Quantum state diffusion with a moving basis: computing quantum-optical spectra

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Abstract

Quantum state diffusion (QSD) as a tool to solve quantum-optical master equations by stochastic simulation can be made several orders of magnitude more efficient if states in Hilbert space are represented in a moving basis of excited coherent states. The large savings in computer memory and time are due to the localization property of the QSD equation. We show how the method can be used to compute spectra and give an application to second harmonic generation.

Stochastic simulation of trajectories of Hilbert-space vectors or quantum trajectories has proved to be a powerful new method for the solution of master equations in quantum optics. The main advantage of stochastic simulation methods over direct numerical solution of the master equation stems from the fact that far less computer memory is needed to store a Hilbert-space vector than to store a density operator. This advantage often far outweighs the main disadvantage of stochastic simulation, namely that many trajectories have to be added to obtain good statistics.

There are two main approaches to quantum trajectories in quantum optics: the relative state method [1–3] and quantum state diffusion (QSD) [4]. In the relative state method, quantum trajectories are conditional on measurement outcomes. Consequently, a single master equation can be “unraveled” into many different stochastic equations, each corresponding to a different measurement scheme. For a given problem, one is free to choose the unraveling that results in the fastest algorithm. This flexibility is a major strength of the relative state method, when the measurement process is the main interaction with the environment. The relative state method is limited, however, to problems with few degrees of freedom and to relatively small photon numbers. For two or more field modes and large photon numbers, the number of basis states needed for a numerical representation of a Hilbert-space vector can become very large, leading to prohibitive computing times.

For the QSD method, on the other hand, there is a unique correspondence between master equations and stochastic equations [4]. Although it has been shown that, under special circumstances, the QSD equation is identical to the relative state equation conditioned on
heterodyne detection of photons \[6\], in general the QSD equation is not derived with respect to any specific measurement scheme. The QSD method can be applied with equal ease whether or not the main interaction with the environment is a measurement process. For an interpretation of the QSD equation, see \[4\].

QSD derives its strength as a computational tool from the localization property of the QSD equation \[4,7–11\]. We have shown \[12\] that representing QSD trajectories in a moving basis of excited coherent states instead of representing them in the usual number-state basis can reduce the number of basis states needed—and thus the computing time—by several orders of magnitude. We call the numerical method based on localization quantum state diffusion with a moving basis (MQSD). MQSD is particularly advantageous for problems with several degrees of freedom and large photon numbers and can be used in regimes extending from the highly quantum mechanical (few photons) to the semiclassical (very many photons).

In this paper, we show how MQSD can be used to compute quantum-optical spectra. Whereas computing spectra using the relative state method is a well established procedure \[13\], quantum state diffusion has not been applied to the practical computation of spectra before. Here we show that using MQSD for the computation of spectra leads to the same savings as using MQSD for the computation of photon numbers as in \[12\], and thus that it can be applied where the relative state method would be impractical.

Many problems in quantum optics can be formulated in terms of a master equation of Lindblad form \[14\]

\[
\frac{d}{dt} \hat{\rho} = \mathcal{L} \hat{\rho} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \sum_m \left( \hat{L}_m \hat{\rho} \hat{L}_m^\dagger - \frac{1}{2} \hat{L}_m^\dagger \hat{L}_m \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{L}_m^\dagger \hat{L}_m \right),
\]

where \(\hat{\rho}\) is the system density operator, \(\hat{H}\) is the system Hamiltonian, and the \(\hat{L}_m\) are Lindblad operators which are generally not Hermitian and represent the effect of the environment on the system in the Markov approximation. The QSD equation \[4\] derived from Eq. (1) is a nonlinear stochastic differential equation for a normalized state vector \(|\psi\rangle\):

\[
|d\psi\rangle = -\frac{i}{\hbar} \hat{H} |\psi\rangle dt + \sum_m \left( \langle \hat{L}_m^\dagger \hat{L}_m - \frac{1}{2} \hat{L}_m^\dagger \hat{L}_m - \frac{1}{2} \langle \hat{L}_m^\dagger \rangle \langle \hat{L}_m \rangle \right) |\psi\rangle dt
\]

\[
+ \sum_m \left( \hat{L}_m - \langle \hat{L}_m \rangle \right) |\psi\rangle d\xi_m .
\]

The first sum in (2) represents the deterministic drift of the state vector due to the environment, and the second sum the random fluctuations. Angular brackets denote the quantum expectation \(\langle \hat{G} \rangle = \langle \psi | \hat{G} | \psi \rangle\) of the operator \(\hat{G}\) in the state \(|\psi\rangle\). The \(d\xi_m\) are independent complex differential Gaussian random variables satisfying the conditions

\[
M d\xi_m = M d\xi_n d\xi_m = 0 , \quad M d\xi^*_m d\xi_m = \delta_{nn} dt ,
\]

where \(M\) denotes the ensemble mean. The density operator is given by the mean over the projectors onto the quantum states of the ensemble:

\[
\hat{\rho} = M |\psi\rangle \langle \psi | .
\]

If the pure states of the ensemble satisfy the QSD equation (2), then the density operator satisfies the master equation (1).
A crucial property of the QSD equation is localization. The Schrödinger evolution of an isolated system usually produces delocalization or dispersion. According to the Schrödinger equation, initially localized wave packets become highly delocalized except under very special circumstances. This effect is also present in the first, Hamiltonian term in the QSD equation (2). The environment terms in the QSD equation, however, have the opposite effect; they tend to make the wave packet narrower. The theory of localization is treated in [4,9]. Numerical simulations [4,8,12,15] show the competition between the delocalizing effect of the Hamiltonian and the localizing effect of the environment. The net effect is often a very well localized wave packet.

One important consequence of the localization of quantum trajectories is that, by continually changing the basis, it is often possible to reduce the number of basis states needed to represent the wave packet by several orders of magnitude. If a wave packet is localized about a point \((q,p)\) in phase space far from the origin, it requires many number states \(|n\rangle\) to represent it. But relatively few excited coherent states \(|q,p,n\rangle = \hat{D}(q,p)|n\rangle\), are needed, with corresponding savings in computer storage space and computation time. The operator \(\hat{D}(q,p)\) is the usual coherent state displacement operator [16],

\[
\hat{D}(q,p) = \exp \frac{i}{\hbar} \left( p\hat{Q} - q\hat{P} \right),
\]

where \(\hat{Q}\) and \(\hat{P}\) are the position and momentum operators. The separation of the representation into a classical part \((q,p)\) and a quantum part \(|q,p,n\rangle\) is called the moving basis [12] or, as in [10], the mixed representation.

The QSD equation (2) can contain both localizing and delocalizing terms. Nonlinear terms in the Hamiltonian tend to spread the wave function in phase space, whereas the Lindblad terms localize. Accordingly, the width of the wave packets varies along a typical trajectory. We use this to reduce the computing time even further by dynamically adjusting the number of basis vectors. Details about the implementation of MQSD can be found in [12].

We now turn to the computation of optical spectra. The method we use simulates the measurement of a spectral component at offset frequency \(\omega\) and is similar in spirit to [17–19]. It involves an auxiliary field mode or filter mode weakly coupled to a system operator \(\hat{c}\), detuned by the frequency \(\omega\), and weakly damped with damping constant \(\kappa\). The master equation describing the system coupled to the filter mode can be written as

\[
\frac{d}{dt} \rho = \mathcal{L} \rho - \frac{i}{\hbar} [\hat{H}_t, \rho] + 2\kappa (\hat{b}\rho\hat{b}^\dagger - \frac{1}{2} \hat{b}^\dagger \hat{b} \rho - \frac{1}{2} \rho \hat{b}^\dagger \hat{b}) ,
\]

where the system superoperator \(\mathcal{L}\) is defined as in [1], \(\hat{b}\) is the annihilation operator for the filter mode, and

\[
\hat{H}_t = \hbar \omega \hat{b}^\dagger \hat{b} + i\hbar \epsilon (\hat{c}\hat{b}^\dagger - \hat{c}^\dagger \hat{b})
\]

is the interaction picture Hamiltonian describing the filter mode and its coupling to the system with coupling constant \(\epsilon\). As in a real experiment, the spectral resolution is limited by the filter damping constant \(\kappa\).
Assuming that the coupling $\epsilon$ is so small that there is a negligible probability for the excitation of more than one photon in the filter mode, we can write the total density operator as

$$\hat{\rho} \simeq \hat{\rho}_{00} \otimes |0\rangle \langle 0| + \hat{\rho}_{01} \otimes |0\rangle \langle 1| + \hat{\rho}_{10} \otimes |1\rangle \langle 0| + \hat{\rho}_{11} \otimes |1\rangle \langle 1| , \tag{8}$$

where the $\hat{\rho}_{ij}$ operate in the system Hilbert space, and the $|i\rangle \langle j|$ operate in the filter Hilbert space. By expanding the solution to the master equation in powers of the coupling $\epsilon$, we obtain the following approximate equations of motion for the system operators $\hat{\rho}_{00}$ and $\hat{\rho}_{01}$ \cite{20}—notice that these equations do not preserve the trace.

$$\frac{d}{dt} \hat{\rho}_{00} = \mathcal{L} \hat{\rho}_{00} + O(\epsilon^2) , \tag{9}$$

$$\frac{d}{dt} \hat{\rho}_{01} = \mathcal{L} \hat{\rho}_{01} + i\omega \hat{\rho}_{01} + \epsilon \hat{\rho}_{00} \hat{c}^\dagger - \kappa \hat{\rho}_{01} + O(\epsilon^3) . \tag{10}$$

These equations can be solved formally to yield

$$\hat{\rho}_{00}(t) = e^{\mathcal{L} t} \hat{\rho}_{00}(0) + O(\epsilon^2) , \tag{11}$$

$$\hat{\rho}_{01}(t) = \epsilon \int_0^t e^{\mathcal{L}(t-t')} \left( \hat{\rho}_{00}(t') \hat{c}^\dagger \right) e^{(i\omega-\kappa)(t-t')} \, dt' + O(\epsilon^3) . \tag{12}$$

We can now obtain an approximation to the Fourier transform of the stationary-state time correlation function $\langle \hat{c}^\dagger(0) \hat{d}(\tau) \rangle_{ss}$ for an arbitrary system operator $\hat{d}$ by computing the expectation $\langle \hat{b}^\dagger \hat{d} \hat{b} \hat{d}^\dagger \rangle$ in the stationary regime (by $\langle \cdots \rangle_{ss}$ we denote the expectation value in the stationary state):

$$\text{tr} \left( \hat{\rho}(t) \hat{b}^\dagger \hat{d} \hat{b} \hat{d}^\dagger \right) = \text{tr} \left( \hat{b}^\dagger \left( \hat{\rho}_{01}(t) \otimes |0\rangle \langle 1| \right) \hat{b} \hat{d} \right) = \text{tr} \left( \left( \hat{\rho}_{01}(t) \otimes |0\rangle \langle 0| \right) \hat{d} \right) = \text{tr} \left( \hat{d} \hat{\rho}_{01}(t) \right)$$

$$\simeq \epsilon \int_0^t \text{tr} \left( \hat{d} e^{\mathcal{L}(t-t')} \left( \hat{\rho}_{00}(t') \hat{c}^\dagger \right) e^{(i\omega-\kappa)(t-t')} \, dt' \right)$$

$$= \epsilon \int_0^t \langle \hat{c}^\dagger(t') \hat{d}(t) \rangle e^{(i\omega-\kappa)(t-t')} \, dt' , \tag{13}$$

where the quantum regression theorem \cite{1,2} has been used in the last line. In the limit $t \to \infty$, one obtains

$$\langle \hat{b}^\dagger \hat{db} \hat{d} \hat{b}^\dagger \rangle_{ss} \simeq \epsilon \int_0^\infty \langle \hat{c}^\dagger(0) \hat{d}(\tau) \rangle_{ss} e^{(i\omega-\kappa)\tau} \, d\tau . \tag{14}$$

Similarly, one finds

$$\langle \hat{b} \hat{db} \hat{d} \rangle_{ss} \simeq \epsilon \int_0^\infty \langle \hat{d}(\tau) \hat{c}(0) \rangle_{ss} e^{(-i\omega-\kappa)\tau} \, d\tau . \tag{15}$$

By computing the expectation values $\langle \hat{b}^\dagger \hat{d} \hat{b} \hat{d}^\dagger \rangle_{ss}$ and $\langle \hat{b}^\dagger \hat{d} \hat{b} \rangle_{ss}$ for various choices of the system operators $\hat{c}$ and $\hat{d}$ using straightforward simulation of the QSD equation, one can thus obtain approximations for various spectral densities at the offset frequency $\omega$. For each value of $\omega$, a new simulation is needed.

In the following, we apply the method outlined above to the problem of second harmonic generation or frequency doubling. The system consists of two optical modes of frequency $\omega_1$
and $\omega_2 = 2\omega_1$ which interact in a cavity driven by a coherent external field with frequency $\omega_1$ and amplitude $E$. The Hamiltonian in the interaction picture is

$$
\hat{H} = i\hbar E (\hat{a}_1^\dagger - \hat{a}_1) + i\hbar \frac{\chi}{2}(\hat{a}_1^{12} \hat{a}_2 - \hat{a}_1^2 \hat{a}_2^1),
$$

where $\hat{a}_1$ and $\hat{a}_2$ are the annihilation operators of the two cavity modes, and $\chi$ describes the strength of the nonlinear interaction between them. Damping of the two cavity modes is described by the Lindblad operators $\hat{L}_1 = \sqrt{2\gamma_1} \hat{a}_1$ and $\hat{L}_2 = \sqrt{2\gamma_2} \hat{a}_2$. The factors of $\sqrt{2}$ are a consequence of the convention used in the master equation (1) which differs from the usual convention in quantum optics.

The master equation for this problem first appeared in [22]. Earlier numerical treatments include [12,23–27]; none of these compute spectra. The main difficulty in a numerical treatment of second harmonic generation is due to the large size of the number-state basis needed to represent a Hilbert-space vector. If $n_1$ number states are needed for mode 1 and $n_2$ number states are needed for mode 2, then the total number of basis states needed is $n_1 n_2$, which can be very large. By using MQSD, and thus exploiting the localization property of the QSD equation, this number can be reduced significantly [12]. We are then in a position to compute spectra with moderate numerical effort.

Of particular interest is the squeezing spectrum in the upconverted mode $\hat{a}_2$ as observed in homodyne detection. Squeezing in the upconverted mode in second harmonic generation has been experimentally observed by Sizmann et al. [28]. The squeezing spectrum $S_{\theta,\kappa}(\omega)$ is defined in terms of the quadrature operators

$$
\hat{A}_\theta(t) = \frac{1}{2} [\hat{a}_2(t)e^{-i\theta} + \hat{a}_2^\dagger(t)e^{i\theta}]
$$

and

$$
\Delta \hat{A}_\theta(t) = \hat{A}_\theta(t) - \langle \hat{A}_\theta(t) \rangle
$$

as

$$
S_{\theta,\kappa}(\omega) = 16\gamma_2 \int_0^\infty d\tau \cos(\omega\tau)e^{-\kappa\tau} \langle \Delta \hat{A}_\theta(0) \Delta \hat{A}_\theta(\tau) \rangle_{ss}.
$$

The notation $\langle \cdots \rangle$ means normal ordering and time ordering of the operator products, and a nonzero value of $\kappa$ results in a limited spectral resolution. A few lines of algebra lead to

$$
S_{\theta,\kappa}(\omega) = 4\gamma_2 \text{Re} \left[ \int_0^\infty d\tau e^{-\kappa\tau} \left( e^{i\omega\tau} + e^{-i\omega\tau} \right) \left( e^{-2i\theta} \langle \hat{a}_2(\tau)\hat{a}_2(0) \rangle_{ss} + \langle \hat{a}_2^\dagger(0)\hat{a}_2(\tau) \rangle_{ss} \right) \right. 
- \left. \frac{2\kappa}{\kappa^2 + \omega^2} \left( e^{-2i\theta} \langle \hat{a}_2 \rangle_{ss}^2 + \langle \hat{a}_2^\dagger \rangle_{ss} \langle \hat{a}_2 \rangle_{ss} \right) \right].
$$

All the quantities in this equation can be easily determined by simulation of the QSD equation with the help of Eqs. (14) and (15).

In this paper, we do not attempt to reproduce the results of Sizmann et al.; instead, we choose a set of parameter values leading to a limit cycle in the corresponding classical dynamics. The numerical treatment of this regime has proven to be particularly challenging.
Figure 1 shows the resulting spectrum Eq. (19) with $\theta = \pi/2$. The spectral density is positive throughout; there is no squeezing in this regime, which agrees with the findings in [23]. The stationary expectation values required for the evaluation of Eq. (20) were generated by computing time averages in the stationary regime, assuming ergodicity. The integration time was $T = 100\kappa^{-1}$. Since the filter decay time $\kappa^{-1}$ was chosen to be the largest decay time in the system, the statistics resulting from an integration time $T = n\kappa^{-1}$ corresponds roughly to the statistics resulting from adding $n$ trajectories. The computing time was about 1 day per data point on a standard Pentium PC running Linux.

In conclusion, we have shown that the method of quantum state diffusion with a moving basis or MQSD can be used to compute quantum optical spectra, with considerable savings in computing time and memory compared with earlier methods.

We thank the EPSRC in the UK and the University of Geneva for essential financial support, and G. Alber, N. Gisin, P. Knight, M. Plenio, W. Strunz and P. Zoller for valuable communications.
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FIGURES

FIG. 1. Homodyne spectrum Eq. (19) with $\theta = \pi/2$ for the upconverted mode in second harmonic generation. The frequency scale on the plot is in units of the decay constant of the fundamental mode, $\gamma_1$. The parameters are $E/\gamma_1 = 20$, $\chi/\gamma_1 = 0.4$, $\gamma_2/\gamma_1 = 1$, $\kappa/\gamma_1 = 0.1$, $\epsilon/\gamma_1 = 10^{-6}$, corresponding to a limit cycle regime of the classical dynamics.
Spectrum $S$ vs $\omega$