefunctions under one or another simulation scheme are radically different, but in a way that does not disturb the statistical agreement with the density matrix.

The stochastic evolution of Monte Carlo wavefunctions may be visualized as a random walk in the space of wavefunction amplitudes $\{c_i\}$. The different simulation schemes lead to different trajectories, *but also* to different probability distributions $P(\{c_i\})$, see, for example, the figures in [21]. All physical information, however, relates to operator expectation values $\langle \phi | A | \phi \rangle$, hence to the bilinear terms $\overline{c_i c_j^*}$, only. These averages are the ‘second moments’ of the $P(\{c_i\})$ distributions, and they are independent of the simulation scheme. Only in the cases where the simulation scheme can be interpreted in terms of measurements on the single quantum system atom + reservoir, do other details of the $P(\{c_i\})$ represent relevant knowledge about the system.

4.3.2. Monte Carlo wavefunctions and macroscopic localization. An ideal measurement on a single quantum system yields an eigenvalue of the operator pertaining to the observed quantity, although a quantum system cannot simultaneously be in an eigenstate of all operators that may hypothetically be subject to measurement. Instead, after detection, the system finds itself in the eigenstate corresponding to the measured operator eigenvalue. This imposes a counterintuitive back-action of the (classical) observer on the observed quantum system, incorporated in the projection postulate of quantum measurements (Copenhagen interpretation).

The probabilistic aspect of the detection process may be incorporated in a density matrix formulation, and, for example, for a continuously monitored system, the density matrix will obey a master equation which is necessarily of the Lindblad form. Indeed, prior to their application to dissipative quantum systems, the density matrix, the Lindblad form master equation *and stochastic wavefunctions* (!) appeared in the very fundamental discussion of

the role of measurements in quantum physics.

In the so-called continuous spontaneous localization model [16, 25], suggested in the mid-eighties by Ghirardi, Rimini and Weber, a position-dependent stochastic field is introduced with parameters ensuring that even on very long time-scales no discrepancy with the results of the usual Schrödinger equation appears for microscopic systems, but when a macroscopic object is studied it will localize in position on a very short time-scale and at random according to the stochastic field. It was emphasized that the stochastic term should not be thought of as the ‘back-action’ of a position measuring aggregate, but as a term always present in the Schrödinger equation [17]: the stochastic evolution takes place irrespective of our observing the system or not. Similar viewpoints are adopted in the quantum state diffusion model [14], which has recently been formally united by another formulation called the decoherent histories approach [25, 26]. The desired consequence of this model is that the back-action by postulate of the meter on the observed system is explicitly avoided. If a system is in a superposition $c_1|1\rangle + c_2|2\rangle$ of two eigenstates of an observable, the coupled system + meter wavefunction would evolve into a coherent superposition state involving two states of the macroscopic meter $|M_1\rangle$, $|M_2\rangle$. According to the Copenhagen interpretation, we do not see this macroscopic superposition state in the classical world, but one of the components is picked at random, and subsequently the observed system is in the pertaining eigenstate. In the continuous spontaneous localization model the macroscopic superposition state is not *a priori* forbidden, it just happens that the non-linear and stochastic equation of evolution of the combined system wavefunction very rapidly suppresses one of the components. No separate treatments of the microscopic and the macroscopic world are needed.

Apart from a criticism based on Occam’s razor principle—that one should not introduce variables in a theory that are not rooted in our knowledge about the system—the continuous spontaneous localization model may meet a problem in tailoring the stochastic terms so that they neither lead to contradictions with the high precision obtainable in modern experiments on atoms and ions nor should they exclude the quantum phenomena observable on still larger scales (mesoscopic quantum physics).

A more severe criticism to the project of ‘localization without the projection postulate’ may, however, come from the work on Monte Carlo wavefunctions: the central equation in the quantum state diffusion model is, indeed, equation (35) of this paper, which is also very similar to the continuous spontaneous localization equation, see e.g. [27]. As we have identified (35) as one out of several equations (16), (34), (35) applicable to the same system, its unique importance in the evolution of a quantum system is questionable. Moreover, we have actually identified the origin of the stochasticity in all of these equations in terms of measurement-induced collapses of the statevector—and, clearly, one cannot by simply ignoring such an interpretation claim that a theory free of this element has been established.

On the other hand, the continuous spontaneous localization model and related theories point out one important feature, namely that macroscopic localization may take place in a continuous manner, and that the only projections or quantum jumps needed for the interpretation may be associated with, e.g. single-photon detection events, see also [28].

Let us finally, in this section, comment on the so-called decoherence obtained when the off-diagonal elements of the density matrix of a system tend to zero. This evolution has been interpreted as a sign of the system choosing randomly between different states [29]. But, just as there is nothing unique about any particular simulation scheme, there is nothing unique about the basis in which a system density matrix is diagonal: one *can* interpret the density matrix as a statistical mixture of such basis states, but one can, just as well, construct statistical mixtures of completely different state vectors, for example, a set of physically motivated Monte Carlo wavefunctions.

5. Beyond master equations of the Lindblad form

As mentioned in the introduction, the arguments leading to the Lindblad form of master equation are quite general, and a few words are needed to motivate studies of equations which are not of this form.

Before turning to non-Lindblad master equations that can be simulated, let us note that in some cases the master equation itself can be pathological. Indeed, the master equation is an approximation to a problem (a Markov assumption and second-order perturbation theory is generally used to derive the equation). An effective treatment in terms of a density matrix may hence not be valid at all or, maybe, a linear equation for ρ can be found which is not of the Lindblad form. Given (un-)suitable initial conditions, such an equation may involve, for example, negative probabilities, on some time-scales or for some special quantum states, but it may still be the most useful equation to apply when one disregards these peculiarities. A well known example is the one of Brownian motion where a particle is subject to a mean friction force linear in velocity [30]. We shall not consider this type of master equation further.

A first extension beyond the calculation of density matrices or selected one-time expectation values is the determination of multi-time correlation functions of observables of the system. This type of problem leads to master equations for a density matrix which is not necessarily positive and to affine master equations. We briefly review the known simulation techniques in subsection 5.1, and we give as an example the derivation of the fluorescence spectrum from an atom.

Second, a physical problem may be so large that approximations may be needed to accomplish a solution, and these approximations may transform a master equation of Lindblad type into one that is not. We show first in subsection 5.2 how to simulate the phenomenological non-homogeneous master equation describing exchange of atoms between the interaction region and an external reservoir of atoms. We consider in subsection 5.3 cases where the final (reduced) problem is not Markovian (because part of the system with a finite correlation time has been eliminated) and in subsection 5.4 cases where the problem is non-linear (e.g. because a mean-field approach is taken to a many-body problem).

5.1. Correlation functions and spectra

We have already explained how to calculate one-time averages with Monte Carlo wavefunctions. Imagine now that the quantity to be calculated is a two-time correlation function

$$g(t_2, t_1) = \langle A(t_2)B(t_1) \rangle \quad (t_2 > t_1) \quad (36)$$

where $A(t_2)$ and $B(t_1)$ are two operators of the system written in the Heisenberg picture at times t_2 and t_1 . From the quantum regression theorem the function g is given by

$$g(t_2, t_1) = \text{Tr}(A\sigma(t_2; t_1)) \quad (37)$$

where the density matrix σ is the solution of

$$\frac{\partial}{\partial t}\sigma(t; t_1) = \frac{1}{i\hbar}[H(t), \sigma(t; t_1)] + \mathcal{L}_{\text{relax}}(t)[\sigma(t; t_1)] \quad (38)$$

$$\sigma(t_1; t_1) = B\rho(t_1). \quad (39)$$

Note that σ as a function of t obeys the same equation (11) as the usual density matrix $\rho(t)$, but the initial condition (39) makes in general σ neither positive nor even Hermitian.

A first suggestion [1] for the calculation of g with Monte Carlo wavefunctions is to write the initial value of σ as a linear combination with coefficients c_α of four positive density matrices $\sigma_\alpha(t_1; t_1)$ that are known as statistical mixtures of pure states from the Monte Carlo representation of $\rho(t_1)$. These positive matrices are evolved according to (38) with the usual Monte Carlo scheme so that $\sigma(t; t_1) = \sum_{\alpha=1}^4 c_\alpha \sigma_\alpha(t; t_1)$ is approximated by Monte Carlo wavefunctions for any $t > t_1$.

A second suggestion [31, 32] is to introduce formally the non-Lindblad master equation

$$\frac{d}{dt}\Pi(t) = \frac{1}{i\hbar}[H(t), \Pi(t)] + \mathcal{L}_{\text{relax}}(t)[\Pi(t)] + h(t)B\Pi(t) \quad (40)$$

where h is a given function of time, and to expand the solution Π in powers of B , $\Pi = \Pi_0 + \Pi_1 + \dots$, with initial conditions (at $t = 0 < t_1$) $\Pi(t = 0) = \rho(t = 0)$. To zeroth order in B the equation (11) is recovered and $\Pi_0(t)$ and $\rho(t)$ coincide. Π_0 is simulated with Monte Carlo wavefunctions:

$$\Pi_0(t) = \langle |\phi_0(t)\rangle \langle \phi_0(t)| \rangle \quad (41)$$

where the brackets denote the average over many realizations. To first order in B an affine master equation is obtained:

$$\frac{d}{dt}\Pi_1 = \frac{1}{i\hbar}[H(t), \Pi_1(t)] + \mathcal{L}_{\text{relax}}(t)[\Pi_1(t)] + h(t)B\Pi_0(t) \quad (42)$$

with the initial condition $\Pi_1(t = 0) = 0$. The key point is now that Π_1 can be represented by stochastic wavefunctions in the following way:

$$\Pi_1(t) = \langle |\phi_1(t)\rangle \langle \phi_0(t)| \rangle. \quad (43)$$

Basically, $|\phi_1\rangle$ is slaved to $|\phi_0\rangle$. During the Hamiltonian evolution of $|\phi_0\rangle$, the evolution of $|\phi_1\rangle$ involves, in addition to the effective Hamiltonian (13), the source term $h(t)B|\phi_0(t)\rangle$. When $|\phi_0(t)\rangle$ makes a quantum jump $|\phi_1(t)\rangle$ undergoes the same quantum jump. Also the normalization factor applied to $|\phi_1(t)\rangle$ coincides with the one applied to $|\phi_0(t)\rangle$. We refer to [31, 32] for the precise description of the evolution of $|\phi_1\rangle$.

$\Pi_1(t_2)$ permits a calculation of the integral over t of $h(t)\langle A(t_2)B(t) \rangle$. The correlation function $g(t_2; t_1)$ is obtained with $h(t) = \delta(t - t_1)$ as a special case. The fluorescence spectrum from an atom at a frequency ν is instead given by the Fourier transform of the correlation function of the atomic dipole at this frequency, so that it is obtained with the choice $h(t) = \exp(i\nu t)$.

In the case of the fluorescence spectrum the appearance of an affine equation and this formal perturbation theory (expansion in powers of B) can be understood physically. Indeed the spectrum may be found in experiments as the intensity built up, e.g. in a Fabry–Pérot cavity illuminated by the fluorescence, i.e. the fluorescence spectrum may be obtained by solving the master equation of the atom + cavity mode and extracting the *one-time average* mean photon number as a function of the eigenfrequency of the Fabry–Pérot cavity. If the coupling between the two sub-systems is weak, we may assume that only density matrix elements with photon numbers of zero and unity are needed, and the steady-state zero- and one-photon components of this density matrix may be obtained successively in a calculation that is formally equivalent to the one performed using the quantum regression theorem treatment of the problem.

A Monte Carlo wavefunction simulation of the spectrum along these lines involves a wavefunction of the type

$$|\psi\rangle = |\phi\rangle \otimes |0_\omega\rangle + |\phi_\omega\rangle \otimes |1_\omega\rangle \quad (44)$$

where one of the field modes in the sum (1) is now retained for closer analysis. The evolution with or without jumps is given by the usual terms (note that the choice of application of an atomic jump operator C_m is determined by the larger zero-photon component of the wavefunction, but the operator affects both (atomic) components $|\phi\rangle$ and $|\phi_\omega\rangle$). The spectrum is proportional to the squared norm of the one-photon component of this wavefunction. These ideas have been developed further in [31, 32] to identify other spectral properties, and to make efficient numerical schemes.

The density matrix-like object evolved in the quantum regression theorem calculation corresponds to the atom + cavity mode density matrix elements between zero- and one-photon field states, $\rho_{i0,j1}$ and $\rho_{i1,j0}$. As the atomic diagonal elements ($i = j$) of these matrices are not populations they do not need to be positive, but there is clearly no problem in obtaining these quantities by the Monte Carlo wavefunction simulations: the field-off-diagonal parts of the total atom + cavity mode density matrix are simulated by the dyads $|\phi\rangle\langle\phi_\omega|$ and $|\phi_\omega\rangle\langle\phi|$ in the wavefunction above.

5.2. Simulation of an inhomogeneous master equation

If, for example, we study a situation where atoms interact with a laser field within a given interaction region, a realistic master equation should also describe the effect of atoms leaving and arriving in this region. In such a problem we may find a steady state, where the loss and feeding terms exactly compensate each other, and if the atoms are not interacting with each other, we may approximate the problem by a single one-particle density matrix, where in addition to the usual terms in the master equation (11), (12) we have a loss term and an inhomogeneous source term:

$$\frac{d}{dt}\rho(t)_{\text{flux}} = -\gamma\rho + \gamma\rho^0. \quad (45)$$

This equation describes how, for example, atoms enter in a state described by the density matrix ρ^0 , and how they leave, in this simple equation, with a probability independent of their internal state. The value of γ and the normalization of ρ , ρ^0 also rely on the real flux of atoms in number per second. Note that the arrival and departure does not need to be in position space, it may also be defined with respect to part of the full space of quantum states of the system, i.e. an excitation by a collision or a discharge may enter an atom in a subspace corresponding to, for example, a two-level system.

A simple and intuitive wavefunction simulation of the system utilizes, apart from the usual treatment of the terms in the master equation not written in (45), knowledge of the eigenvalues π_λ and eigenstates $|\chi_\lambda\rangle$ of ρ^0 : at each time step dt , with a probability γdt the Monte Carlo wavefunction is replaced by one of the $|\chi_\lambda\rangle$'s (chosen according to the probability law $\{\pi_\lambda\}$). If the inhomogeneous term ρ^0 is itself the result of a Monte Carlo wavefunction calculation featuring statevectors $|\phi_i^0\rangle$, $i = 1, \dots, n$ we implement the random element by the simpler random choice of one of these statevectors (each having probability $1/n$).

A more technical derivation of this intuitive simulation scheme relies on the fact that (45) can be replaced by the homogeneous master equation

$$\frac{d}{dt}\rho(t)_{\text{flux}} = -\gamma\rho + \gamma\rho^0 \text{Tr}(\rho) \quad (46)$$

which can be shown to be of the Lindblad form. In the same way one shows also that the more general form of inhomogeneous master equations

$$\frac{d}{dt}\rho(t)_{\text{flux}} = -\frac{1}{2}(W\rho + \rho W) + \rho_0 \text{Tr}(\rho W) \quad (47)$$

can be simulated provided that W is positive.

5.3. Non-Markovian problems

There are cases in which it is not allowed to apply a Markovian hypothesis to obtain a simple local-in-time master equation for a system density matrix. Here, we cannot take a general approach to this problem, but we may consider two different situations that can be treated, and that may be combined into approximations of less restricted problems.

One should also mention that in a number of quantum optics systems it is possible to apply a perturbation to a system that depends on a certain measured quantity. Such a feedback, is for example, applied to stabilize the phase or intensity of output optical signals. In [33], the non-Markovian behaviour of systems with feedback is discussed.

5.3.1. Noisy classical terms in system Hamiltonian. If, for example, an atom is excited by a classical laser field with an intensity or phase, or both, that fluctuate in time, the set of linear equations, coupling the density matrix elements, will have coefficients (detuning or Rabi frequency) fluctuating with time. This implies that the density matrix itself becomes a stochastic variable whose mean (over the fluctuations of the classical terms) will be the quantity of interest. It is thus of interest, when possible, to find an equation for this mean, denoted by $\bar{\rho}$ in the following. This kind of problem has, of course, received considerable interest for its practical relevance; when the noisy term is δ -correlated in time a Markovian assumption may be applied and a new effective master equation is obtained of the usual type (but typically with new damping rates for coherences, reflecting the fluctuations in their oscillation frequencies). For different kinds of coloured noise an analytical treatment is possible [34] which may lead to a master equation of the form

$$\frac{d}{dt}\bar{\rho}(t) = \int_{-\infty}^t K(t-s)\bar{\rho}(s) ds \quad (48)$$

where the kernel $K(t-s)$ couples $\bar{\rho}(t)$ to its value at previous times. $K(t-s)$ may be determined from the parameters of the problem.

It is unclear how one could simulate (48) directly, but a Monte Carlo wavefunction simulation may readily be suggested by noting that we wish to simulate a master equation which is at each instant of time of Lindblad type. To treat the problem, we simply have to use random elements both to produce the instantaneous values of the fluctuating coefficients and as criteria for the jump or no-jump evolution.

5.3.2. System coupled to a finite width reservoir. The Markov property of the master equation comes from the coupling to states within a wide energy range, cf the discussion below (1): if the surroundings into which the system dissipates energy has a finite bandwidth, one may not simply evaluate the amplitude $b(t')$ in (3) at the fixed time t . Instead of decaying exponentially away, the energy may be exchanged back and forth between the system and the reservoir, yielding in the limit of a very narrow reservoir continuum the usual Rabi oscillations [35].

As in our discussion of correlation functions, here it may also be a good idea to examine the physical problem further. The finite bandwidth may result from the system being indirectly coupled to a broad-band reservoir, but the resonant structure of the intermediate system ‘filters’ the energy continuum as seen by the system of interest. Physical examples are an atom coupled to a leaky cavity field mode and a cavity field mode coupled to an atomic transition. Instead of just dissipating energy into the narrow-band reservoir, a system may also be excited by the output from another quantum system which may not be represented by c -numbers, and which may not be δ -correlated in time, a situation made the subject

of recent studies by Gardiner *et al* [36] and by Carmichael *et al* [37]. In both cases the system forms part of a *cascaded* open system, and the total system may be described by a master equation of the usual Lindblad type (11). A simulation of the evolution of this larger system is then straightforward. One essentially applies a wavefunction of the same kind as in (44), possibly with more components. Decay terms may be absent from the evolution of the $|\phi_i\rangle$'s, but, for example, an amplitude on an excited state in $|\phi\rangle$ may be transferred to a ground state component in $|\phi_\omega\rangle$, and a 'jump', de-exciting the adjacent system, now puts this ground state in place of $|\phi\rangle$. The physics in this sequence of events corresponds, e.g. to an excited atom transferring its excitation to a cavity field mode which subsequently loses the quantum of energy by dissipation to its environment (mirror-loss). Depending on the jump (mirror-loss) rate the population may oscillate back and forth among the involved states before the jump takes place and relieves the combined system of the energy, or before the no-jump evolution has had the same effect. This shows the non-Markovian character of the dynamics of the atomic part of the system.

Here the Monte Carlo wavefunction method may be an important tool, as the degrees of freedom added enlarges the problem, and may make it hard to treat by density matrices. Imamoglu [38] has suggested to approximate arbitrary reservoirs by a finite number of damped harmonic oscillators, each contributing a Lorentzian continuum function. When a few oscillators are sufficient to model the density of states and the energy-dependent coupling strengths, and when their excitation number may be kept low, a wide range of problems should become tractable.

5.4. Non-linear master equations

Non-linear master equations result, for example, if one attempts a 'mean-field theory' treatment of a many-body problem. Many-body problems in quantum optics have become relevant with, e.g. the increased phase space density of atoms achievable in laser cooled or evaporatively cooled samples. The first non-linear master equations have already been suggested and non-linear matter-wave effects similar to known non-linear optical effects have been studied.

We have revealed the close analogy between non-linear optics and non-linear atom optics starting from the coupled Maxwell-Bloch equations for the propagation of light through an atomic gas [39]: assuming the atoms at location \vec{r} to be in their internal steady state, we obtain the macroscopic polarization of the medium $\vec{P}(\vec{r})$ as a function of the field amplitude, and as this is coupled back to the field in the Maxwell equations, the propagation of light becomes non-linear. Alternatively, assuming that the position distribution of atoms in the gas is given by $N\langle\vec{r}|\rho|\vec{r}\rangle$, where N is the total number of atoms, and ρ is the internal *and* external state density matrix, the coupling between the light and the component of the atomic system at position \vec{r} is sensitive to the damping and refraction of the light beam as it propagates through the medium, i.e. to the value of the density matrix at other positions \vec{r}' . Now eliminating the field, one obtains a non-linear atomic master equation for ρ [39]. The same equation is obtained by a Hartree approximation of the full N -atom problem, cf [40, 41].

Phenomenological or approximate non-linear master equations have been around for some time and represent equations that it may be interesting to treat by the Monte Carlo wavefunction method. However, unlike the case in the previous sections, here we cannot perform a large number of independent wavefunction simulations and in a simple way obtain the correct density matrix averages. Assume that a Monte Carlo wavefunction is represented by amplitudes $c_i(t)$. A density matrix element, ρ_{ij} is approximated by the

average over many realizations of $c_i c_j^*$, and any part of the jump/no-jump evolution leads to a rate of change of these averaged quantities given by a linear combination of similar products $c_k c_l^*$. The simulations reproduce the master equation because the coefficients in this combination coincide with the factors multiplying ρ_{kl} in the master equation. Now, in a nonlinear problem, some of these coefficients are functions of the density matrix elements themselves, thus we have to express them in terms of the simulated wavefunction amplitudes. The problem is that the statistical agreement between wavefunctions and the density matrix only assures that the ensemble average of products $c_k c_l^*$ have the correct values; the average of a general nonlinear term $f(\{c_i c_j^*\}) c_k c_l^*$ will not necessarily yield an approximation to $f(\{\rho_{ij}\}) \rho_{kl}$.

To take a specific example, consider the rate equation for the excited state population of a two-level atom

$$\frac{d}{dt} \rho_{ee} = -\Gamma \rho_{ee} - \Gamma(N-1)(1-\rho_{ee})\rho_{ee} \quad (49)$$

that has been used as a model to describe superradiance [42, 43]. The equation is similar to the usual Lindblad master equation for one-atom decay, if one replaces the constant decay rate Γ by the ρ_{ee} -dependent $\Gamma(\rho) = \Gamma(1 + (N-1)(1-\rho_{ee}))$. The solution to equation (49) is not an exponential decay curve for ρ_{ee} . If, however, we simulate the problem by a single wavefunction initially in the excited state, we note that as long as it stays there, Γ will have its usual one-atom value, thus the non-linear term never comes into play and the simulation is wrong.

The natural solution to the problem is to evolve a number of wavefunctions simultaneously. At every instant, the whole ensemble then provides an approximation to the density matrix, and this approximation (involving all state vectors) determines the nonlinear terms which are then applied in the propagation of each wavefunction. Such an approach applies whenever the master equation may be written on the Lindblad form with operators (H and C_m) that depend parametrically on the density matrix elements.

A simple analysis of the superradiance model involving just two wavefunctions already shows a modification in the correct direction: starting with both state vectors equal to the excited state, both wavefunctions evolve as in the normal decay problem until one of the states has been set equal to the ground state. The remaining excited state wavefunction now experiences an increased decay rate, because the effective Γ has increased, as ρ_{ee} decreases to the value of one half, and the nonlinear term in (49) is no longer suppressed. With even more simultaneously propagated wavefunctions, one obtains the characteristic behaviour of superradiance: first a period with a usual decay rate, then a rapid, almost simultaneous, jump of all Monte Carlo wavefunctions. For numerical examples, see [43].

In the nonlinear atom optics problem, and in the superradiance model, equation (49), the master equation ‘coefficients’ are affine functions in the density matrix elements. For this type of problem we have proven [43] that the suggested procedure of using the whole ensemble of stochastic wavefunctions will, indeed, lead to results approaching the correct solution to the nonlinear problem. With a finite sample, there will be a systematic error, as it is seen by the example of only one wavefunction in the superradiance model, but the error scales as $1/n$ where n is the number of wavefunctions, hence it will for large n be smaller than the error bar due to sampling, which still scales as $1/\sqrt{n}$ [43].

6. Conclusion

Since Monte Carlo wavefunctions emerged as a tool to describe dissipation in quantum optics systems a variety of systems has been studied with this method. The concept of a

conditioned wavefunction evolution has been applied to interpret the evolution of a simpler quantum system and as a starting point for entirely new analytical and numerical treatments. The formulation in terms of wavefunctions may provide a short-cut to the derivation of master equations, and for numerically demanding problems a direct formulation in terms of wavefunctions can be applied in simulations without ever writing the explicit master equation for the density matrix.

Many examples have appeared in the literature, and in this paper we have attempted to illustrate some of the main applications of Monte Carlo wavefunctions. We have chosen to focus on a few examples and to discuss features that we believe are universal for the application of this alternative to density matrices.

The Monte Carlo wavefunctions provide information about dissipation and decoherence in quantum physics supplementary to the one from the density matrix, and we anticipate that this approach may contribute further both to our understanding of the evolution of open quantum systems, and to discussions of the foundations of quantum physics beyond the brief comments in this paper.

The method has turned out to be extremely well suited to describing the dynamics of laser cooling, and as this topic has now evolved towards situations with dense and cold samples in which the interaction among the particles may no longer be safely ignored, there is an increasing interest in studying atom–atom interactions in this domain. Monte Carlo wavefunctions have already been successfully applied to the problem of binary atomic interactions in laser fields [44, 45], and the generalization of the method to simulate effective nonlinear master equations describing an N -atom system may become important.

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