Stochastic Wave-function Simulation of Two-time Correlation Functions

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We propose an optimized algorithm for the numerical simulation of two-time correlation functions by means of stochastic wave functions. As a first application, we investigate the two-time correlation function of a nonlinear optical parametric oscillator.

I. INTRODUCTION

Spurred by the ever increasing speed of commercially available desk-top computers, the analysis of dissipative quantum dynamics in terms of stochastic Schrödinger equation was recently promoted as an interesting alternative to the more traditional approach which is based on the solution of the system’s master equation. This is because workstations are usually strong in in simulating a couple (say 100) runs of a N-dimensional wave function, but — because of memory limitations — perform rather weak in propagating the $O(N^2)$ matrix elements of the statistical operator [1]. In particular in quantum optics, where $N$ may be of the order $N = 1000$ or larger, stochastic techniques enjoy increasing popularity.

The technique is based on the “unraveling” [2] of a given master equation

$$\frac{d}{dt} \rho = L \rho,$$

in terms of a stochastic Schrödinger equation, which propagates a state vector $\psi_r(t)$ in such a way, that the solution of the master equation $\hat{\rho}(t) = e^{Lt} \hat{\rho}(0)$, is recovered in the stochastic average,

$$\hat{\rho}(t) = \langle \psi_r(t) | \psi_r(t) \rangle.$$

Here, the subscript $r$ labels a particular realization of the stochastic process, and $\langle ... \rangle$ denotes the average over all realizations, including a weighted sum over pure initial states.

A given master equation may be unraveled by a variety of stochastic methods, which involve either appropriate generalizations of the continuous Wiener stochastic processes, discontinuous jump processes, or a mixture of both. The mathematical foundation of the various representations, their relation to a specific physical set-up and their connection to the quantum measurement problem is nicely reviewed in Refs. [3,4]. For a semi-popular account, including some historical and philosophical issues, see Ref. [5].

Even though the individual trajectories $|\psi_r(t)\rangle$ enjoy great popularity for the illustration of a quantum systems’ dynamics, the only physical quantities which may reliably be predicted using the set of $|\psi_r(t)\rangle$ are the time dependent expectation values of quantum mechanical operators, $\langle \hat{A}(t) \rangle \equiv \text{tr} \left( \hat{A} \hat{\rho}(t) \right)$, viz.

$$\langle \hat{A}(t) \rangle = \langle \psi_r(t) | \hat{A} | \psi_r(t) \rangle.$$

In particular, multi-time correlation functions may not be computed by means of the representation (3). The two-time correlation function

$$\langle \hat{A}(t) \hat{B}(0) \rangle = \text{tr} \left( \hat{A} e^{Lt} \hat{B} \hat{\rho}(0) \right),$$

for example, can not be evaluated by the recipe “measure $\hat{B}$ in a suitably selected initial state, propagate the post-measurement state to time $t$, measure $\hat{A}$, repeat and average”. The Heisenberg operators on the left hand side of Eq. (4) must be treated with special care in open systems with non-unitary time evolution, as algebraic properties are generally not preserved by transformation to the Heisenberg picture (i.e. $(\hat{A}\hat{B})(t) \neq \hat{A}(t)\hat{B}(t)$ [6]). It turns out that for non-commuting $\hat{A}(t)$, $\hat{B}(0)$, the evaluation of Eq. (4) requires an intricate algorithm involving, at least, one pair of coupled stochastic Schrödinger equations.
Indeed, the correlator (4) may be viewed as the single-time expectation value of $\hat{A}$ with respect to an improper state $\hat{\chi}(t)$, $\langle \hat{A}(t) \hat{B}(0) \rangle = \text{tr} \left( \hat{A} \hat{\chi}(t) \right)$, where

$$\hat{\chi}(t) = e^{t \hat{H}} \hat{\rho}(0).$$

(5)

For a pure initial state, $\hat{\rho}(0) = |\psi(0)\rangle \langle \psi(0)|$, the initial value of $\hat{\chi}(t)$ is given in terms of a dyadic product of two state vectors $|\psi(0)\rangle$ and $|\phi(0)\rangle \equiv \hat{B}|\psi(0)\rangle$,

$$\hat{\chi}(0) = |\phi(0)\rangle \langle \psi(0)|.$$

(6)

This indicates that the evaluation of (4) may be reduced to the simulation of a single-time expectation value of $\hat{A}$ with respect to $\hat{\chi}(t)$, which comes, however, at the expense of dealing with two different wave functions simultaneously.

In the past, several stochastic wave function algorithms have been proposed which support the numerical simulation of a two-time correlation function $\langle \chi(t) \rangle^2$. Since all these algorithms are build to yield the correct result in the limit of infinitely many runs, they are effective, but they are usually not very efficient. The scheme proposed by Castin et al [7], for example, is threatened by numerical instability as it relies on the subtraction of possibly large numbers. The particular scheme proposed by Gardiner and Zoller [3] and Gisin [8], on the other hand, is exponentially inefficient, that is the number of trajectories which are needed for a reliable estimate of the desired correlation function is bound from below by an increasing exponential function of the correlator’s time $t$. The somewhat more intricate algorithm which may be extracted from the work of Breuer and collaborators [9] does not suffer from this particular kind of inefficiency, but it is not yet optimized. To date no systematic investigation has addressed the issue of how to tailor an algorithm which is both effective and efficient.

In the present paper we construct an optimal algorithm for a class of stochastic representations which are characterized by pseudo-linear Ito differential equations involving jump processes. The paper is organized as follows. In Sec. II we review the unraveling of the master equation for a genuine statistical operator using Ito stochastic calculus. In Sec. III, we extend our analysis for the stochastic representation of the dynamics of skew-symmetric state operators, and we indicate an optimal algorithm. Using the simple example of spontaneous emission of a two-state system we analyse the efficiency of alternative algorithm, including the Gardiner-Zoller [3] and Breuer-Kappler-Petruccione [9] method. As a non-trivial example, we apply our algorithm to the problem of tunneling in the degenerate optical parametric oscillator. The methods of Castin and collaborators [7], and of Breuer and collaborators [9] are revied in Appendices A and B.

II. PROPAGATION OF PROPER STATE OPERATORS

In this section we seek the unraveling of the model master equation,

$$\frac{d}{dt} \hat{\rho} = 2\hat{\sigma} \hat{\rho} \hat{\sigma}^\dagger - \hat{\sigma}^\dagger \hat{\rho} \hat{\sigma} - \hat{\rho} \hat{\sigma}^\dagger \hat{\sigma},$$

(7)

which – dependent on the algebraic properties of the operators $\hat{\sigma}$, $\hat{\sigma}^\dagger$ – describes spontaneous emission of a 2-level atom or the damping of a cavity mode. Generalizations to other systems will be covered in Sec. III B.

We unravel the master equation (7) in terms of an Ito stochastic differential equation

$$|d\psi_r(t)\rangle = d\xi(t)|\psi_r(t)\rangle - d\mu(t)\hat{\sigma}^\dagger|\psi_r(t)\rangle + d\eta(t)\hat{\sigma}|\psi_r(t)\rangle,$$

(8)

where $\xi(t)$, $\mu(t)$ and $\eta(t)$ are, in general complex, stochastic processes, and differentials are forward oriented, $d\psi(t) = \psi(t + dt) - \psi(t)$ etc. Note that the equation is pseudo-linear, as the stochastic increments $d\xi(t)$, $d\mu(t)$ and $d\eta(t)$ may depend on $\psi_r(t)$.

A stochastic process like $\xi(t)$ is, in general, not differentiable and the stochastic increment $d\xi(t)$ does not have the properties of an ordinary differential, i.e. it can not, in general, be treated as “infinitesimal”. However, from Eq. (4) and the assumed smoothness of $\hat{\rho}(t)$ it follows that the stochastic average of the dyadic product $|\psi_r(t)\rangle \langle \psi_r(t)|$ must be well-behaved and differentiable,

$$d \left( |\psi_r(t)\rangle \langle \psi_r(t)| \right) = d|\psi_r(t)\rangle \langle \psi_r(t)| + |\psi_r(t)\rangle d\langle \psi_r(t)| + d|\psi_r(t)\rangle \langle \psi_r(t)|.$$

(9)

Note that we are not allowed to drop the last term as would be the case if $d|\psi_r(t)\rangle$ were an ordinary differential.
By virtue of Eq. (2), the differential \( \rho(t) \) equals the forward differential of the density operator, \( d\rho(t) = \rho(t + dt) - \rho(t) \). For our particular model, \( \dot{\rho}(t) \)

\[
\frac{d\dot{\rho}(t)}{dt} = 2\dot{\sigma}\dot{\rho}(t)\dot{\sigma}^\dagger dt - \dot{\sigma}^\dagger \dot{\sigma}\rho(t) dt - \dot{\rho}(t)\dot{\sigma}^\dagger dt.
\]

(10)

Since Eqs. (9) and (10) must coincide regardless of the value of \( \rho(t) \), they must coincide for any individual member of the ensemble \( \rho(t) \), say \( \psi_r(t) \). Hence we set \( \rho(t) = |\psi_r(t)\rangle\langle\psi_r(t)| \) in Eq. (10), and in Eq. (9) consider \( \psi_r(t) \) as fixed. As we make no assumptions on the action of the operators \( \dot{\sigma} \) and \( \dot{\sigma}^\dagger \), respectively, we insert the stochastic ansatz into Eq. (9) and compare coefficients of the right hand sides of Eqs. (9) and (10). The result reads

\[
\frac{d\xi(t) + d\xi^*(t) + d\xi(t) d\xi^*(t)}{(d\xi(t) + 1) d\mu^*(t)} = dt, \quad \frac{d\xi(t) d\xi^*(t)}{(d\xi(t) + 1) d\eta^*(t)} = 0, \quad \frac{d\mu(t) d\mu^*(t)}{(d\mu(t) d\eta^*(t))} = 0, \quad \frac{d\eta(t) d\eta^*(t)}{(d\eta(t) d\eta^*(t))} = 2dt,
\]

(11)

where \[\ldots\] denotes an average over the stochastic increments for fixed \( \psi_r(t) \).

The unraveling (2) conserves the norm square \(|\psi_r(t)|^2\) in stochastic average, as is obvious when taking the trace in Eq. (2),

\[
\langle\psi_r(t)|\psi_r(t)\rangle = 1.
\]

(12)

In fact, all well-established algorithms preserve the norm even for every single realization:

\[
\forall t, r : \quad \langle\psi_r(t)|\psi_r(t)\rangle = 1.
\]

(13)

As a rule, algorithms which have been derived from some theory of continuous measurement respect norm conservation in the strong version, as they deal with proper states which admit a physical interpretation at any time.

If numerical efficiency rather than merely effectiveness is an issue, algorithms which respect the stronger condition of norm conservation (13) ought to be preferred. This is because they generate trajectories of equal weight, avoiding waste of CPU time on simulating a large number of trajectories when only a few “heavy” ones actually contribute to the result. A more formal proof of this requirement is given in Sec. III A.

The strong conservation law imposes additional constraints on the stochastic increments. Taking the stochastic differential of Eq. (13) we obtain

\[
\langle\psi_r(t)|d\psi_r(t)\rangle + \langle d\psi_r(t)|\psi_r(t)\rangle + \langle d\psi_r(t)|d\psi_r(t)\rangle = 0,
\]

(14)

which — using the stochastic ansatz and dropping the time arguments for readability — amounts to the following constraint:

\[
d\xi + d\xi^* - (d\mu + d\mu^*)Q + d\eta P + d\eta^* P^* + d\xi^* d\xi - d\mu^* d\xi Q + d\xi d\eta P - d\eta^* d\eta Q = 0,
\]

(15)

where \( P := \langle\psi_r|\dot{\sigma}|\psi_r\rangle, Q := \langle\psi_r|\dot{\sigma}^\dagger \dot{\sigma}|\psi_r\rangle, R := \langle\psi_r|\dot{\sigma}^\dagger \dot{\sigma}^\dagger \dot{\sigma}|\psi_r\rangle, \) and \( S := \langle\psi_r|\dot{\sigma}^\dagger \dot{\sigma}^\dagger \dot{\sigma}^\dagger \dot{\sigma}|\psi_r\rangle \).

Even if supplemented by the strong condition of norm conservation (13), the conditions (11) and (13) still offer quite some freedom in the choice of a correspondig stochastic model.

Most prominent are the models of quantum state diffusion, where the stochastic Schrödinger equation assumes the form of a Langevin equation with Wiener stochastic increments, and models of quantum jumps, where the time evolution is mostly deterministic, only interrupted by discontinuous jumps at random times. Since jump methods seem to be favoured in numerical applications we concentrate on the jump processes in the following.

In a simple two-branch jump process, at any time \( t \), the tripel \((d\xi, d\mu, d\eta)\) can take on one of two different values,

\[
(d\xi, d\mu, d\eta) = \begin{cases} (\xi_3, \mu_3, \eta_1) & \text{with probability } dp \\ (\xi_3, \mu_3, 0) & \text{with probability } 1 - dp \end{cases}
\]

(16)

1 Sometimes this is not obvious at first glance: in some recipes for unraveling (2), norm conservation may be violated temporarily; however, explicit renormalization will then become necessary, at the latest when expectation values are computed.
Most of the time, $d\eta$ is zero while $d\xi$ and $d\mu$ take on well-defined, infinitesimal, values, so that the state evolves continuously, denoted by the index $c$. With a certain probability $dp \propto dt$, a “jump” occurs, corresponding to a finite-valued triplet $(\xi_j, \mu_j, \eta_j)$. Such processes are often derived from a theory of measurement, where jumps correspond to “clicks” of some photo detector.

Note that while Eq. (8) contains stochastic differentials $d\xi$, $d\mu$, $d\eta$, we are now left with 6 parameters $\xi_j, \mu_j, \eta_j, d\xi_c, d\mu_c$, and $dp$, which are deterministic functions of the state vector $|\psi_r(t)\rangle$; the only stochastic element in (10) is the decision which branch to take. We have retained the differential notation for the parameters $d\xi$ and $d\mu$, which will be of order $dt$, in contrast to $\xi_j, \mu_j$ and $\eta_j$, which will be of order 1.

The most simple jump process is obtained by choosing $\xi_j = -1$, $\mu_j = 0$; from this, and the strong condition of norm conservation (13), one readily derives the remaining parameters

$$\eta_j = |\hat{\sigma} |\psi_r\rangle|^{-1}, \quad dp = 2dt |\hat{\sigma} |\psi_r\rangle|^2, \quad d\xi_c = \frac{dp}{2}, \quad d\mu_c = dt.$$ (17)

The stochastic process (8) now reads

$$|d\psi_r\rangle = \left\{ \begin{array}{ll} \left( -\mathbb{1} + |\hat{\sigma} |\psi_r\rangle|^{-1} \hat{\sigma} \right) |\psi_r\rangle, & dp \\
\left( \langle \psi_r \hat{\sigma}^\dagger |\psi_r\rangle - \hat{\sigma}^\dagger \hat{\sigma} \right) dt |\psi_r\rangle, & 1 - dp, \end{array} \right.$$(18)

and the vector $|\psi_r(t)\rangle$ will be mapped according to $|\psi_r(t)\rangle \rightarrow |\psi_r(t + dt)\rangle$,

$$|\psi_r(t + dt)\rangle = \left\{ \frac{|\hat{\sigma} |\psi_r(t)\rangle|^{-1} \hat{\sigma} |\psi_r(t)\rangle}{(\mathbb{1} - dt\hat{\sigma}^\dagger \hat{\sigma})} \frac{dp}{(\mathbb{1} - dt\hat{\sigma}^\dagger \hat{\sigma}) |\psi_r(t)\rangle}, & 1 - dp \right.$$ (19)

This algorithm and its generalizations are quite popular in the quantum optics community, where they have been applied to a variety of problems, see Refs. [1-6].

### III. PROPAGATION OF NON-SYMMETRIC OPERATORS

#### A. Construction of an efficient general-purpose algorithm

As indicated in the introduction, numerical simulation of the two-time correlation function $\langle A(t)B(0) \rangle$ requires the unraveling of the skew-symmetric operator $\hat{\chi}(t) = e^{-t\hat{B}}\hat{B}\hat{\rho}(0)$. Here, a naive generalization of recipes like (18) can not succeed, as there is no obvious way to define the jump probability for an operator like $\hat{\chi}(t)$ which is neither definite nor hermitian.

Recall, however, that the unraveling is only required for a pure initial state, $\hat{\rho}(0) = |\psi(0)\rangle \langle \psi(0)|$, since the case of mixed initial state is easily obtained by means of a suitable weighted sum over such pure states. Denoting $|\phi(0)\rangle = \hat{B}|\psi(0)\rangle$, one has $\hat{\chi}(0) = |\phi(0)\rangle \langle \phi(0)|$, which is the dyadic product of two state vectors $\phi$ and $\psi$. Thus unraveling may well proceed along the lines of Sec. 4.1, this time however for a pair $\langle |\phi_r(t)\rangle, |\psi_r(t)\rangle \rangle$ of vectors, such that the skew-symmetric $\hat{\chi}(t)$ is recovered in the stochastic average:

$$\hat{\chi}(t) = \frac{|\phi_r(t)\rangle \langle \psi_r(t)|}{\langle A(t)B(0) \rangle} = \frac{\langle \psi_r(t) |A| \phi_r(t) \rangle}{\langle \psi_r(t) |A| \phi_r(t) \rangle}.$$ (20)

We start the unraveling of $\hat{\chi}(t)$ from an ansatz similar to (8), but now for a pair of wave functions:

$$|d\phi_r\rangle = d\xi_1 |\phi_r\rangle - d\mu_1 \hat{\sigma}^\dagger |\phi_r\rangle + d\eta_1 \hat{\sigma} |\phi_r\rangle,$$

$$|d\psi_r\rangle = d\xi_2 |\psi_r\rangle - d\mu_2 \hat{\sigma}^\dagger |\psi_r\rangle + d\eta_2 \hat{\sigma} |\psi_r\rangle.$$ (21)

Analogous to Eq. (11), we can again derive a set of necessary conditions for the stochastic increments:

$$\frac{d\xi_1}{d\xi_2} + d\xi_3 = 0,$$ (22a)

$$d\xi_1 + d\mu_2 = (d\xi_2 + 1)d\mu_1 = dt.$$ (22b)
We restrict ourselves to a jump process similar to \((18)\), but with free parameters:

\[
\begin{align*}
\frac{d\xi_1+1}{d\mu_2} &= \frac{d\xi_2^*+1}{d\eta_1} = 0, \\
\frac{d\mu_1 d\mu_2}{dt} &= 0, \\
\frac{d\mu_1 d\eta_2}{dt} &= \frac{d\mu_2 d\eta_1}{dt} = 0, \\
\frac{d\eta_1 d\eta_2}{dt} &= 2dt.
\end{align*}
\] (22c)

(22d)

(22e)

(22f)

As above, the indices \(c\) and \(J\) denote the continuous branch and the jump branch, respectively. The ansatz \((23)\), although less general than in Eq. \((21)\), still contains enough degrees of freedom to allow for a wide range of jump algorithms, including many of those suggested in the literature \([1,3,4]\); it has the advantage of being easier to implement, and it will automatically fulfill the conditions \((22c)\) and \((22e)\).

There are two degrees of freedom in the choice of the free parameters in \((23)\) which are mere gauge freedoms with no relevance to the efficiency of the process (this has already been observed by Diósi, see \([3]\)): for some complex number \(c \neq 0\), the transformation

\[
(d\xi_{1,c}, d\mu_{1,c}, d\xi_{2,c}, d\mu_{2,c}) \mapsto (c^* d\xi_{1,c}, c^* d\mu_{1,c}, c^{-1} d\xi_{2,c}, c^{-1} d\mu_{2,c})
\] (24)

will leave \((22e)\) invariant and leads to a process which is equivalent in the sense that it predicts identical trajectories for all observable quantities. Similarly, there is another gauge freedom for \(\eta_{1,1}, \eta_{2,1}\): for any complex number \(\tilde{c} \neq 0\), the transformation

\[
(\eta_{1,1}, \eta_{2,1}) \mapsto (\tilde{c}^* \eta_{1,1}, \tilde{c}^{-1} \eta_{2,1})
\] (25)

leads to an equivalent stochastic process.

We are therefore free to choose the symmetric gauge:

\[
\forall r, t: \quad |\phi_r(t)| = |\psi_r(t)|.
\] (26)

As this must hold for both the continuous and the jump branch in Eq. \((23)\), it fixes the modulus of both gauge parameters \(c\) and \(\tilde{c}\) in \((24)\) and \((25)\). The phase can be fixed by demanding that \(d\xi_{1,c}\) and \(\eta_{1,2,1}\) be real numbers; from \((22c)\) it follows that \(d\mu_{1,2,c}\), too, will be then real-valued.

We are now left with 7 real-valued parameters to be determined; since \((22c)\) and \((22e)\) are always satisfied by our ansatz \((23)\), we have to fulfill the following 7 conditions:

\[
\begin{align*}
(1 - dp)(d\xi_{1,c} + d\xi_{2,c}) &= dp, \quad \text{(22a)} \\
(1 - dp)(d\xi_{1,c} + 1) d\mu_{2,c} &= dt, \quad \text{(22b)} \\
(1 - dp)(d\xi_{2,c} + 1) d\mu_{1,c} &= dt, \quad \text{(22c)} \\
(1 - dp)(d\mu_{1,c} d\mu_{2,c}) &= 0, \quad \text{(22d)} \\
\eta_{1,1} d\eta_{2,1} &= 2dt, \quad \text{(22e)} \\
|\eta_{1,1} \sigma | |\phi_r| &= |\eta_{2,1} \sigma | |\psi_r|, \quad \text{(26)} \\
|((d\xi_{1,c} + 1) - d\mu_{1,c} \sigma)| |\phi_r| &= |((d\xi_{2,c} + 1) - d\mu_{2,c} \sigma)| |\psi_r|, \quad \text{(26)}
\end{align*}
\] (27)

Taking into account that \(d\xi_{1,c}, d\xi_{2,c}, d\mu_{1,c}, d\mu_{2,c}\) and \(dp\) are quantities of order \(dt\), while \(\eta_{1,1}\) and \(\eta_{2,1}\) will be quantities of order 1, these conditions can be simplified: the values

\[
d\mu_{1,c} = d\mu_{2,c} = dt
\] (28)

are already determined, and we are left with just 4 constraints for the 5 remaining parameters \(dp, d\xi_{1,c}, d\xi_{2,c}, \eta_{1,1}, \eta_{2,1}\):
\[
\begin{align*}
\frac{d\xi_{1,c} + d\xi_{2,c}}{c} &= dp \\
\eta_{1,1}\eta_{2,1}dp &= 2dt \\
|\eta_{1,1}\hat{\sigma}| |\phi_r\rangle &= |\eta_{2,1}\hat{\sigma}| |\psi_r\rangle \\
\left|\left((d\xi_{1,c} + 1) - d\mu_{1,c}\hat{\sigma}\hat{\sigma}^\dagger\right)|\phi_r\rangle\right| &= \left|\left((d\xi_{2,c} + 1) - d\mu_{2,c}\hat{\sigma}\hat{\sigma}^\dagger\right)|\psi_r\rangle\right|
\end{align*}
\]

We are thus free to impose exactly one additional arbitrary constraint; since all conditions listed above are either required (within our ansatz for the jump process) or mere gauge conditions with no effect on the trajectories of observable quantities, it will be this single condition which will determine the efficiency of the algorithm.

**B. Minimizing the error of an jump algorithm**

In a simulation of \(K\) trajectories \(\hat{\chi}_j := |\phi_j\rangle \langle \psi_j|\), \(j = 1, \ldots, K\), the true skew operator \(\hat{\chi}\) will be approximated by

\[
\hat{\chi} = \frac{1}{K} \sum_{j=1}^K \hat{\chi}_j .
\]

For any correct algorithm, we have

\[
\hat{\chi} = \hat{\chi}. \tag{31}
\]

At the same time, we would like the error to be minimal:

\[
\|\hat{\chi} - \chi\|^2 = \text{minimal}. \tag{32}
\]

If we use the norm \(\|\chi\|^2 := \text{tr} (\chi^\dagger \chi)\), then we find for our ensemble of \(K\) trajectories:

\[
\|\hat{\chi} - \chi\|^2 = \frac{1}{K^2} \sum_{j, l=1}^K \text{tr} \left( \hat{\chi}_j^\dagger \hat{\chi}_l \right) - \text{tr} (\hat{\chi}^\dagger \hat{\chi}) . \tag{33}
\]

For independent trajectories \(\hat{\chi}_j\) and \(\hat{\chi}_l\), where \(j \neq l\), we have

\[
\text{tr} \left( \hat{\chi}_j^\dagger \hat{\chi}_k \right) = \sum_{r, r'} P(r) P(r') \text{tr} \left( \hat{\chi}_j^\dagger \hat{\chi}_{r'} \right) = \text{tr} \left( \left( \sum_r P(r) \hat{\chi}_r^\dagger \right) \left( \sum_{r'} P(r') \hat{\chi}_{r'} \right) \right) = \text{tr} (\hat{\chi}^\dagger \hat{\chi}) , \tag{34}
\]

where we sum over all realizations \(r\) of the stochastic process and denote with \(P(r)\) the probability of the realization \(r\). Thus, Eq. (33) becomes:

\[
\|\hat{\chi} - \chi\|^2 = \frac{1}{K^2} \left( \sum_{j=1}^K \text{tr} \left( \hat{\chi}_j^\dagger \hat{\chi}_j \right) + \sum_{j, l=1}^K \text{tr} \left( \hat{\chi}_j^\dagger \hat{\chi}_l \right) \right) - \text{tr} (\hat{\chi}^\dagger \hat{\chi}) = \frac{1}{K} \left( \text{tr} (\hat{\chi}_r^\dagger \hat{\chi}_r) + \frac{K-1}{K} \text{tr} (\hat{\chi}^\dagger \hat{\chi}) - \text{tr} (\hat{\chi}^\dagger \hat{\chi}) \right) = \frac{1}{K} \text{tr} (\hat{\chi}_r^\dagger \hat{\chi}_r) - \frac{1}{K} \text{tr} (\hat{\chi}^\dagger \hat{\chi}) . \tag{35}
\]

The condition (32) now reads:

\[
\text{tr} \left( \hat{\chi}_r^\dagger \hat{\chi}_r \right) = \langle \phi_r | \phi_r \rangle \langle \psi_r | \psi_r \rangle = \text{minimal} . \tag{36}
\]

By minimizing

\[
\text{tr} \left( \hat{\chi}_r^\dagger \hat{\chi}_r \right) = \langle \phi_r | \phi_r \rangle \langle \psi_r | \psi_r \rangle = \text{minimal} .
\]
under the constraints
\[ \sum_r P(r) = 1 \quad \text{and} \quad \sum_r P(r) \dot{\chi}_r = \dot{\chi}, \]
(38)

(36) turns out to be equivalent to
\[ \forall r, r' : \quad \text{tr} \left( \dot{\chi}_r \dot{\chi}_{r'} \right) = \text{tr} \left( \dot{\chi}_r \dot{\chi}_{r'} \right). \]
(39)

We see that it is indeed desirable to avoid algorithms containing rare but “large” trajectories. Unfortunately, ensuring Eqs. (36) or (39) will be in general impossible, so we replace it by a weaker condition which is necessary but not sufficient for Eq. (39) to hold, but which will nevertheless suffice as the last missing constraint required by the one remaining degree of freedom in (29):
\[ \forall \langle \phi \rangle, \langle \psi \rangle : \quad \frac{d}{dt} \langle \phi \langle \phi \rangle \langle \psi \rangle \rangle = \text{minimal}. \]
(40)

Here, the ensemble average \( \langle \phi \rangle, \langle \psi \rangle \) is taken only over the two possible branches in (29), not over an ensemble of possible states before performing the time step: we want this condition to be fulfilled for every member of the ensemble individually. We will show below that this will even guarantee a monotonically decreasing of the norm of both \( \langle \phi \rangle \) and \( \langle \psi \rangle \) in every single realization.

We can now proceed to derive a jump algorithm fulfilling (40). The time derivative can be evaluated separately for the jump branch and the continuous branch in (29); for the jump branch we find:
\[
d (\langle \phi \langle \phi \rangle \langle \psi \rangle \rangle) = \eta^2 \left[ 2 \langle \phi \rangle \langle \dot{\psi} \rangle \langle \psi \rangle \rangle - \langle \phi \langle \phi \rangle \langle \psi \rangle \rangle \right] = \frac{4dt^2}{dp^2} \Phi^2 \Psi^2 - s^2 ,
\]
(41)

where
\[
s := \langle \phi \langle \phi \rangle \rangle \equiv \langle \psi \rangle \rangle , \quad \Phi := \langle \dot{\phi} | \phi \rangle , \quad \Psi := \langle \dot{\psi} | \psi \rangle \rangle .
\]
(42)

For the continuous branch, we have:
\[
d (\langle \phi \langle \phi \rangle \langle \psi \rangle \rangle) = 2 (d\xi_{1,c} + d\xi_{2,c}) \langle \phi \rangle \langle \phi \langle \psi \rangle \rangle
- 2dt \left( \langle \phi \dot{\phi} \langle \phi \rangle \rangle + \langle \psi \dot{\psi} \langle \psi \rangle \rangle \right)
= 2 (d\xi_{1,c} + d\xi_{2,c}) s^2 - 2dt (\Phi^2 + \Psi^2) s
= 2dp s^2 - 2dt (\Phi^2 + \Psi^2) s .
\]
(43)

So we have on average:
\[
\langle d (\langle \phi \langle \phi \rangle \langle \psi \rangle \rangle) \rangle = dp d (\langle \phi \langle \phi \rangle \langle \psi \rangle \rangle) + (1 - dp)d (\langle \phi \langle \phi \rangle \langle \psi \rangle \rangle) = \frac{4dt^2}{dp} \Phi^2 \Psi^2 + dp s^2 - 2dt (\Phi^2 + \Psi^2) s .
\]
(44)

Minimizing this with respect to the only remaining parameter \( dp \) yields our choice for the jump probability \( dp \):
\[
dp = \frac{2}{s} \Phi \Psi dt .
\]
(45)

The remaining parameters can now readily be derived from (29):
\[
\eta_{1,J} = \frac{\sqrt{s}}{\Phi} , \quad \eta_{2,J} = \frac{\sqrt{s}}{\Psi} ,
\]
\[
d\xi_{1,c} = \left( \Phi \Psi + \frac{1}{2} \Phi^2 - \frac{1}{2} \Psi^2 \right) dt , \quad d\xi_{2,c} = \left( \Phi \Psi - \frac{1}{2} \Phi^2 + \frac{1}{2} \Psi^2 \right) dt ,
\]
\[
d\mu_{1,c} = dt , \quad d\mu_{2,c} = dt .
\]
(46)
C. Comparison with other algorithms

We are going to compare several alternative algorithms by analyzing the radiative decay of a two-level atom. The atom is prepared in its excited state $|e\rangle$ from where it decays into its ground state $|g\rangle$ by means of spontaneous emission. The corresponding master equation is given by Eq. (49) with the specification $\sigma = \sqrt{\gamma}|g\rangle\langle e|$. 

We wish to compute the correlation function

$$g(t) = \langle \hat{\sigma}^\dagger(t)\hat{\sigma} \rangle ,$$

which for this particular problem should result in $g(t) = e^{-\gamma t}$.

Starting with the initial state

$$(|\phi(0)\rangle , |\psi(0)\rangle) = (|g\rangle , |e\rangle) ,$$

we observe that the continuous branch in Eq. (23) will leave the state unchanged except for scalar factors changing the norm of $\phi_r$ and $\psi_r$. The first jump maps $|\phi_r(t)\rangle$ onto 0. As this value can never change again, only trajectories with no jump up to time $t$ will contribute to $g(t)$.

1. The Gardiner-Zoller algorithm

In Ref. [3] an algorithm is suggested which is characterized by the following choice of parameters:

$$dp = 2\Psi^2 dt , \quad \eta_{1,1} = \eta_{2,1} = \frac{1}{\Psi} ,$$
$$d\xi_{1,1} = d\xi_{2,1} = \Psi^2 dt , \quad d\mu_{1,1} = d\mu_{2,1} = dt ,$$

with $\Psi = |\sigma|\psi|$, see Eq. (12). Note that this algorithm displays a certain asymmetry in favour of $|\psi_r\rangle$, as it will keep $|\psi_r\rangle$ strictly normalized, but exerts little control over the norm of $|\phi_r\rangle$. This may pose a serious problem, as the following analysis demonstrates.

Using the parameters (49), trajectories with no jump evolve according to

$$(|\phi_{n,1}(t)\rangle , |\psi_{n,1}(t)\rangle) = (|g\rangle e^{\gamma t}, |e\rangle) ,$$

and the probability of getting a trajectory without jumps up to time $t$ is

$$p_{n,1} = e^{-2\gamma t} .$$

The expectation value

$$g(t) = p_{n,1} \langle \psi_{n,1}(t)|\hat{\sigma}^\dagger|\phi_{n,1}(t)\rangle = e^{-\gamma t}$$

is predicted correctly, but it requires the simulation of at least

$$N_{GZ} \gg p_{n,1}^{-1} = e^{2\gamma t}$$

trajectories to get a statistically significant result. In view of the exponential growth of the right-hand side of Eq. (53), the algorithm (49) is not suited for investigation of the long-time dynamics of $g(t)$.

2. The doubled-Hilbertspace method

A different choice of parameters which is symmetric with respect to $|\psi_r\rangle$ and $|\phi_r\rangle$ is suggested in Ref. [3]:

$$dp = 2dt \left( \langle \psi_r|\hat{\sigma}^\dagger \hat{\sigma}|\psi_r\rangle + \langle \phi_r|\hat{\sigma}^\dagger \hat{\sigma}|\phi_r\rangle \right) , \quad \eta_{1,1} = \eta_{2,1} = \left( \langle \psi_r|\hat{\sigma}^\dagger \hat{\sigma}|\psi_r\rangle + \langle \phi_r|\hat{\sigma}^\dagger \hat{\sigma}|\phi_r\rangle \right)^{-1} ,$$
$$d\xi_{1,1} = d\xi_{2,1} = \langle \psi_r|\hat{\sigma}^\dagger \hat{\sigma}|\psi_r\rangle + \langle \phi_r|\hat{\sigma}^\dagger \hat{\sigma}|\phi_r\rangle , \quad d\mu_{1,1} = d\mu_{2,1} = dt .$$

Note that in this formulation the normalization $\langle \psi_r|\psi_r\rangle + \langle \phi_r|\phi_r\rangle \equiv 1$, which is required for $t = 0$, will be preserved by the dynamics. A more detailed account of this algorithm is given in Appendix A.
For the example of the radiative decay of a 2-level atom, we find that in this algorithm, trajectories with no jumps evolve like
\[
\begin{pmatrix}
|\phi_{nJ}(t)\rangle \\
|\psi_{nJ}(t)\rangle
\end{pmatrix}
= \frac{1}{\sqrt{1 + e^{-2\gamma t}}}
\begin{pmatrix}
|g\rangle \\
|e^{\gamma t}\rangle
\end{pmatrix}.
\] (55)

The probability to simulate such a trajectory is given by
\[
p_{nJ} = \frac{1}{2} (1 + e^{-2\gamma t}).
\] (56)

Therefore, one needs
\[
N_{\text{BKP}} \gg \frac{2}{1 + e^{-2\gamma t}}
\] (57)

trajectories to predict \(g(t)\).

The analysis of the algorithm proposed in [7], which we review in Appendix B, leads to an identical estimate for this example. This is no coincidence, as both algorithms are equivalent for any system where \(\hat{\sigma}|\phi_r\rangle\) and \(\hat{\sigma}|\psi_r\rangle\) are always orthogonal.

The estimate (57), although already much better than Eq. (53), can still be improved, as we shall now demonstrate.

3. The optimized algorithm

If we apply our algorithm, defined by the choice of parameters (45) and (46), to the example of the spontaneously emitting 2-level atom, it turns out that the algorithm degenerates and the evolution becomes deterministic: Trajectories with no jump evolve like
\[
|\phi(t)\rangle = e^{-\frac{\gamma}{2} t} |g\rangle, \quad |\psi(t)\rangle = e^{-\frac{\gamma}{2} t} |e\rangle.
\] (58)

As \(dp\) vanishes for all times, no jumps will ever occur. The trajectory (58) is the only possible one, and the value of the correlation function \(g(t)\),
\[
g(t) = \langle \Psi(t)|\hat{\sigma}|\Phi(t)\rangle = e^{-\gamma t},
\] (59)
is predicted exactly by just this single trajectory.

D. Introduction of a “no-jump-probability”

As it is desirable not to have to check for jumps in every elementary time interval \(dt\), one needs a more efficient way to find the time of the next jump.

We label the jump times by \(\tau_1, \tau_2, \tau_3, \ldots\), and define the quantities \(q_k(t), t > \tau_k\), by
\[
q_k(\tau + t) := P\left(\text{"no jump in } [\tau_k, \tau_k + t]\right),
\] (60)
where \(P\) denotes a probability. Clearly, the \(q_k(t)\) are monotonically decreasing, starting from \(q_k(\tau_k) = 1\), and they obey the differential equation
\[
q_k(t + dt) = q_k(t) (1 - dp(t)).
\] (61)

For the time \(\tau_{k+1}\) of the next jump after the jump at \(\tau_k\), we have for \(t > \tau_k\),
\[
dP(\tau_{k+1} \in [t, t + dt]) = q_k(t) dp(t) = |dq_k(t)|,
\] (62)
(Probability of the jump not occurring before \(t\), multiplied by the probability of any jump occurring in \(dt\)). If \(r\) is a random number with uniform distribution in \([0, 1]\), then we find that for any \(t > \tau_k\),
\[
dP(r \in [q_k(t), q_k(t) + dq_k(t)]) = |dq_k(t)| = dP(\tau_{k+1} \in [t, t + dt]).
\] (63)
The inverse function \(q_k^{-1}(r)\) can therefore be used to map uniformly distributed random numbers \(r \in [0, 1]\) onto jump times \(\tau_{k+1}\) with the correct distribution. This allows to simulate the process (25) by integrating equation (61) in parallel to the continuous branch of (25), and performing a jump whenever \(q_k(t)\) drops below a previously chosen random number \(r \in [0, 1]\).
E. Generalization for arbitrary master equations

If we generalize this to a master equation containing several loss channels, as well as an Hamiltonian interaction,

\[
\frac{d}{dt} \chi(t) = \sum_{k=1}^{n} \left( 2\tilde{\sigma}_k \chi(t) \tilde{\sigma}^\dagger_k - \tilde{\sigma}^\dagger_k \tilde{\sigma}_k \chi(t) - \chi(t) \tilde{\sigma}^\dagger_k \tilde{\sigma}_k - i \left[ \tilde{H}, \chi(t) \right] \right),
\]  

(64)

with

\[
\chi(0) = |\phi(0)\rangle \langle \psi(0)|, 
\]

(65)

we arrive at the following recipe for unraveling:

Initialization:

- Use a gauge transformation \(|\phi(0)\rangle \mapsto c|\phi(0)\rangle, |\psi(0)\rangle \mapsto c^{-1}|\psi(0)\rangle\), such that \(\langle \phi(0)|\phi(0)\rangle = \langle \psi(0)|\psi(0)\rangle\);
- initialize the real-valued auxiliary variable \(q(0) := 1\);
- choose a random number \(r \in [0,1]\).

The continuous evolution between jumps is governed by the following pseudo-linear equations of motion:

\[
\frac{d}{dt} q = -\frac{2}{s} q \sum_{k=1}^{n} \Phi_k \Psi_k, \\
\frac{d}{dt} |\phi_r\rangle = \frac{1}{s} \sum_{k=1}^{n} \left( \Phi_k \Psi_k + \frac{1}{2} \Phi_k^2 - \frac{1}{2} \Psi_k^2 \right) |\phi_r\rangle - \left( \sum_{k=1}^{n} \tilde{\sigma}^\dagger_k \tilde{\sigma}_k + i\tilde{H} \right) |\phi_r\rangle, \\
\frac{d}{dt} |\psi_r\rangle = \frac{1}{s} \sum_{k=1}^{n} \left( \Phi_k \Psi_k - \frac{1}{2} \Phi_k^2 + \frac{1}{2} \Psi_k^2 \right) |\psi_r\rangle - \left( \sum_{k=1}^{n} \tilde{\sigma}^\dagger_k \tilde{\sigma}_k + i\tilde{H} \right) |\psi_r\rangle, 
\]

(66)

where, as above,

\[
s := \langle \phi_r|\phi_r\rangle \equiv \langle \psi_r|\psi_r\rangle, \quad \Phi_k := |\tilde{\sigma}_k|\phi_r\rangle, \quad \Psi_k := |\tilde{\sigma}_k|\psi_r\rangle. 
\]

Whenever the variable \(q\) drops below the previously chosen random number \(r\), a jump occurs according to the following scheme:

- Choose randomly one jump operator \(\tilde{\sigma}_k\) using the statistical weights \(\Phi_k \Psi_k\) for the individual channels;
- apply the following map:

\[
q \mapsto 1, \quad |\phi_r\rangle \mapsto \sqrt{s} \Phi_k \tilde{\sigma}_k |\phi_r\rangle, \quad |\psi_r\rangle \mapsto \sqrt{s} \Psi_k \tilde{\sigma}_k |\psi_r\rangle; 
\]

(68)

- choose a new random number \(r \in [0,1]\).

F. Some properties of the proposed algorithm

From the map (68), it can be seen that jumps have no influence on the norms of \(|\phi_r(t)\rangle\) and \(|\psi_r(t)\rangle\) (which is the local equivalent to the global condition (69)). The continuous evolution, however, will cause the norms to decrease monotonically:

\[
\frac{d}{dt} \langle \phi_r|\phi_r\rangle = 2 \langle \phi_r| \sum_{k=1}^{n} \left( \frac{1}{s} \left( \Phi_k \Psi_k + \frac{1}{2} \Phi_k^2 - \frac{1}{2} \Psi_k^2 \right) - \tilde{\sigma}^\dagger_k \tilde{\sigma}_k \right) |\phi_r\rangle \\
= 2 \sum_{k=1}^{n} \left( \sqrt{\langle \phi_r|\tilde{\sigma}^\dagger_k \tilde{\sigma}_k|\phi_r\rangle \langle \psi_r|\tilde{\sigma}^\dagger_k \tilde{\sigma}_k|\psi_r\rangle} - \frac{1}{2} \left( \langle \phi_r|\tilde{\sigma}^\dagger_k \tilde{\sigma}_k|\phi_r\rangle + \langle \psi_r|\tilde{\sigma}^\dagger_k \tilde{\sigma}_k|\psi_r\rangle \right) \right). 
\]

(69)
From the properties of geometric and arithmetic means, we find:

\[
\frac{d}{dt} \langle \phi_r | \phi_r \rangle = \frac{d}{dt} \langle \psi_r | \psi_r \rangle \leq 0. \tag{70}
\]

According to Eq. 33, the absolute error is bounded from above by \( K^{-1} \langle \phi_r | \phi_r \rangle \langle \psi_r | \psi_r \rangle \), and from Eq. 70 it follows that this upper bound is decreasing with time.

An implementation of our algorithm is available via web-download, see Ref. [11]. In order to demonstrate its reliability, we have simulated the two-time correlation function of a driven 2-level atom. The coupling to the classical driving field is described by the Hamiltonian \( \hat{H} = \frac{i}{2} \Omega (|e\rangle \langle g| + |g\rangle \langle e|) \). Spontaneous emission is described by the Lindblad operator \( \hat{S} \), with \( \hat{S} = \sqrt{2} \langle e | \phi \rangle \langle \phi | e \rangle \). In Fig. 1 we compare the results of our simulation with the exact solution. We find excellent agreement between the results of the simulation and the exact formula for both the correlation function. A somewhat larger model system is considered in the next section.

IV. THE OPTICAL PARAMETRIC OSCILLATOR

We consider a system of two resonant optical modes \( \hat{a}_1 \) (fundamental) and \( \hat{a}_2 \) (second harmonic), interacting in a \( \chi^{(2)} \)-medium via the Hamiltonian

\[
\hat{H}_I = i \frac{\kappa}{2} \left( \hat{a}_1^\dagger \hat{a}_2^\dagger - \hat{a}_2 \hat{a}_1 \right), \tag{71}
\]

where \( \kappa \) is the coupling constant. The second harmonic mode is pumped by a coherent field of amplitude \( \epsilon \):

\[
\hat{H}_P = i \left( \epsilon \hat{a}_2^\dagger - \epsilon^* \hat{a}_2 \right), \tag{72}
\]

and both modes are damped, with rates \( \gamma_1 \) and \( \gamma_2 \), respectively:

\[
\mathcal{L} \hat{\rho} = \gamma_1 \left( 2 \hat{a}_1 \hat{a}_1^\dagger - \hat{a}_1^\dagger \hat{a}_1 - \hat{p}_1 \hat{p}_1^\dagger + \hat{p}_1^\dagger \hat{p}_1 \right) + \gamma_2 \left( 2 \hat{a}_2 \hat{a}_2^\dagger - \hat{a}_2^\dagger \hat{a}_2 - \hat{p}_2 \hat{p}_2^\dagger + \hat{p}_2^\dagger \hat{p}_2 \right). \tag{73}
\]

A detailed discussion of this system can be found in Ref. [12]. For pump field amplitudes above the threshold \( \epsilon_{th} = \gamma_1 \gamma_2 / \kappa \), there exist two classical steady state solutions for the fundamental mode amplitude:

\[
\alpha_1 = \pm \sqrt{\frac{2}{\kappa} \frac{\epsilon - \epsilon_{th}}{\kappa}}. \tag{74}
\]

The quantum state resembles this classical solution: above threshold, the Wigner function consists of two peaks close to the classical solutions. The superposition of these peaks is incoherent, so the steady state is a classical mixture of two states both of which are well localized and have a well-defined quantum phase. However, tunneling between the two stable states is possible, corresponding to a change of the phase angle by \( \pi \). Therefore, above threshold the tunneling events will be the main reason for the decay of the correlation function \( g(t) := \frac{\langle a_1^\dagger(t) a_2 \rangle}{\langle a_1^\dagger a_2 \rangle} \) in the long-time regime. Following [13], the tunneling is modeled to be a telegraph noise process with a characteristic time \( T \), which leads to an exponential decay

\[
g(t) = e^{- \frac{t}{T}}. \tag{75}
\]

By adiabatic elimination of the second harmonic mode (the pump mode), which is a good approximation only in the case of a rapidly decaying pump mode, i. e. for \( \gamma_2 \gg \gamma_1 \), Kinsler and Drummond [13] found the following analytical expression for the tunneling time \( T \):

\[
T \approx \frac{\pi}{\gamma_1} \sqrt{\frac{\lambda + \sigma}{\lambda(\lambda - \sigma)^2}} \exp \left\{ \frac{2}{G^2} \left[ \lambda - \sigma - \sigma \ln \left( \frac{\lambda}{\sigma} \right) \right] \right\}. \tag{76}
\]

where \( \lambda := \epsilon / \epsilon_{th} \) is the normalized pump field amplitude, \( G := \kappa \sqrt{2 \gamma_1 \gamma_2}^{-1} \) is the scaled coupling constant, and \( \sigma := 1 - G^2 / 2 \). Eq. (76) is obtained in the “potential-barrier approximation” which is valid in the limit of large threshold photon numbers, i. e., for \( G \ll 1 \), and a large potential barrier, i. e., it fails for \( \lambda \) very close to or below the threshold \( \lambda = 1 \).
We carried out numerical simulations of the full quantum dynamics specified in Eqs. (71-73), i.e., without adiabatic elimination of the pump mode, using a truncated number state representation of the state vectors. Classical analysis predicts a photon number $N_2 = 1$ for the pump mode above threshold, and $N_1 = 8$ for the fundamental mode at $\lambda = 2$ for the chosen values $\gamma_1 = \kappa$, $\gamma_2 = 4\kappa$. Since photon number fluctuations are enhanced by the nonlinear interaction, the truncation values of a number state representation have to be chosen considerably higher than these values. We used truncation values for the fundamental mode between a photon number $N_1 = 24$ for $\lambda \approx 1$, and $N_1 = 48$ for $\lambda \approx 2$. Tests with truncation values up to $N_1 = 64$ indicated that no significant error was caused by this truncation. The Hilbert space of the second harmonic mode was truncated at a photon number $N_2 = 16$.

Results of our numerical simulations of $g(t)$ are depicted in Fig. 2 and Fig. 3. Quite generally, $g(t)$ displays a fast transient, which decays on a small time scale $\propto \kappa \epsilon \gamma_2^{-1}$, followed by a slow exponential decay $\propto \exp(-2t/T)$ which governs the behavior of $g(t)$ in the limit $t \to \infty$.

In Fig. 3 we depict the tunneling times $T$ which we extracted from our numerical data as a function of the normalized pump field amplitude $\lambda$. We see a good agreement between our simulation and the prediction of Eq. (76), for intermediate values of $\lambda$. For larger values of $\lambda$, the tunneling times predicted by our simulations are consistently shorter than predicted by Eq. (76). This may be due to the full quantum dynamics of the pump mode which is taken into account in our simulations.

V. SUMMARY

We have derived an efficient method for the numerical simulation of quantum mechanical two-time correlation functions which is based on stochastic wave function propagation. In comparison with other algorithms, our algorithm was demonstrated to be generally more efficient, i.e., requiring less runs for a reliable prediction of $g(t)$. We have successfully applied our method for the simulation of $g(t)$ of a nonlinear optical parametric oscillator.

The tests indicate that our algorithm is stable and efficient, even for “large” (i.e., having large Hilbert spaces) problems: despite the seemingly more complicated pseudolinear equations of motion (66), a proper implementation need not be slower but can be of of faster convergence than previously published algorithms. This stems from the fact that the most time consuming operations are the application of operators to vectors (operations of the type “matrix times vector”), and all algorithms require the computation of $\hat{\sigma}_k^\dagger \hat{\sigma}_k \langle \Phi |$ and $\hat{\sigma}_k^\dagger \hat{\sigma}_k \langle \Psi |$ for every computation of a time derivative to be used in the numerical integration of the continuous (no-jump) part of the evolution. All other quantities required in our algorithm can be obtained by computing scalar products of vectors and purely scalar operations, which are comparatively cheap operations.

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APPENDIX A: THE DOUBLED-HILBERTSPACE METHOD

The algorithm proposed in [9] is based on the observation, that the problem of propagating the skew-symmetric $\hat{\chi}(t)$, as defined in Sec. IIIA, can be reduced to solving a master equation for a positive symmetric operator in a Hilbert space of twice the dimension of the original space.

The new density operator $\hat{\Omega}(t)$ in this doubled space is defined by the initial condition

$$\hat{\Omega}(0) = \left( \begin{array}{cc} |\phi(0)\rangle \langle \phi(0)| & |\phi(0)\rangle \langle \psi(0)| \\ |\psi(0)\rangle \langle \phi(0)| & |\psi(0)\rangle \langle \psi(0)| \end{array} \right)$$

(A1)

and the equation of motion

$$\frac{d}{dt} \hat{\Omega}(t) = \mathcal{L} \hat{\Omega}(t) := \left( \begin{array}{cc} L & 0 \\ 0 & L \end{array} \right) \hat{\Omega}(t).$$

(A2)

The superoperator $\mathcal{L}$ is again a Lindblad operator:

$$\mathcal{L} \hat{\Omega} = 2\hat{\Sigma}^\dagger \hat{\Omega} \hat{\Sigma} - \hat{\Sigma}^\dagger \hat{\Sigma} \hat{\Omega} - \hat{\Omega} \hat{\Sigma}^\dagger \hat{\Sigma},$$

(A3)
where
\[ \hat{\Sigma} := \left( \begin{array}{cc} \hat{\sigma} & 0 \\ 0 & \hat{\sigma} \end{array} \right). \] (A4)
The initial value \( \hat{\Omega}(0) \) can be written as a symmetric dyadic product,
\[ \hat{\Omega}(0) = |\Upsilon(0)\rangle \langle \Upsilon(0)|, \] (A5)
where
\[ |\Upsilon(0)\rangle = \left( \begin{array}{c} |\phi(0)\rangle \\ |\psi(0)\rangle \end{array} \right) \] is a normalized pure state in the doubled Hilbert space. Standard algorithms can now be used to unravel (A2) into a stochastic process for a state vector \( |\Upsilon_r(t)\rangle \) in this doubled Hilbert space, e. g. the jump algorithm (18) can be used:
\[ |d\Upsilon_r(t)\rangle = \begin{cases} \left( -1 + \hat{\Sigma} |\Upsilon_r(t)\rangle \right)^{-1} \hat{\Sigma} |\Upsilon_r(t)\rangle, & dp = 2dt \langle \Upsilon_r(t)|\hat{\Sigma}^\dagger \hat{\Sigma}|\Upsilon_r(t)\rangle, \\ \left( \langle \Upsilon_r(t)|\hat{\Sigma}^\dagger \hat{\Sigma}|\Upsilon_r(t)\rangle - \hat{\Sigma}^\dagger \hat{\Sigma} \right) dt |\Upsilon_r(t)\rangle, & 1 - dp. \end{cases} \] (A7)
The jump probability is computed as the arithmetic mean,
\[ dp = 2dt \langle \Upsilon_r(t)|\hat{\Sigma}^\dagger \hat{\Sigma}|\Upsilon_r(t)\rangle = 2dt \left( \langle \phi_r(t)|\hat{\sigma}^\dagger \hat{\sigma}|\phi_r(t)\rangle + \langle \psi_r(t)|\hat{\sigma}^\dagger \hat{\sigma}|\psi_r(t)\rangle \right), \] (A8)
as opposed to the geometric mean suggested in our algorithm (15). However, unlike (19), this algorithm is symmetric with respect to the two components \( |\phi_r(t)\rangle \) and \( |\psi_r(t)\rangle \). Moreover, the condition
\[ \langle \phi_r(t)|\phi_r(t)\rangle + \langle \psi_r(t)|\psi_r(t)\rangle = 1, \] (A9)
which is the proper normalization of vectors in the doubled Hilbert space, will be fulfilled for all realizations, so exponential growth of the norm of one of the vectors as in (50) cannot occur.

Noteworthy, the condition (A9) is actually more restrictive than necessary: in the doubled Hilbert space, we are only interested in expectation values of operators of the Form
\[ \mathcal{A} = \left( \begin{array}{cc} 0 & 0 \\ A & 0 \end{array} \right); \] (A10)
in particular, the expectation value of the identity operator
\[ \mathcal{I} = \left( \begin{array}{cc} \mathbb{I} & 0 \\ 0 & \mathbb{I} \end{array} \right) \] (A11)
is irrelevant, and norm conservation in the stochastic average,
\[ \langle \phi_r(t)|\phi_r(t)\rangle + \langle \psi_r(t)|\psi_r(t)\rangle = 1, \] (A12)
is not required. Therefore, condition (A9) is less well justified than the corresponding condition (13) in the unraveling of master equation (7) for a symmetric operator, and we believe that it should be replaced by condition (40).

2 Consequently, a constant factor must usually be applied when computing expectation values, to compensate for this normalization.
APPENDIX B: THE MöLMER-CASTIN-DALIBARD ALGORITHM

Already in [7], the following stochastic jump process was proposed (although formulated as in Eq. (B2)):

\[
\begin{align*}
\left( \frac{d\phi_r(t)}{dt} \right) &= \left( -1 + |\hat{\sigma} \psi_r(t) + \nu \phi_r(t)|^{-1} \hat{\Sigma} \right) \left( \frac{\phi_r(t)}{\psi_r(t)} \right), & dp &= 2 dt |\hat{\sigma} \psi_r(t) + \nu \phi_r(t)|^2 \\
\left( \frac{d\psi_r(t)}{dt} \right) &= \left( |\hat{\sigma} \psi_r(t) + \nu \phi_r(t)|^2 - \hat{\Sigma}^\dagger \hat{\Sigma} \right) dt \left( \frac{\phi_r(t)}{\psi_r(t)} \right), & 1 - dp
\end{align*}
\]  

(B1)

Here, \( \nu \) is a phase factor with \( |\nu| = 1 \), \( \hat{\Sigma} \) is the operator defined in Eq. (A4), and we use the abbreviation \( |\phi_r(t) + \nu \psi_r(t)| = |\phi_r(t)| + \nu |\psi_r(t)| \). The vectors are normalized such that \( ||\phi_r(t) + \nu \psi_r(t)|| = 1 \); it is easy to verify that the process (B1) will conserve this normalization. In the original formulation of this method [7], it was suggested not to propagate the pair \( (|\psi_r(t)|, |\phi_r(t)|) \), but the linear combination \( |\psi_{\nu,r}(t)| = |\phi_r(t) + \nu \psi_r(t)| \); this is possible, as all coefficients appearing in both branches of Eq. (B1), as well as the jump probability \( dp \), are functionals of \( |\psi_{\nu,r}(t)| \), and we can write:

\[
\begin{align*}
\left| \frac{d\psi_{\nu,r}(t)}{dt} \right| &= \left\{ \left( -1 + |\hat{\sigma} |\psi_{\nu,r}(t)|^{-1} \hat{\sigma} \right) |\phi_{\nu,r}(t)|, & dp &= 2 dt |\hat{\sigma} |\psi_{\nu,r}(t)|^2 \\
\left( \frac{d\psi_{\nu,r}(t)}{dt} \right) &= \left( |\hat{\sigma} |\psi_{\nu,r}(t)|^2 - \hat{\Sigma}^\dagger \hat{\Sigma} \right) dt |\phi_{\nu,r}(t)|, & 1 - dp
\end{align*}
\]  

(B2)

However, merging of both vectors \( |\psi_r| \) and \( |\phi_r| \) into one only allows for a simulation of

\[
\hat{\chi}_\nu(t) := \frac{\langle \psi_{\nu,r}(t) | \psi_{\nu,r}(t) \rangle}{|\psi_{\nu,r}(t)|^2} = \frac{\langle \psi_{\nu,r}(t) | \psi_{\nu,r}(t) \rangle}{|\psi_{\nu,r}(t)|^2} + \nu \langle \psi_{\nu,r}(t) | \phi_{\nu,r}(t) \rangle + \nu^* \langle \psi_{\nu,r}(t) | \phi_{\nu,r}(t) \rangle + |\phi_{\nu,r}(t)|^2.
\]  

(B3)

To extract the quantity of interest, \( \hat{\chi}(t) = \frac{1}{4} \langle \phi_{\nu,r}(t) | \psi_{\nu,r}(t) \rangle \), one has to perform the simulation for four different values of \( \nu \):

\[
\hat{\chi}(t) = \frac{1}{4} \left( \hat{\chi}_{+1}(t) - \hat{\chi}_{-1}(t) - i \hat{\chi}_{+i}(t) + i \hat{\chi}_{-i}(t) \right).
\]  

(B4)

Since (B2) is just the simple jump process (B3), applied to \( |\psi_{\nu,r}(t)| \), the problem of propagating the skew object \( \hat{\chi}(t) \) has been reduced to the problem of unraveling 4 proper, positive definite density operators.

Clearly, the extra work can be avoided (at the cost of having to propagate two separate vectors instead of a single one) by not merging the vectors and using the stochastic process (B1) directly.

APPENDIX C: A CONCEIVABLE IMPROVEMENT WHICH TURNS OUT TO FAIL

The algorithm derived in Sec. IIIA was based on the requirement to simulate all operators of the type (A10), disregarding more general operators in the doubled Hilbert space.

If all we want to compute is the expectation value

\[
g(t) = \langle \psi_r(t) | \hat{A} | \phi_r(t) \rangle
\]  

(C1)

for just one special operator \( \hat{A} \), we could ask whether one can formulate an even more specialized algorithm fitted to exactly this problem. More specifically, instead of the error (B2) of the estimate of the skew operator \( \hat{\chi} \), we could wish that the mean square of the error of our estimate of \( g(t) \) should be minimized. Again, we cannot obtain the global minimum and have to resort to a local condition, analogous to Eq. (10):

\[
\forall \langle \phi \rangle, \langle \psi \rangle : \frac{d}{dt} \left| \langle \psi | \hat{A} | \phi \rangle \right|^2 = \text{minimal}.
\]  

(C2)

An algorithm fulfilling (C2) can be derived in much the same way as from Eq. (10). In particular, the corresponding jump probability is:
\[
dp = 2 \sum_{k=1}^{n} \left| \frac{\langle \psi_r | \hat{\sigma}_k^\dagger \hat{A} \hat{\sigma}_k | \phi_r \rangle}{\langle \psi_r | \hat{A} | \phi_r \rangle} \right| dt. \tag{C3}
\]

Jumps will not change the value of \(|g_r(t)|\) in this algorithm. At first glance, this method looks promising: when applied to the simulation of the correlation function \(g(t) = \langle \hat{\sigma}^\dagger \hat{\sigma} \rangle\) of a 2-level atom, then we have to choose \(\hat{A} \equiv \hat{\sigma}^\dagger\) and \(\hat{\sigma} \hat{\sigma}^\dagger \equiv 0\). Therefore, no jumps will ever occur for any states \(|\phi_r\rangle, |\psi_r\rangle\), and the algorithm becomes deterministic even for the driven 2-level atom. Unfortunately, the results will be incorrect. In general, the method derived from condition \((C2)\) turns out to be highly unstable at best, and produces completely wrong results in some cases. This happens because it does not possess a property analogous to \((70)\); rather, \(|g_r(t)|^2\) may very well grow large for certain trajectories during the deterministic continuous evolution. Moreover, the algorithm will completely avoid to jump into states for which \(g_r(t)\) vanishes, although such states can be important as \(g_r(t)\) may very well take on finite values at a later time.

\[3\] Even the phase of \(g_r(t)\) can be conserved if we relax the requirement of our parameters \(\eta_{1,3}\) and \(\eta_{2,3}\) to be real-valued.
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FIG. 1. Time evolution of the correlation function $g(t) = \langle \hat{\sigma}^\dagger(t)\hat{\sigma} \rangle$ for the driven 2-level atom, with $\Omega = 8\gamma$. The inset shows the corresponding spectrum. The solid line is the result of a Monte Carlo simulation with 5000 trajectories, while the crosses represent exact analytical values.
FIG. 2. The correlation function $g(t)$ of the optical parametric oscillator for system parameters $\gamma_1 = \kappa = 1$, $\gamma_2 = 4\kappa$, and a normalized pump amplitude $\lambda = \frac{\kappa}{\kappa_{th}} = 2.0$, derived from 500 simulated trajectories. The inset displays a close-up view for different values of $\lambda$, showing the fast initial decay before the slow tunneling regime.

FIG. 3. Comparison of numerical values for the tunneling times of the optical parametric oscillator and the analytical approximation for system parameters as in Fig. 2.