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Quantum state diffusion, localization and computation

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Abstract. Numerical simulation of individual open quantum systems has proven advantages over density operator computations. Quantum state diffusion with a moving basis (MQSD) provides a practical numerical simulation method which takes full advantage of the localization of quantum states into wavepackets occupying small regions of classical phase space. Following and extending the original proposal of Percival, Alber and Steimle, we show that MQSD can provide a further gain over ordinary QSD and other quantum trajectory methods of many orders of magnitude in computational space and time. Because of these gains, it is even possible to calculate an open quantum system trajectory when the corresponding isolated system is intractable. MQSD is particularly advantageous where classical or semiclassical dynamics provides an adequate qualitative picture but is numerically inaccurate because of significant quantum effects. The principles are illustrated by computations for the quantum Duffing oscillator and for second-harmonic generation in quantum optics. Potential applications in atomic and molecular dynamics, quantum circuits and quantum computation are suggested.

1. Introduction

Most quantum systems are not even approximately isolated, but open, so that they are significantly affected by the environment. This interaction is important for atoms and molecules in gaseous or condensed matter environments, which broaden spectral lines. It affects the motion of molecules and the rates of chemical reactions. It is important for signalling near the quantum limit, where the environment produces the noise through which the signal must be detected, and it is important in quantum optics, where it produces the dissipation that destroys coherence.

Quantum state diffusion with a moving basis (MQSD) is a method of representing and computing the evolution of individual open quantum systems. It has already been used by Percival *et al* [39] to analyse the motion of a particle in a Penning trap. Here we provide a general theory of the method, and provide a guide as to when it should be used in preference to other methods. Second-harmonic generation in optics and the quantum Duffing oscillator are used as illustrations.

Because stochastic environmental fluctuations affect the evolution of an individual open quantum system, it is represented traditionally by a density operator ρ, which satisfies a linear master equation. No attempt is made to represent the evolution of individual pure states explicitly. This approach is adequate when the master equation has analytic solutions, or when the number of basis states N of Hilbert space required for numerical solution is not too large. But for large N it often breaks down in practice long before the corresponding numerical solution of the Schrödinger equation, because the number of elements of a density matrix increases as N^2.

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Numerical simulation of individual open quantum systems, represented by pure states which move along quantum trajectories, has proven advantages over density operator computations. Quantum state diffusion (QSD) provides such a numerical simulation, in which each state diffuses continuously in the state space and satisfies a nonlinear Langevin–Itô diffusion equation, determined uniquely by the master equation as shown in [25] and described in section 2. This diffusion often produces a localization of quantum states into wavepackets that occupy small moving regions R of classical phase space. Such localization is a special characteristic of QSD that is usually absent in other quantum state simulation methods [16].

For a system of f freedoms, a Planck cell of volume $(2\pi\hbar)^f$ corresponds to one quantum state. The number of basis states used to represent a system need not be much greater than the number of Planck cells in the region R, *provided* that the basis follows the motion of the wavepacket in phase space. Quantum state diffusion with a moving basis (MQSD) provides a practical numerical simulation method which takes full advantage of the localization, by referring the quantum state to a moving origin (q, p) in phase space. This origin lies at the phase space centroid of the quantum state, determined by the current quantum expectations $\langle \mathbf{Q} \rangle$ and $\langle \mathbf{P} \rangle$.

Numerical methods for solving the time-dependent Schrödinger equation for an isolated system using moving wavepackets have long been used in chemical physics [31, 33, 6, 32]. But as the ordinary Schrödinger equation disperses wavepackets instead of localizing them in phase space, the applicability of these wavepacket approaches is very restricted.

For some systems, computation using MQSD is orders of magnitude more economical in terms of computer storage space and computation time than other quantum state simulation methods, or the solution of master equations for the density operator. We give examples in which it is very difficult to see how any other current method of numerical solution could be used.

Section 2 presents the basic QSD equations and their derivation. The problems of the choice of boundary between system and environment are described. There is a brief comparison with other quantum trajectory methods, sometimes called quantum jump or relative state methods [5, 7, 14, 15]. Localization is defined and discussed in section 3, with reference to localization theorems and numerical examples. This is followed by the definition of the moving basis, using excited coherent states, and the derivation of the MQSD equations.

Section 4 applies MQSD to two challenging examples, the Duffing oscillator and second-harmonic generation. These two examples show how effective MQSD can be in bridging the gap between those quantum problems where the number of basis states required in a fixed basis is relatively small, and the quasiclassical limit where the number of *fixed* basis states would be so large as to rule out any practical use. This section is completed by a crude analysis of comparative computing times for the solution of an open system problem using MQSD and the numerical solution of the Schrödinger equation for a similar isolated system.

Section 5 concludes with a comparison of methods for open systems and some recommendations for their use, followed by the prospects for using MQSD in various applications.

2. Quantum state diffusion (QSD)

Quantum state diffusion represents the evolution of a quantum system through a correspondence between the solutions of the master equation for the ensemble density operator ρ and the solutions of a Langevin–Itô diffusion equation for the normalized pure

state vector $|\psi\rangle$ of an individual system of the ensemble [25].

An analogy is helpful. A solution of the Langevin–Itô equation for the motion of an individual Brownian particle in position space represents a single member of an ensemble whose distribution function satisfies the corresponding Fokker–Planck equation. Similarly, a solution of the QSD equation for the diffusion of a pure quantum state in state space represents a single member of an ensemble whose density operator satisfies the corresponding master equation. In each case the effect of the environment can be represented either by the stochastic evolution of an individual system or by the deterministic evolution of the distribution. For Brownian motion the evolution of the individual system gives a more detailed picture of what happens to an individual particle than the evolution of the distribution function. Similarly, for open quantum systems, the evolution of the individual pure states of QSD gives a more detailed picture of what happens to an individual quantum system than the evolution of the density operator. This is particularly important for applications like single-particle traps, quantum noise in gravitational wave detection, quantum circuits and quantum computers.

In QSD, *quantum expectations* $\langle\cdots\rangle$ for individual systems, and *ensemble means* M are distinct. The traditional quantum expectation $\mathrm{Tr}\,\rho\mathbf{G}$ of an operator $\mathbf{G}$ for a mixed state of an open system is equivalent in QSD to an ensemble mean over the quantum expectations of the pure states $|\psi\rangle$. That is

$$\mathrm{Tr}\,\rho\mathbf{G} = M\langle\mathbf{G}\rangle = M\langle\psi|\mathbf{G}|\psi\rangle\,. \tag{1}$$

If the master equation has the standard Lindblad [34] form

$$\dot{\rho} = -\frac{\mathrm{i}}{\hbar}[\mathbf{H},\rho] + \sum_m \left(\mathbf{L}_m\rho\mathbf{L}_m^\dagger - \tfrac{1}{2}\mathbf{L}_m^\dagger\mathbf{L}_m\rho - \tfrac{1}{2}\rho\mathbf{L}_m^\dagger\mathbf{L}_m\right) \tag{2}$$

then the corresponding QSD equation is a nonlinear stochastic differential equation for the normalized state vector $|\psi\rangle$ of the ensemble, whose general differential form is [25]

$$\begin{aligned}|\mathrm{d}\psi\rangle = -\frac{\mathrm{i}}{\hbar}\mathbf{H}|\psi\rangle\mathrm{d}t + \sum_m \left(\langle\mathbf{L}_m^\dagger\rangle\mathbf{L}_m - \tfrac{1}{2}\mathbf{L}_m^\dagger\mathbf{L}_m - \tfrac{1}{2}\langle\mathbf{L}_m^\dagger\rangle\langle\mathbf{L}_m\rangle\right)|\psi\rangle\mathrm{d}t \\ + \sum_m \left(\mathbf{L}_m - \langle\mathbf{L}_m\rangle\right)|\psi\rangle\mathrm{d}\xi_m\end{aligned} \tag{3}$$

where $\mathbf{H}$ is a Hamiltonian and $\mathbf{L}_m$ are Lindblad operators which represent the effect of the environment on the system in a Markov approximation.

The first sum in (3) represents the 'drift' of the state vector in the state space and the second sum the random fluctuations. The $\mathrm{d}\xi_m$ are independent complex differential random variables, with normalized independent white noise in their real and imaginary parts, leading to an isotropic Brownian motion or Wiener process in the complex ξ_m-plane. These satisfy the conditions

$$M\,\mathrm{d}\xi_m = 0 \qquad M\,\mathrm{d}\xi_n\,\mathrm{d}\xi_m = 0 \qquad M\,\mathrm{d}\xi_n^*\,\mathrm{d}\xi_m = \delta_{nm}\,\mathrm{d}t \tag{4}$$

where M represents a mean over the ensemble. The complex Wiener process is normalized to $\mathrm{d}t$, so the independent real and imaginary Wiener processes are each normalized to $\mathrm{d}t/2$. This is the same normalization as in [26, 27, 38], but is different from that of [25]. The distribution (4) is invariant under unitary transformations in the linear space of the $\mathrm{d}\xi_m$.

$\langle\mathbf{L}_m\rangle = \langle\psi|\mathbf{L}_m|\psi\rangle$ is the quantum expectation of $\mathbf{L}_m$ for state $|\psi\rangle$. The density operator is given by the mean over the projectors onto the quantum states of the ensemble:

$$\rho = M|\psi\rangle\langle\psi|\,. \tag{5}$$

It can be verified that if the pure states of the ensemble satisfy the QSD equation (3), then the density operator (5) satisfies the master equation (2). There are many diffusion equations for pure states $|\psi\rangle$ which give the same master equation for the density operator. The uniqueness of the QSD equations follows from a principle of unitary invariance in operator space.

This is most clearly illustrated by a QSD equation with a single Lindblad operator $\mathbf{L}$. In that case unitary transformation in operator space is multiplication by a scalar phase factor u of modulus unity. Then it is obvious by inspection that if $\mathbf{L}$ is replaced by $u\mathbf{L}$, the master equation, and hence the solution of the master equation, is unchanged. In the corresponding QSD equation, the replacement of $\mathbf{L}$ by $u\mathbf{L}$ is the same as the replacement of $d\xi$ by $u\,d\xi$, but since the distribution of the elementary differential fluctuations $d\xi$ is invariant for multiplication by a phase factor, the QSD equations are also unchanged. This is not true if the fluctuations are real or otherwise do not satisfy unitary invariance in fluctuation space, as in [19, 22]. The QSD equations are in this respect the only diffusion equations that respect this unitary invariance property in the one-dimensional operator space, and they are unique up to a physically irrelevant external time-dependent phase factor for the state vector.

This result generalizes to an arbitrary number of Lindblad operators if u is taken to be a general unitary transformation in the linear space of the Lindblad operators. The general result was first given for QSD equations in [25], following the statement of an invariance principle by Diósi [9], and the derivation for a Fokker–Planck equation in state space in [37].

In either the traditional or QSD formulation for open systems, there is always a problem as to where to put the boundary between system and environment. If the system is made too small, then important effects are neglected, and errors are made. If it is made too large by including too much of the environment, then the dimension N of the basis state space becomes too large for the equations to be solved. In practice there is a compromise. Often, in addition, the problem is simplified by approximating the effects of complicated environments by simple operators.

Because of the localization property discussed in the next section, QSD has the property that it has no need of a separate measurement hypothesis, as shown in detail with examples in [25–27]. A measuring apparatus is just one type of environment, and its effects can be represented by simple operators. Alternatively, measurement can be represented in detail by pushing the boundary between system and environment out so far that the system includes the measuring apparatus. This is useful in establishing the representation of measurement by operators, but results in a system too complicated to solve directly. Localization and the representation of measuring apparatus are needed for comparison with the relative state or quantum jump methods.

QSD theory followed from research that was motivated by the desire to find an explicit physical representation of the measurement process. Following pioneering work of Bohm and Bub [2] and Pearle [35, 36], Gisin [20] introduced a simple example of quantum state diffusion with real fluctuations that was generalized by Diósi [9] and Gisin [21]. The complex Itô form of QSD was introduced in [25]. The detailed QSD theory and its applications are described in [25–27, 38]. Diffusion in the space of quantum states also appears in connection with the theory of continuous quantum measurements as shown, for example, in the many references in [1, 5].

Gisin and Percival [24] used QSD to describe a quantum jump experiment. Goetsch and Graham [28] used it to describe some nonlinear optical processes. Garraway and Knight [17] compared QSD and quantum jump simulations for two-photon processes, and in [18]

they compared the phase space picture of QSD and quantum jumps, showing that the former gives localization and the latter does not. Spiller and his co-workers applied QSD to thermal equilibrium [44], studied chaos in a simple open quantum system [45] and investigated open angular systems, such as quantum capacitors and rotors [46]. Gisin [23] investigated the Heisenberg picture for QSD. Further examples are given in [25–27, 40].

3. Localization and the moving basis

For a quantum system in a pure state, localization refers to dynamical variables and operators like position, momentum, energy and angular momentum which have classical equivalents. It is helpful to picture the localization in classical phase space. There are many phase space representations of quantum systems, such as the Wigner distribution, but these are not necessary to obtain a classical picture of the phase space localization of a quantum system. For that, it is only necessary to consider the expectations and variances of quantum dynamical variables, and then to picture these expectations and variances *as if* they represented the expectations and variances of classical quantities.

The general theory of localization is treated in [25] and in [38]. The Schrödinger evolution of a system usually produces *de*localization or dispersion. The interaction of the system with its environment, by contrast, produces localization.

It is convenient to consider these competing processes separately before considering them together. The dispersion is well known, since it occurs in isolated systems. The opposite extreme is an open system which interacts with its environment so strongly that the Schrödinger evolution can be neglected. This is a *wide open* system, and the theory of localization for these systems has been treated in detail in [38].

For simple systems, earlier papers [25–27] had built up a picture in which interaction with the environment produced localization, sometimes to an eigenstate of an operator corresponding to a surface in phase space, but more commonly to a state which is localized to a wavepacket in phase space whose Heisenberg indeterminacy products are of the order of $\hbar$. In [38] that picture was confirmed and extended. A general theory was presented, lower bounds were put on rates of self-localization, and bounds were put on asymptotic states.

For a pure state $|\psi\rangle$, the expectation of a self-adjoint operator $\mathbf{G}$ is denoted

$$\langle \mathbf{G} \rangle = \langle \psi | \mathbf{G} | \psi \rangle \tag{6}$$

and the variance of the operator $\mathbf{G}$ is

$$\sigma^2(\mathbf{G}) = \langle \mathbf{G}^2 \rangle - \langle \mathbf{G} \rangle^2 . \tag{7}$$

The localization Λ is defined as the inverse of the mean of the variance for the ensemble:

$$\Lambda = \left(M \sigma^2(\mathbf{G}) \right)^{-1} . \tag{8}$$

The simplest theorem is for a wide open system in which there is only one self-adjoint Lindblad operator $\mathbf{L}$ in the state diffusion equation. It is shown that the rate of localization of $\mathbf{L}$ is at least as fast as 2 ([38], section 3):

$$\mathrm{d}\Lambda/\mathrm{d}t \geqslant 2 . \tag{9}$$

Because Lindblad operators have the dimension of time$^{-1/2}$, the rate is dimensionless.

This localization is towards a *surface* in phase space defined by the dynamical variable L, and is characteristic of interaction with apparatus that measures L. More general and more interesting is the case where there are at least $2f$ operators, where f is the number of

freedoms, and the surfaces for the corresponding dynamical variables define points in phase space. In that case at least f pairs of operators will not commute. The simplest example is a one freedom system with two conjugate variables X, Y whose operators satisfy

$$[\mathbf{X}, \mathbf{Y}] = \mathrm{i}\hbar\,. \tag{10}$$

In this case it is shown that the state localizes and asymptotically approaches a wavepacket with minimum Heisenberg indeterminacy product. It is also shown that operators that are not self-adjoint, such as annihilation and creation operators, can localize to wavepackets. In the more realistic examples that we study numerically in the following section, the localization has to compete with the dispersion due to the Schrödinger evolution, the wavepacket is more dispersed, and its dispersion often varies considerably as a function of time.

For general open systems there is a physical competition between the dispersion due to the Hamiltonian and the localization due to the state diffusion. There is no general theory for this, but there are many numerical examples of localization, such as [25] for the forced damped oscillator and [27] for localization in one well of a double well, and phase space localization by position localization and Hamiltonian coupling of position and momentum. Halliwell and Zoupas [30] have provided a general theory for the evolution of Gaussian wavepackets for an important model, generalizing a result of Diósi [8].

From the theorems and the numerical examples it would appear that the localization of wavepackets to relatively small regions of phase space is the norm, so that the limiting behaviour on a classical scale is the direct representation of classical states as points in phase space, rather than the more abstract surfaces defined by action functions that satisfy the Hamilton–Jacobi equation.

For our purposes the most important consequence of the localization of quantum trajectories around phase space trajectories is, that by continually changing the basis, it is often possible to reduce the number of basis states needed to represent the wavepacket by many orders of magnitude. If a wavepacket is localized about a point (q, p) in phase space far from the origin, it requires a great many of the usual number states $|n\rangle$ to represent it. But fewer *excited coherent* basis states $|q, p, n\rangle = \mathbf{D}(q, p)|n\rangle$, are needed, with corresponding savings in computer storage space and computation time. These states are defined using the coherent state displacement operator,

$$\mathbf{D}(q, p) = \exp\frac{\mathrm{i}}{\hbar}\Big(p\mathbf{Q} - q\mathbf{P}\Big)\,. \tag{11}$$

The separation of the representation into a classical part (q, p) and a quantum part $|q, p, n\rangle$ is called the *moving basis*, or, as in [39], the *mixed* representation.

In this basis, the usual creation and annihilation operators are modified:

$$\mathbf{a} = \mathbf{a}(q, p) + (q + \mathrm{i}p)\mathbf{I}/\sqrt{2} \qquad \mathbf{a}^\dagger = \mathbf{a}^\dagger(q, p) + (q - \mathrm{i}p)\mathbf{I}/\sqrt{2} \tag{12}$$

where $\mathbf{a}(q, p)$ is the local annihilation operator (with (q, p) as the origin) and $\mathbf{I}$ is the identity operator. The effect of the local operators on the excited coherent states is given by

$$\mathbf{a}(q, p)|q, p, n\rangle = \sqrt{n}|q, p, n-1\rangle \qquad \mathbf{a}^\dagger(q, p)|q, p, n\rangle = \sqrt{n+1}\,|q, p, n+1\rangle\,. \tag{13}$$

Similarly,

$$\mathbf{Q} = \mathbf{Q}(q, p) + q\mathbf{I} \qquad \mathbf{P} = \mathbf{P}(q, p) + p\mathbf{I} \tag{14}$$

where

$$\mathbf{Q}(q, p) = (\mathbf{a}(q, p) + \mathbf{a}^\dagger(q, p))/\sqrt{2} \qquad \mathbf{P}(q, p) = -\mathrm{i}(\mathbf{a}(q, p) - \mathbf{a}^\dagger(q, p))/\sqrt{2}\,. \tag{15}$$

Care must be taken to avoid ambiguity in the external phase factors. Normally, different displacement operators do not commute; nor is the product of two displacement operators a standard displacement operator. In both cases there is an additional phase factor:

$$\mathbf{D}(q', p')|q, p, n\rangle = |q + q', p + p', n\rangle e^{i(qp' - pq')/2}. \tag{16}$$

In order to retain an unambiguous relation to the standard fixed basis states, this additional phase factor must be removed. Fortunately this is simple, as it is the same for all the moving basis states.

The numerical algorithm follows directly. As the integration proceeds, the phase point expectation

$$(\delta q, \delta p) = (\langle \mathbf{Q}(q, p)\rangle, \langle \mathbf{P}(q, p)\rangle) \tag{17}$$

drifts away from zero. The basis is then shifted,

$$|\psi\rangle \to \mathbf{D}(-\delta q, -\delta p)|\psi\rangle \tag{18}$$

and the classical phase point (q, p) adjusted:

$$(q, p) \to (q + \delta q, p + \delta p). \tag{19}$$

The time between basis adjustments can be optimized in various ways, depending on the problem, the degree of localization, and the difficulty of carrying out the basis change.

In principle, there is another way to make the basis change. If the phase space point

$$(q, p) = (\langle \mathbf{Q}\rangle, \langle \mathbf{P}\rangle) \tag{20}$$

and state $|\psi\rangle$ *relative to* (q, p) *as origin* are used to define the state, then we can include the change of basis in the evolution equation for $|\psi\rangle$. This leads to a set of simultaneous differential equations in q, p, and $|\psi\rangle$; in integrating these equations, both the QSD evolution and the basis shift are done automatically. This *simultaneous moving basis* method is attractive for a number of reasons; the states always remain in an optimally 'localized' basis, and therefore can take the best advantage of the QSD localization effects to minimize the number of necessary basis states. There is no need for an additional step for the basis change. In practice, the simultaneous moving basis method results in a considerable increase in programming complexity, and may have numerical stability problems. As yet the method has not proved itself sufficiently, so we have not used it.

Implementing the moving basis algorithm on a computer is straightforward. Each set of normalized fluctuations $d\xi_m$ determines a quantum trajectory through (3), which can be simulated using discrete time steps δt, using a Runge–Kutta algorithm for the deterministic part, and an Euler method for the stochastic part (but see also [47]). Suppose that at time $t = t_0$ the state $|\psi(t_0)\rangle$ is represented in the basis $|q_0, p_0, n\rangle$, centred at

$$(q_0, p_0) = (\langle\psi(t_0)|\mathbf{Q}|\psi(t_0)\rangle, \langle\psi(t_0)|\mathbf{P}|\psi(t_0)\rangle). \tag{21}$$

Then after one discrete time step, the expectations in this basis shift to

$$(q_1, p_1) = (\langle\psi(t_0 + \delta t)|\mathbf{Q}|\psi(t_0 + \delta t)\rangle, \langle\psi(t_0 + \delta t)|\mathbf{P}|\psi(t_0 + \delta t)\rangle) \neq (q_0, p_0). \tag{22}$$

The computational advantage of a small number of basis states is then retained by changing the representation to the shifted basis $|q_1, p_1, n\rangle$ centred at q_1 and p_1. This shift in the origin of the basis represents the elementary single step of the moving basis of MQSD.

The components of $|\psi(t_0 + \delta t)\rangle$ can be computed using the expressions given above. The computing time needed for the basis shift is of the same order of magnitude as for computing a single discrete time step of (3). Shifting the basis once every discrete time step could therefore double the computing time, depending on the complexity of the Hamiltonian

and the number of degrees of freedom. On the other hand, the reduced number of basis vectors needed to represent states in the moving basis can lead to savings far larger than a factor of 2.

In one example of second-harmonic generation described in the following section, two modes of the electromagnetic field interact. Using the moving basis reduces the number of basis vectors needed by a factor of 100 in each mode. The total number of basis vectors needed is thus reduced by a factor of 10 000, leading to reduction in computing time by a factor of $10\,000/2 = 5000$. Furthermore, the fixed basis would exceed the memory capacity of most existing computers.

The QSD equation (3) can contain both localizing and delocalizing terms. Nonlinear terms in the Hamiltonian tend to spread the wavefunction in phase space, whereas the Lindblad terms localize. Accordingly, the width of the wavepackets varies along a typical trajectory. We use this to reduce the computing time even further by dynamically adjusting the number of basis vectors. Our criterion for this adjustment depends on parameters $\epsilon \ll 1$, the *cut-off probability*, and N_{pad}, the *pad size*, which represents the number of boundary basis states that are checked for significant probability. We require the total probability of the top N_{pad} states to be no greater than ϵ, increasing and decreasing the number of states actually used accordingly, as the integration proceeds along the quantum trajectory.

4. Examples: the Duffing oscillator and second-harmonic generation

The quantum mechanics of systems whose classical limit exhibits dissipative chaos is an interesting problem. Dissipation is relatively difficult to treat in quantum mechanics. The best of the commonly used techniques is the solution of the master equation, but as we have pointed out, solving the master equation numerically can be an extremely difficult problem. Perhaps because of this, quantum dissipative chaos has been neglected by comparison with quantum Hamiltonian chaos. Clearly the QSD method for open systems is eminently suitable for such dissipative systems. Recently Spiller and Ralph [45] applied QSD to a dissipative chaotic system.

The Duffing oscillator is particularly appropriate for applying MQSD, as the classical system has been widely studied [29]. This system has also been treated quantum mechanically in the decoherent histories formalism [3, 4], which has been shown to have connections to QSD [10]. This oscillator consists of a particle moving in one dimension in the two-welled potential

$$V(x) = \frac{x^4}{4} - \frac{x^2}{2}. \tag{23}$$

Dissipative chaos can be produced by adding both dissipation (of the form $-2\Gamma\dot{x}$) and a periodic driving force (of the form $g\cos(t)$).

By using either the master equation or QSD, it is relatively simple to calculate the evolution of this system far from the classical limit, for example, when $\hbar = 1$. But it is also very important to study the classical limit of quantum chaos, to see how the relatively well understood properties of classical chaos appear in quantum systems. This limit is conveniently represented by decreasing $\hbar$, which increases the number of fixed basis states required. With $\hbar = 1$, about ten states are needed to simulate the system with accuracy. On approaching the classical limit, the number of states quickly becomes impractical. In a semiclassical regime with $\hbar \approx 10^{-4}$, more than 10 000 states are needed; the density operator method would require storage and computation with a prohibitive 10^8 real numbers. This, like most nonlinear problems, is exacerbated by the fact that the potential needs much more

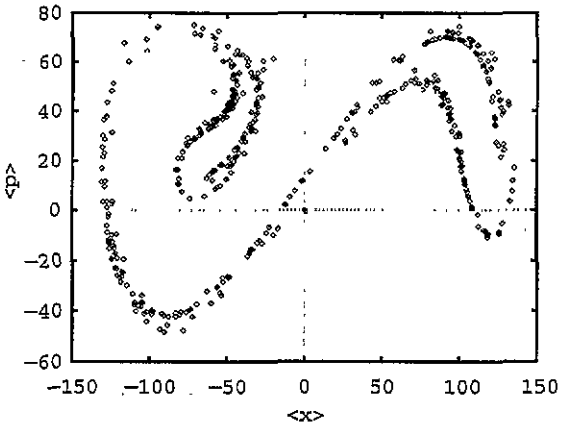

Figure 1. Poincaré surface for expectation values of x versus p for the forced, damped Duffing oscillator, plotted at times of constant phase $t_n = 2\pi n$. This is in the chaotic regime, with constants $g = 0.3$ and $\Gamma = 0.125$, and scaled up by a factor of 100 in x and p, effectively reducing $\hbar$ by a factor of 10^4. The system is initially in the ground state. Note that it would take ~50 000 states to represent this system with a non-moving basis. The cut-off probability is $\epsilon = 5 \times 10^{-3}$.

computation than, for example, the simple harmonic oscillator.

Using MQSD, however, this problem becomes tractable. In a chaotic system, the delocalizing forces are particularly strong in the neighbourhood of hyperbolic fixed points, where the dynamics spreads the wavepacket in phase space. However, the localizing effects of the environment always predominate. MQSD picks out a good local time-dependent basis, and the method rarely requires more than twenty states, usually about ten, just as in the small-scale quantum limit. This is easy to see by examining figure 1.

Our second example is frequency doubling or second-harmonic generation, which is a standard process in quantum optics. The system consists of two optical modes of frequency ω_1 and $\omega_2 \simeq 2\omega_1$ which interact in a cavity driven by a coherent external field with frequency $\omega_f \simeq \omega_1$ and amplitude f. The cavity modes are slightly damped and detuned, with detuning parameters $\delta_1 = \omega_1 - \omega_f$ and $\delta_2 = \omega_2 - 2\omega_f$.

The Hamiltonian in the interaction picture is

$$\mathbf{H} = \hbar\delta_1\mathbf{a}_1^\dagger\mathbf{a}_1 + \hbar\delta_2\mathbf{a}_2^\dagger\mathbf{a}_2 + i\hbar f(\mathbf{a}_1^\dagger - \mathbf{a}_1) + i\hbar\frac{\chi}{2}(\mathbf{a}_1^{\dagger 2}\mathbf{a}_2 - \mathbf{a}_1^2\mathbf{a}_2^\dagger) \tag{24}$$

where $\mathbf{a}_1$ and $\mathbf{a}_2$ are the annihilation operators of the two cavity modes, and χ describes the strength of the nonlinear interaction between them. Damping of the two cavity modes is described by the Lindblad operators $\mathbf{L}_1 = \sqrt{2\kappa_1}\mathbf{a}_1$ and $\mathbf{L}_2 = \sqrt{2\kappa_2}\mathbf{a}_2$. The factors of $\sqrt{2}$ are a consequence of normalization conventions used in the master equation (2) which differ from those commonly used in quantum optics. The master equation for this problem first appeared in [12, 13].

A direct numerical solution of the master equation for this problem is difficult because, in the Fock basis, the dimension of the effective Hilbert space is equal to the product of the photon number cut-offs in both modes and easily becomes very large. The problem becomes intractable even for moderate numbers of photons in each mode. Earlier treatments of this problem include [11, 41, 43, 28, 48].

The QSD method was employed for studying second-harmonic generation by Gisin and Percival [25] and Goetsch and Graham [28]. Both used a fixed Fock-state basis, and rather limited photon numbers. Gisin and Percival [25] improved the method slightly by using a lower as well as an upper cut-off. More recently, Zheng and Savage [48] applied the quantum jump method to the chaotic regime [42] of second-harmonic generation for large photon numbers. Using hundreds of hours on a 32-processor supercomputer, they succeed in simulating cases where the expectation of the photon number is of the order of 200 in

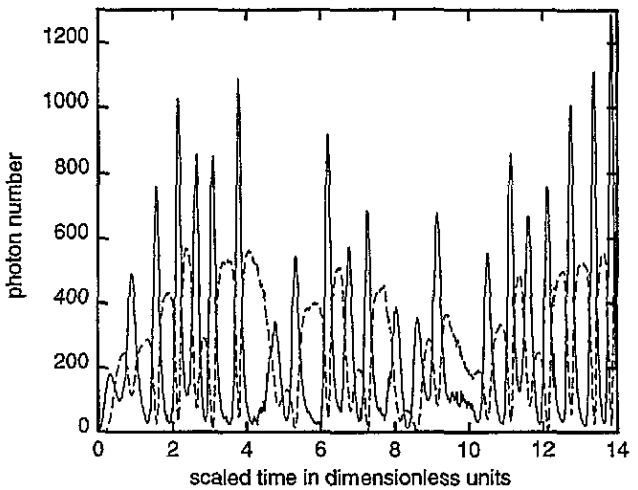

Figure 2. Photon number versus dimensionless scaled time $\tau = \kappa_1 t$ for a single second-harmonic generation trajectory. Full curve: fundamental mode $\langle \mathbf{a}_1^\dagger \mathbf{a}_1 \rangle$; broken curve: second harmonic mode $\langle \mathbf{a}_2^\dagger \mathbf{a}_2 \rangle$. The parameters are $\kappa_2/\kappa_1 = 0.25$, $\delta_1/\kappa_1 = \delta_2/\kappa_1 = -1$, $\chi/\kappa_1 = 0.5$, and $f/\kappa_1 = 62$. At time $t = 0$, the system is in the vacuum state. These parameters lie in the chaotic regime of the corresponding classical system. The cut-off probability is $\epsilon = 10^{-3}$.

each mode. Their Fock basis has 512 basis states in each mode, i.e. a total of 250 000 basis states, a *tour-de-force* near the limits of their method.

To illustrate the power of MQSD, we have computed trajectories for second-harmonic generation with parameters similar to the ones used by Zheng and Savage [48], but leading to photon numbers on average six times as large. For this problem, Zheng and Savage would have needed approximately $36 \times 250\,000 \simeq 10^7$ basis states. Using the moving basis with an adaptive basis size, we computed a single trajectory in a few hours on a PC. The results shown in figure 2 were obtained using a cut-off probability $\epsilon = 10^{-3}$. The total number of basis states needed in the simulation varied between approximately 50 and 1000. Changing the cut-off probability to $\epsilon = 10^{-2}$ lowered the number of basis states needed to between approximately 40 and 200, clearly a strong dependence on ϵ. Surprisingly, the choice of cut-off probability affected the simulated expectation values only very slightly.

It is interesting to compare estimates of computation space and time of a single MQSD run for an open system and the numerical solution of the Schrödinger equation for the same system isolated from its environment. The former has diffusion and drift terms that increase the computation time for a single step of integration, but the localization reduces significantly the size of the basis needed for computation. The latter has fewer terms in the equation, but the Schrödinger dispersion increases the number of states needed for the representation. Clearly, for systems with more than one degree of freedom the advantage of MQSD is even greater, the savings in number of states going as the power of the number of freedoms. We can make this semiquantitative by the following analysis.

Consider computing times. For each computation, let N_j be the arithmetic mean of the number of basis states required for the jth freedom. Let $\bar{N}$ be the geometric mean of all the N_j, which is a useful measure for the number of basis states. Let f be the number of freedoms. Then an estimate of the computing time T_{comp} is given by $K\bar{N}^f$, where the constant K is much larger for MQSD but $\bar{N}$ is much larger for Schrödinger. The ratio of

computing times is then

$$\frac{T_{\text{comp}}(\text{Sch})}{T_{\text{comp}}(\text{MQSD})} \approx \frac{K(\text{Sch})}{K(\text{MQSD})}\left[\frac{\bar{N}(\text{Sch})}{\bar{N}(\text{MQSD})}\right]^{f}. \tag{25}$$

The values of these numbers are highly problem-dependent. Clearly, for a problem with a complicated Hamiltonian and one simple Lindblad operator (as in the Duffing oscillator), the difference in time between the QSD and Schrödinger calculations will be much less than it would be for a simple Hamiltonian with several Lindblad operators (as in second-harmonic generation).

One can estimate the values of these numbers for the problems described. For the Duffing oscillator, $K(\text{Sch})/K(\text{MQSD}) \approx 2/3$, $\bar{N}(\text{Sch})/\bar{N}(\text{MQSD}) \approx 1500$, and $f = 1$. From equation (25) we expect that the ratio of computing time between MQSD and the Schrödinger equation is roughly 10^{-3}. In the case of second-harmonic generation, we have $K(\text{Sch})/K(\text{MQSD}) \approx 1/2$, $\bar{N}(\text{Sch})/\bar{N}(\text{MQSD}) \approx 100$ and $f = 2$, yielding a ratio of computing times of approximately 2×10^{-4}. Clearly, the advantage for multi-freedom problems is very great.

5. Conclusions and prospects

For the simplest open system problems, where analytic solutions are available, or the number N of basis states that are needed for the solution of the master equation is small, a density operator method is to be preferred. This method may be the only one available when very high accuracy is needed, because of the inevitable statistical errors in Monte Carlo simulations.

Otherwise a method that simulates individual states is to be preferred.

Where the main interaction of the open system is with a measuring apparatus, which records the quantum state by counting, as with a photon counter, then the relative state or quantum jump method is the natural one and the best to use for numerical computations. The application of QSD produces rapid changes in state that look like quantum jumps [25, 24], but this is numerically inefficient.

When measurement is not the main interaction with an environment, then QSD is often more efficient. Examples are the types of thermal interaction that are often represented by heat baths, interactions with a radiation field, and also continuous interactions with condensed matter or gaseous environments that are not to be considered as part of the system, such as in line broadening, molecular dynamics, noise in quantum circuits, etc. In these cases it is often simplest to use QSD with a fixed basis, and this is likely to be more efficient numerically than jumps.

Where the interaction with the environment is sufficiently strong to produce strong localization during a significant part of the evolution, then MQSD is to be preferred. This is a very common situation, as the greater the environmental interaction, the greater the localization becomes. MQSD is feasible where there are several degrees of freedom, and there would be no hope of using other simulation methods. In some limiting cases quasiclassical methods can be used instead. MQSD is likely to be valuable in those situations that lie between those that are sufficiently simple to be simulated by other numerical means, and those for which a quasiclassical method can be used.

Monte Carlo trajectory methods for open systems have been developed largely in connection with quantum optics, but they have been extended using QSD and MQSD to particles in traps [39], while Spiller and his collaborators [46] have carried out some

interesting QSD studies of quantum circuit elements with a view to applications to Josephson junctions.

The potential range of useful applications is far greater. In particular, there has been no application to quantum effects in the dynamics of molecules which interact strongly with gases or liquids. For isolated molecules, there are often transitions between many potential energy surfaces, and no clear way of localizing the molecule on one surface out of many. But in QSD, the interaction with the environment localizes the molecule into a small region around a phase point on one of many possible surfaces, so that MQSD for a molecule interacting with its environment would have considerable advantages over the numerical solution of the Schrödinger equation for an isolated molecule.

It is also clear that the noise in quantum circuits is an environmental effect that could well be simulated by MQSD. This applies even more strongly to quantum computation, where the potentially rapid decoherence produced by thermal interaction could be a crucial limitation. In these cases a lot could be learned from individual MQSD runs, without the need to make the large number of simulations required to get good statistics.

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