5 Discussion

5.1 The Quantum Monte Carlo method as a numerical tool

Averaged over a large ensemble of stochastic wave functions the QMC method yields results in agreement with those of the density matrix treatment. With a finite number n of wavefunctions one may thus obtain an estimate of any operator expectation value, and as the number n increases, the uncertainty decreases as $a/\sqrt{n}$. When the dimension N of the system Hilbert space is large, satisfactory precision may thus be obtained more easily from a calculation involving $N \cdot n$ rather than N^2 variables. The consideration concerns both computing *time* and computer *memory*, and details about the computer (scalar or vector processor ?) may well determine the competition between a density matrix calculation and the QMC treatment.

As the numerically most demanding problem, we have considered laser cooling of atoms in three dimensions. Laser cooling is a topic that has achieved considerable experimental and theoretical interest, and it is an excellent example of a process where the interplay between coherent evolution (atom-laser interaction, kinetic energy) and dissipation (spontaneous emission, recoil) combined with the large dimension of the problem lends itself to a treatment based on Monte Carlo wave functions. We have demonstrated that a time evolution towards steady state of N amplitudes, with N on the order of 300.000, is feasible. This large number is required to describe laser cooling of Cs on the $J_g = 4 - J_e = 5$-transition. The results are promising, and they represent a step forward compared to dealing with a density matrix with $\simeq 50 \cdot 10^9$ elements.

A number of aspects about the method should be mentioned, and some open questions should be raised:

Simple programming: It is easier to write a routine that propagates wave functions than density matrices because the equations are fewer and simpler. With just a few wave functions one gets a "quick and dirty" estimate of the evolution of the system. Furthermore, it is very easy to use this method to generalize coherent evolution problems to include dissipative effects: one only needs to make minor corrections in the Hamiltonian in the coherent evolution routine, e.g. Eqs.(78,79) without the Γ-term, and then to add the jumps.

Symmetries and selection rules: Many density matrix problems benefit from selection rules that make certain coherences $\rho_{i_0 j_0}$ 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 wave functions as well, so that e.g. no wave function 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 wave function formalism.

Different simulations of the same problem: We have shown that different QMC simulations may be applied, leading to the same mean values. A continuous stochastic

evolution was found for an atom whose fluorescence was observed in a homodyne or heterodyne setup, and a general continuous stochastic wave function simulation of the master equation can be derived as a limit of the simulations of jump-type. For a numerical application it is relevant to know which simulation is the most efficient in terms of having an uncertainty $a/\sqrt{n}$ with the smallest possible a. On beforehand, it is usually not clear which simulation is the best one. The fluctuations in parts c) and d) of Fig. 11 show that there *is* a difference.

Error bars, local and global operators: With n wave functions we obtain n operator expectation values. Their mean is an estimate of the exact density matrix average, and their spread divided by $\sqrt{n}$ is the uncertainty of this estimate. The procedure hence provides its own error bars, a very important fact when one has to accept less accurate results for practical reasons. The error depends on the type of operator: the value of a global operator such as the kinetic energy of laser cooled atoms will fluctuate less than the value of a local operator such as the population of a specific state, a $\vec{p} = \vec{0}$ momentum state, say. The "broader" the wave functions, the better the estimate of the expectation value, the limit being a wave function as broad as the density matrix so that one wave function suffices to yield the required quantity. "Broad" should be understood in the sense of the spectrum of the operator of interest, and we may to some extent control this width by the choice of simulation scheme.

Time averages for stationary problems: For systems approaching a stationary state one may benefit from averaging the individual wave function results over time before performing the statistics involving all n wavefunctions. The time-averaged quantities fluctuate much less; in fact, a single wave function result averaged over a long time is sufficient to determine the correct mean [9]. By keeping a *number* of wave functions, however, we are still able to produce an error bar. For the laser cooling problem we have been able to reduce our error bar by about a factor of two, compared to the typical size as shown in Fig.7, corresponding to a gain in computing efficiency of a factor of four.

5.2 Insights gained from applications to simple systems

The QMC method may also be applied to simple systems for which density matrix solutions may readily be obtained. In this way one may get additional insight in the mechanisms leading to certain phenomena. It is of course a personal matter whether a certain description adds to one's understanding of a phenomenon or not. I felt much more comfortable with the simple decay of a two-level atom after having appreciated the mechanisms described in Section 3.1.2, and also for slightly more complicated systems it may be useful to confront the density matrix results with simulations.

Dark states and velocity selective coherent population trapping. The evolution of an effective three level Λ system as the one shown in Fig.10 towards a dark state is obtained very easily with the density matrix. A question is: how can the system ap-

proach a coherent superposition of the two ground states, when spontaneous emission does not feed the corresponding coherence, and when the laser light is not coupled to the state ? As we saw in Section 4.2.2 the "no-jump" evolution does the job, the same way as it brings the ground state fraction of two-level atoms into the ground state without emission of photons. In problems with dissipation this emphasizes a dynamics towards the least dissipating states (the other wave function components decay away faster due to the non-hermitian part of the effective Hamiltonian). The dark state appears in the phenomenon of velocity selective coherent population trapping, yielding very narrow velocity distributions of atoms in laser fields, and the dynamics has been studied with the QMC approach providing further information about this process [52]. Also very recently simulations have been applied in numerical tests of a new treatment of this process [53].

Quantum jumps. The experimentally observed quantum jumps [54] are difficult to account for by density matrices, since the elements of ρ are averages, describing large ensembles or many measurements, whereas the experimental situation refers to a single system being watched "here and now". Applying the quantum regression theorem it is possible to show that the expected intensity correlations of fluorescence light are in agreement with the observed signal, consisting of periods of fluctuating duration with either no light at all or a fairly constant intensity [55]. A simulation with a single atom, yields *directly* a fluctuating signal (number of emission events per unit time) as in the experiments, but it should be noticed that our simulations are equivalent to an experiment detecting *all* fluorescence photons and the real experiments only detect within a small solid angle.

Quantum Zeno effect. The quantum Zeno effect experiment in which the evolution of a system away from or towards a certain state is prevented by frequent measurements of the corresponding population [56], can be reproduced by density matrix calculations. As in the case of quantum jumps, we have in the QMC method a picture of the evolution, close to the one applied in a qualitative explanation of the phenomenon, but this one is exact in an average sense or under the assumption of the complete detection of the light emitted from the system.

Hegerfeldt [10] actually developed the stochastic wave functions to deal with precisely this kind of phenomena. His approach is equivalent to our jump treatment when applied to these systems.

Lasing without inversion. For certain ratios between incoherent and coherent pumping parameters in the dynamics of three-level atoms, one has observed the possibility of lasing without inversion [57]. The demonstration of this phenomenon by means of solutions to the master equation has been supplemented by a QMC approach [58], which, apart from giving the proper mean values, also provides dynamical mechanisms (atoms enter this state by absorption of an incoherent pump photon and thereafter, via that state, they transfer their population to this level through stimulated emission

in the lasing mode ...).

Photon detection and evolution of cavity fields. In his beautiful lecture notes describing the evolution of stochastic wave functions, "quantum trajectories" [6], Carmichael considers a number of applications to situations where the quantum system involves a quantized field mode, e.g. in a cavity. In particular the question of shot noise reduction in connection with squeezed light, which he poses as a riddle, is a good example of insight rather than numerical information obtained from the wave function ideas.

Of course, these examples of additional insights have to be seen in the light of the simulation/"detection" scheme applied, however, taking this into consideration, one may obtain an even more profound understanding of the system dynamics.

5.3 The mathematical development of theory, independent of quantum optics

In Eq.(18), the relaxation terms in the master equation were postulated to be of the Lindblad form. This form is actually the result of a mathematical derivation, a *Theorem* in Lindblad's paper [19]. A number of master equations for different physical systems had already been derived, when Lindblad proved his theorem, and they could all be brought on this form. For our applications this expression makes it possible to infer the generality of the simulation approach to dissipative systems, and it even provides an automatic way of implementing this treatment.

In the mathematical literature on Hilbert space theory, C^*-algebra, and semigroups, the ideas developed further, and the idea of realizing the evolution with stochastic wave functions came up quite early. After the publication of our first paper [3], Gisin drew our attention to his work [11], and his applications of the equation (111) to very different aspects of physics, and to parts of the more extensive literature with contributions by Barchelli [59], Belavkin [60] and Dioisi [61] (I am not familiar with the chronology or the milestones in this research, so I give some recent references to these authors from which the interested reader may backtrack through the original developments). Unfortunately the lack of communication between the apparently well-separated fields of mathematical physics and quantum optics, prevented the parties from profiting at a much earlier stage from the insight and practical means which were readily available .

5.4 "Classical" quantum mechanics questions in new light

This work confronts two very different definitions of the density matrix: (i) a reduction, via a trace, of the state of the combined system+reservoir which cannot be described by a pure state in the small system, and (ii) a statistical description of an ensemble of systems populating different states with some probability law. The two are joined, if we by *ensemble* understand a large number of realizations of an experiment, rather

than a large number of simultaneously existing systems. The density matrix is then the average over the different detection sequences (with weight factors inferred from the wave functions attached to each sequence).

In this spirit stochastic approaches have also been introduced in the context of standard [62, 63] or quantum non demolition [64, 65, 66] measurements of photon numbers in cavities. A sequence of quantum jumps resulting from successive measurements, e.g. on atoms leaving the cavity, leads to a reduction of the field state, sometimes into a Fock state $|n\rangle$. The interest of these stochastic approaches is to give explicit individual histories of the quantum field state in a measurement sequence, and this is particularly valuable if one wants to optimize the measurement sequence in order to get complete information on the field state with a minimum number of measurement processes [65, 67]. It is noteworthy that in these cavity problems the evolution may be unitary when the atom traverses the cavity, the dissipative element is the projection of the field state when the final atomic state is detected. Instead of considering the state of the field conditioned on the detection process, one may determine the density matrix, and in some cases its evolution may even be approximated by a master equation as the one discussed here, see e.g. Ref.[13].

It is an important aspect of quantum mechanics how wavefunctions relate to observations. You may consider two components evolving in parallel: the quantum system, represented by a wavefunction $|\psi\rangle$, which is propagated according to Schrödinger's equation, and the detector which "clicks" and gives numbers in a classical manner. These two components are coupled: the detector readings are determined in a random manner, following probabilities determined by the current value of $|\psi\rangle$; every reading of the detector (also a null-measurement) causes a change of the wavefunction, a collapse on some appropriate eigenstate. As a result of this, one cannot observe a system without modifying its evolution. The reason that the QMC method works, is that the system is already being "observed" by the quantized field before we enter our hypothetical detectors: the atom-field coupling causes the same average decoherence of atomic properties as we enforce by the simulated detection. In this respect the QMC method does not add anything new to our interpretation of quantum mechanics, it only brings in some tools in the discussion of dissipative effects. These effects, however, play important roles in any real detector, and a better understanding may help demystifying part of the collapse postulate of quantum mechanics. Gisin and Percival [12] and Carmichael [41] have by means of examples studied how dissipative elements cause localization of wavefunctions, and how, for example, superpositions of "macroscopic" states choose between the components. By such a study of the so-called Schrödinger cat states (superpositions of coherent states of the harmonic oscillator) Carmichael [41] has shown that the elementary collapses introduced at the level of single photon events, as in the QMC method, are sufficient to make a macroscopic superposition state chose betweeen its "classical" components on a very fast time scale. The macroscopic collapse has been explained, the elementary collapse, however, remains as an essential

and unexplained ingredient of the theory.

A real advantage of the QMC method: We can be sitting there discussing its philosophical implications and the deep questions of quantum physics while the computer is cranking out numbers which we need for practical purposes and which we could never obtain in any other way. What more can we ask for ?

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