Moment hierarchies and cumulants in quantum optics

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Nonlinear problems in quantum optics can be described by an infinite hierarchy of ordinary differential equations for the moments. We discuss different truncation schemes involving cumulants. For illustration the method is applied to second-harmonic generation. We prove that all but second-order cumulants are equal for any quasiprobability distribution P_s , especially for the P, Q, and W functions.

I. INTRODUCTION

Nonlinear processes are among the most interesting problems in quantum optics and have been discussed by many authors. Optical bistability¹ or subharmonic generation² are only two important examples. Unfortunately, there exists no general computational method to solve these problems. Very few exact solutions are known. Linearization works only well away from threshold. Matrix continued fractions,³ though very successful in many cases,⁴ cannot be used for problems involving more than a single complex field mode. The complex *P* representation⁵ has been applied successfully only to some special systems. Finally, the positive *P* representation,⁵ a method designed to work in a straightforward fashion, still awaits an explanation of the wrong results it gives for some particular models.⁶⁻⁸

We want to discuss another approach, based on moment hierarchies, which, though it shares the property that it does not work in all cases, sometimes can be applied with success where all other methods fail.

The paper is organized as follows. Section II introduces the notion of moment hierarchies for different operator orderings and shows relations between them. In Sec. III we review the Gaussian approximation which consists in assuming that only first- and second-order cumulants are nonzero. Cumulants corresponding to operator products of different ordering are defined. Section IV extends the approximation to higher orders. The consistency of this approach as well as its limits are discussed. In Sec. V we try to find an improved approximation by considering different orderings, which leads to a theorem about cumulants. A proof is given as well as some implications. In Sec. VI, we apply the method to second-harmonic generation, a problem which is unsolved so far in the parameter regime we consider.

II. MOMENT HIERARCHIES

Our starting point is a master equation for the density matrix ρ where the atomic degrees of freedom have been adiabatically eliminated:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [H,\rho] + \left[\frac{d\rho}{dt} \right]_{\rm irr} . \tag{1}$$

The Hamiltonian H describes the linear and nonlinear interactions between the field modes, whereas the irreversible term includes damping via the interaction with an external reservoir. An example for the explicit form of Hand $(d\rho/dt)_{irr}$ can be found in Sec. VI.

In general, it is impossible to solve the operator equation (1) directly, except for some simple cases. If ρ is expanded in Fock states in the case of two field modes, even moderate photon numbers will lead to matrices that do not fit into the memory of the biggest computer. This is why one introduces the concept of quasiprobabilities. Being *c*-number functions, they obey partial differential equations of the following form:

$$\frac{\partial}{\partial t} P_{s}(\alpha, \alpha^{*}, t) = \left(\frac{\partial}{\partial \alpha} (\cdots) + \frac{\partial}{\partial \alpha^{*}} (\cdots) + \frac{\partial^{2}}{\partial \alpha^{2}} (\cdots) + \cdots \right) + \cdots \right) P_{s}(\alpha, \alpha^{*}, t) , \qquad (2)$$

where P_s stands for the one-parameter family of general quasiprobability distributions introduced by Cahill and Glauber,⁹ and the complex variable α corresponds to a field mode described by Bose operators a and a^{\dagger} . Equation (2) is easily generalized to more than one field mode (Sec. VI).

 P_s can be used to calculate the following expectation values:

$$\langle [a^{\dagger m} a^{n}]_{s} \rangle(t) = \langle \alpha^{*m} \alpha^{n} \rangle_{P_{s}}(t)$$

$$= \int d^{2} \alpha \, \alpha^{*m} \alpha^{n} P_{s}(\alpha, \alpha^{*}, t) , \qquad (3)$$

where the s-ordered operator products $[a^{\dagger m}a^n]_s$ are defined as

$$[a^{\dagger m}a^{n}]_{s} = \frac{\partial^{m}}{\partial (i\beta^{*})^{m}} \frac{\partial^{n}}{\partial (i\beta)^{n}} \times e^{i\beta^{*}a^{\dagger} + i\beta a - (s/2)\beta\beta^{*}} \Big|_{\beta = \beta^{*} = 0}.$$
 (4)

The expression $[a^{\dagger m}a^n]_0$ is called the symmetrically ordered product, and the corresponding quasiprobability $W(\alpha) = P_0(\alpha)$ is the Wigner function. Using the Baker-Haussdorf theorem, one finds normal ordering for s = -1

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$$[a^{\dagger m}a^{n}]_{-1} = \frac{\partial^{m}}{\partial (i\beta^{*})^{m}} \frac{\partial^{n}}{\partial (i\beta)^{n}} e^{i\beta^{*}a^{\dagger}} e^{i\beta a} \bigg|_{\beta=\beta^{*}=0}$$
$$= a^{\dagger m}a^{n}, \qquad (5)$$

and antinormal ordering for s = +1

$$[a^{\dagger m}a^{n}]_{1} = \frac{\partial^{m}}{\partial(i\beta^{*})^{m}} \frac{\partial^{n}}{\partial(i\beta)^{n}} e^{i\beta a} e^{i\beta^{*}a^{\dagger}} \bigg|_{\beta=\beta^{*}=0}$$
$$= a^{n}a^{\dagger m}.$$
(6)

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Normally and antinormally ordered products are related to the diagonal P function $P(\alpha) = \pi^{-1}P_{-1}(\alpha)$ and to $Q(\alpha) = P_1(\alpha)$, respectively.

With the appropriate choice of P_s , we can now use partial integration to derive from Eq. (2) hierarchies of linear ordinary differential equations for moments of any ordering. For the diagonal P function, we get

$$\frac{d}{dt}\langle \alpha^{*m}\alpha^{n}\rangle_{P} = \frac{d}{dt}\langle a^{\dagger m}a^{n}\rangle = \sum_{i,j} c_{ij}^{mn}\langle \alpha^{*i}\alpha^{j}\rangle_{P} , \quad (7)$$

and for the Q function

$$\frac{d}{dt} \langle \alpha^{*m} \alpha^n \rangle_Q = \frac{d}{dt} \langle a^n a^{\dagger m} \rangle = \sum_{i,j} d_{ij}^{mn} \langle \alpha^{*i} \alpha^j \rangle_Q .$$
(8)

At first glance, it might appear confusing that one can transform a general nonlinear problem into a set of linear equations like (7) or (8). But the important point is that these sets are infinite, which means that one cannot solve them using the standard theory of linear initial value problems. In fact, no general method of solution is known. The method of Carleman embedding¹⁰ can be used only in some special cases. So one must try to find a suitable approximation scheme, which is the purpose of Secs. III and IV.

Moment hierarchies like Eqs. (7) and (8) can also be derived directly from the master equation (1). One only has to remember the definition of expectation values in terms of the density matrix ρ , e.g.,

$$\frac{d}{dt}\langle a^n a^{\dagger m}\rangle = \frac{d}{dt} \operatorname{Tr}(\rho a^n a^{\dagger m}) = \operatorname{Tr}\left[\frac{d\rho}{dt} a^n a^{\dagger m}\right] . \tag{9}$$

This means that Eqs. (7) and (8) must be equivalent, although they may look quite different. It is always possible to calculate the coefficients c_{ij}^{mn} from the d_{ij}^{mn} and vice versa by using the commutation relations between a and a^{\dagger} . In the general case, when arbitrary powers of a and a^{\dagger} are involved, the following explicit formulas are helpful:

$$a^{\dagger m} a^{n} = \sum_{k=0}^{\min(m,n)} (-1)^{k} k! \binom{m}{k} \binom{n}{k} a^{n-k} a^{\dagger m-k} ,$$

$$a^{n} a^{\dagger m} = \sum_{k=0}^{\min(m,n)} k! \binom{m}{k} \binom{n}{k} a^{\dagger m-k} a^{n-k} .$$
(10)

These formulas, which can be proven by induction, do not appear to be in the literature. Similar results hold for any operator ordering, i.e., for any P_s .

If we use the positive P representation P_P instead of the diagonal P, the only thing which changes in Eqs. (2) and (3) is that we have to replace α^* by the independent variable β and P by P_P . Therefore, the moment hierarchy derived from the positive P representation is identical to Eq. (7), which is a general result. In a recent publication,¹¹ this was derived only for mean and variance and only in a linearized approach. From this, the authors conclude that the use of P_P instead of the diagonal Ppresents no advantage. This, of course, is true only in the framework of linearization, because one can find exact solutions to linearized problems in any representation (see Ref. 12 for an example where P is expressed in terms of distributions). But until now, little has been known that could be used as a general tool to treat nonlinear problems including quantum noise, which is the aim of the positive P representation. In cases where the Hamiltonian H is at most bilinear in the fields, the problem is linear and Eq. (7) does not link moments on the left-hand side to higher-order moments on the right-hand side. So, for any order, one obtains a closed finite system of linear equations for which an exact solution can immediately be written down. As was already mentioned above, only very few exact solutions to infinite hierarchies are known. This means that in the general case, we have to recur to some simplifying assumption in order to truncate the hierachy. Such a truncation procedure will turn the problem from an infinite set of linear equations into a finite set of nonlinear equations which can be solved numerically by some standard algorithm for initial value problems.

III. GAUSSIAN APPROXIMATION

Let us first define *s*-ordered cumulants. They are denoted by double brackets in order to stress the close formal analogy to the definition of the corresponding moments:

$$\langle \langle [a^{\dagger m} a^{n}]_{s} \rangle \rangle = \langle \langle \alpha^{* m} \alpha^{n} \rangle \rangle_{P_{s}}$$
$$= \frac{\partial^{m}}{\partial (i\beta^{*})^{m}} \frac{\partial^{n}}{\partial (i\beta)^{n}}$$
$$\times \ln[\chi_{P_{s}}(\beta,\beta^{*})] \Big|_{\beta=\beta^{*}=0}.$$
(11)

Here, χ_P denotes the family of characteristic functions:

$$\chi_{P_{s}}(\beta,\beta^{*}) = \operatorname{Tr}(e^{i\beta^{*}a^{\top} + i\beta a - (s/2)\beta\beta^{*}}\rho)$$
$$= \int d^{2}\alpha \, e^{i\beta^{*}\alpha^{*} + i\beta\alpha} P_{s}(\alpha,\alpha^{*}) \,. \tag{12}$$

Cumulants of order n can be expressed by moments of order less or equal to n. An example for a normally ordered cumulant is

$$\langle \langle a^{\dagger 2}a \rangle \rangle = \langle a^{\dagger 2}a \rangle - 2 \langle a^{\dagger} \rangle \langle a^{\dagger}a \rangle - \langle a^{\dagger 2} \rangle \langle a \rangle + 2 \langle a^{\dagger} \rangle^{2} \langle a \rangle .$$
(13)

One method of truncation of Eq. (7) consists in assuming that P is a generalized Gaussian at all times.¹³ By generalized Gaussian we mean a distribution which is not

necessarily Gaussian, but which has a Gaussian Fourier transform. For such a distribution, only the first- and second-order cumulants are nonzero. The vanishing of all cumulants higher than second order now means that we can express all moments of order higher than two by first- and second-order ones. So, we get a closed set of equations for the mean and variance of our distribution. These equations are nonlinear. From this it follows that the Gaussian approximation is not equivalent to a linearization where we would also get a Gaussian distribution, but with mean and variance obeying linear equations. So we expect the truncated set of equations to be able to describe a more general behavior than linearization.

One could ask which kind of partial differential equation corresponds to this truncated set of equations. However, it is easily shown that in the general case, the assumed time-dependent Gaussian distribution does not even obey a generalized Fokker-Planck equation containing higher-order derivatives.

This crude approximation works astonishingly well even in cases where the distribution is quite far from being Gaussian, e.g., where it is doubly peaked. On the other hand, there is presently no known way to predict whether it will work for a particular problem or not. More precisely, one does not know how to estimate the numerical error one makes when using it.

An example where it does not work is shown in Sec. VI. The question how the truncation scheme can be improved is explored in the following two sections.

not be a quasiprobability, as it was the case for the Gaussian approximation.

Of course, this does not mean that higher-order truncation is always a bad approximation. For example, a function which assumes small negative values in some restricted interval can be an excellent approximation to a probability distribution for many purposes. Although higher-order truncation has no systematic mathematical foundation, it can be justified by the often very good results it gives. These can be checked in cases where independent methods of solution are known. In Sec. VI the method is applied to the problem of second-harmonic generation. Unphysical features of the Gaussian approximation to this problem, e.g., that the solutions do not become stationary, are removed if the order of truncation is increased. As in the parameter regime we consider, i.e., above the bifurcation to a limit cycle in classical dynamics, no other method has been applied successfully, the truncated moment hierarchy proves to be a useful tool. Since the size of the equations becomes very large for more than one field and for higher orders, a symbolic manipulation program for performing the tedious calculations is almost indispensible.

In cases where the distribution is suspected to be sharply peaked at a single point, the assumption that higher-order moments simply factorize can lead to a valid truncation scheme. Reference 17 compares both schemes in a simple one-dimensional case.

IV. HIGHER-ORDER APPROXIMATION

It is tempting to extend the method described above by allowing for nonzero third-order cumulants and setting equal to zero fourth- and higher-order ones. We will talk about "*n*th order truncation" if n is the order of the highest nonvanishing cumulants. In this sense, the Gaussian approximation is a second-order truncation. Third-order truncation is discussed for the field of turbulence theory in Ref. 14; there it is called "quasi-normal approximation."

One intuitive justification of higher-order truncation comes from the idea that in a physical system, correlations should become less important with increasing order. This should be reflected by cumulants becoming smaller with increasing order. Unfortunately, this is not true in all cases, as is shown by an example in Ref. 3.

Another difficulty is related to the Marcinkiewicz theorem.¹⁵ This theorem states that a function with a finite cumulant expansion cannot be positive if the order of the highest nonvanishing cumulant is larger than 2. This alone would not imply that such a function cannot be a quasiprobability because quasiprobabilities are not necessarily positive. However, there exists a generalization of the Marcinkiewicz theorem¹⁶ which can be put in the following form: a quasiprobability with a finite cumulant expansion must be a generalized Gaussian. For a simple proof of this generalization, see Sec. V. In other words, any higher-order truncation is inconsistent in the sense that the underlying approximate distribution can-

V. CUMULANTS AND COMMUTATION RELATIONS

In Sec. II we had seen that the moment hierarchies for the P function [Eq. (7)] and for the Q function [Eq. (8)] are equivalent. As it is well known that the Q function is usually smooth and much better behaved than the P function, one could come to think that Q is better approximated by a Gaussian than P, and expect to get a better approximation by setting equal to zero Q cumulants than by setting equal to zero P cumulants as it is done in Sec. VI. The use of Q would imply that one has to work with antinormally ordered products. However, physically measurable quantities which correspond to normal ordering can easily be obtained from the latter, e.g., with the help of Eq. (10).

But if one works out this idea for a particular problem, e.g., in the case of Sec. VI, one finds a surprising result. After applying the commutation relations, one gets exactly the same numerical values for the moments as before. Both approximation schemes are completely equivalent. The following theorem shows that this is a general feature.

Theorem. Only the second-order cumulants $\langle \langle [a^{\dagger}a]_s \rangle \rangle$ depend on the ordering parameter s. All the other cumulants are identical for different values of s. More specifically,

$$\langle \langle [a^{\dagger}a]_{s} \rangle \rangle = \frac{1}{2}(1-s)\langle a^{\dagger}a \rangle + \frac{1}{2}(1+s)\langle aa^{\dagger} \rangle - \langle a^{\dagger} \rangle \langle a \rangle$$

for any $s (-1 \le s \le 1)$ (14)

and

$$\langle \langle [a^{\dagger m} a^n]_s \rangle \rangle = \langle \langle [a^{\dagger m} a^n]_{s'} \rangle \rangle$$

for any $s, s' \ (-1 \le s, s' \le 1)$ if $n \ne 1$ or $m \ne 1$.
(15)

The quasiprobability functions P_s , in particular P, W, and Q, therefore differ only in their second-order cumulants. A generalization to more than one field is straightforward.

The next example is given to illustrate the theorem. We write down the definition of an antinormally ordered third-order cumulant, e.g.,

$$\langle \langle aa^{\dagger 2} \rangle \rangle = \langle aa^{\dagger 2} \rangle - 2 \langle aa^{\dagger} \rangle \langle a^{\dagger} \rangle - \langle a \rangle \langle a^{\dagger 2} \rangle + 2 \langle a \rangle \langle a^{\dagger} \rangle^{2} .$$

then we apply the commutation relation in the first and second term

$$\langle\langle aa^{\dagger 2} \rangle\rangle = \langle a^{\dagger 2}a + 2a^{\dagger} \rangle - 2\langle a^{\dagger}a + 1 \rangle \langle a^{\dagger} \rangle - \langle a \rangle \langle a^{\dagger 2} \rangle + 2\langle a \rangle \langle a^{\dagger} \rangle^{2} ,$$

and after noticing that the additional terms cancel, we rediscover the definition of the normally ordered cumulant [Eq. (13)]

$$\langle\langle aa^{\dagger 2}\rangle\rangle = \langle\langle a^{\dagger 2}a\rangle\rangle$$

This, at first glance, is an astonishing result as the definition of cumulants has nothing to do with quantum mechanics and commutation relations. However, the proof is very short.

Proof. Equation (15) follows immediately after inserting Eq. (12) into Eq. (11):

$$\langle \langle [a^{\dagger m} a^{n}]_{s} \rangle \rangle = \frac{\partial m}{\partial (i\beta^{*})^{m}} \frac{\partial n}{\partial (i\beta)^{n}} \\ \times [-(s/2)\beta\beta^{*} + \ln \operatorname{Tr}(e^{i\beta^{*}a^{\dagger} + i\beta a}\rho)]_{\beta=\beta^{*}=0}.$$
(16)

For n = m = 1 one finds

$$\langle \langle [a^{\dagger}a]_{s} \rangle \rangle = s/2 + \langle \langle [a^{\dagger}a]_{0} \rangle \rangle$$

$$= s/2 + \langle \langle a^{\dagger}a + \frac{1}{2} \rangle \rangle$$

$$= (s+1)/2 + \langle a^{\dagger}a \rangle - \langle a^{\dagger} \rangle \langle a \rangle$$

which is equivalent to Eq. (14).

This theorem has some interesting implications.

(i) The singularities that are often encountered when using the diagonal P function do not reflect any higherorder effects. They are entirely due to negative secondorder cumulants, i.e., negative variances. We do not expect any new insight when switching between the singular P and the very smooth Q. The choice of a particular P_s is entirely a question of taste.

(ii) There still remains some doubt whether it is consistent to keep third-order derivatives in the partial differential equation for the Wigner function W [Eq. (2)] when performing a linearization. This procedure presents no difficulty when performed for the P function for which one gets either a Gaussian or a generalized Gaussian, i.e., a function with a cumulant expansion that stops after the second order. Therefore, the Wigner function must also be Gaussian, and its linearized equation cannot contain third-order derivatives.

(iii) The fact that the Marcinkiewicz theorem (see Sec. IV) also holds for nonpositive quasiprobability functions can now be deduced effortlessly: as it can be applied to the Q function which is always positive, one sees immediately that it remains valid for P, W, and the whole family P_s .

VI. APPLICATION

Here we want to apply the cumulant method to the problem of second-harmonic generation. We will use the following Hamiltonian² in the interaction picture:

$$H = i\hbar \frac{\chi}{2} (a_1^{\dagger 2} a_2 - a_2^{\dagger} a_1^2) + i\hbar (a_1^{\dagger} F_1 - a_1 F_1^*) + i\hbar (a_2^{\dagger} F_2 - a_2 F_2^*) , \qquad (17)$$

where a_1, a_1^{\dagger} and a_2, a_2^{\dagger} are the Bose operators describing the fundamental and second-harmonic modes, respectively. F_1 and F_2 are the corresponding classical driving fields, detuned by δ_1 and δ_2 , respectively. Damping is included via coupling to a reservoir of zero temperature. This leads to the well-known irreversible term in the master equation (1) of the form

$$\left| \frac{d\rho}{dt} \right|_{\rm irr} = \frac{\gamma_1}{2} [a_1, \rho a_1^{\dagger}] + \frac{\gamma_1}{2} [a_1 \rho, a_1^{\dagger}] + \frac{\gamma_2}{2} [a_2, \rho a_2^{\dagger}] + \frac{\gamma_2}{2} [a_2 \rho, a_2^{\dagger}] .$$
(18)

Partial integration of the quasi-Fokker-Planck equation for the diagonal P function on the one hand or tracing over the master equation on the other hand leads to the following moment hierarchy:



FIG. 1. Photon numbers in the fundamental mode (solid line) and the second-harmonic mode (dashed line) as a function of time (in dimensionless units). The parameters are $F_1=20$, $F_2=0$, $\chi=0.4$, $\gamma_1=\gamma_2=1$, and $\delta_1=\delta_2=0$. (For these parameters, the threshold of bifurcation to a limit cycle in the classical dynamics is $F_1=15$). Result of a simulation of the Langevin equations derived from the positive P representation. The spikes are due to nonphysical instabilities of the method. The number of trajectories is 2000.

$$\frac{d}{dt} \langle a_{1}^{\dagger k} a_{2}^{\dagger l} a_{1}^{m} a_{2}^{n} \rangle = \operatorname{Tr} \left[\frac{d\rho}{dt} a_{1}^{\dagger k} a_{2}^{\dagger l} a_{1}^{m} a_{2}^{n} \right]
= -[k(\gamma_{1} - i\delta_{1}) + l(\gamma_{2} - i\delta_{2}) + m(\gamma_{1} + i\delta_{1}) + n(\gamma_{2} + i\delta_{2})] \langle a_{1}^{\dagger k} a_{2}^{\dagger l} a_{1}^{m} a_{2}^{n} \rangle
+ k(\chi \langle a_{1}^{\dagger k} - ia_{2}^{\dagger l} + ia_{1}^{m+1} a_{2}^{n} \rangle + F_{1} \langle a_{1}^{\dagger k} - ia_{2}^{\dagger l} a_{1}^{m} a_{2}^{n} \rangle)
+ l \left[-\frac{\chi}{2} \langle a_{1}^{\dagger k} + 2a_{2}^{\dagger l-1} a_{1}^{m} a_{2}^{n} \rangle + F_{2} \langle a_{1}^{\dagger k} a_{2}^{\dagger l-1} a_{1}^{m} a_{2}^{n} \rangle \right]
+ m(\chi \langle a_{1}^{\dagger k} + ia_{2}^{\dagger l} a_{1}^{m-1} a_{2}^{n+1} \rangle + F_{1} \langle a_{1}^{\dagger k} a_{2}^{\dagger l} a_{1}^{m-1} a_{2}^{n} \rangle)
+ n \left[-\frac{\chi}{2} \langle a_{1}^{\dagger k} a_{2}^{\dagger l} a_{1}^{m+2} a_{2}^{n-1} \rangle + F_{2} \langle a_{1}^{\dagger k} a_{2}^{\dagger l} a_{1}^{m-2} a_{2}^{n+1} \rangle \right]
+ k(k-1) \frac{\chi^{2}}{4} \langle a_{1}^{\dagger k} - 2a_{2}^{\dagger l+1} a_{1}^{m} a_{2}^{n} \rangle + m(m-1) \frac{\chi^{2}}{4} \langle a_{1}^{\dagger k} a_{2}^{\dagger l} a_{1}^{m-2} a_{2}^{n+1} \rangle . \tag{19}$$

These equations do not look very nice, and things get only worse when one applies second- or third-order truncation, which can be seen by a brief look at a typical fourth order cumulant:

$$\langle \langle a_{1}^{\dagger}a_{1}^{2}a_{2} \rangle \rangle = \langle a_{1}^{\dagger}a_{1}^{2}a_{2} \rangle - \langle a_{1}^{\dagger} \rangle \langle a_{1}^{2}a_{2} \rangle - \langle a_{1}^{\dagger}a_{1}^{2} \rangle \langle a_{2} \rangle - 2 \langle a_{1}^{\dagger}a_{1}a_{2} \rangle \langle a_{1} \rangle - 2 \langle a_{1}^{\dagger}a_{1} \rangle \langle a_{1}a_{2} \rangle - \langle a_{1}^{\dagger}a_{2} \rangle \langle a_{1}^{2} \rangle + 2 \langle a_{1}^{\dagger} \rangle \langle a_{1}^{2} \rangle \langle a_{2} \rangle + 4 \langle a_{1}^{\dagger}a_{1} \rangle \langle a_{1} \rangle \langle a_{2} \rangle + 4 \langle a_{1}^{\dagger} \rangle \langle a_{1} \rangle \langle a_{1}a_{2} \rangle + 2 \langle a_{1}^{\dagger}a_{2} \rangle \langle a_{1} \rangle^{2} - 6 \langle a_{1}^{\dagger} \rangle \langle a_{1} \rangle^{2} \langle a_{2} \rangle .$$

$$(20)$$

Handling those equations seems only possible by using an algebraic manipulation program. We derived the truncated moment hierarchies with the help of a program written in REDUCE, consisting of two main parts. The first one expresses cumulants in terms of moments for a given number of variables and for a given order. It is based on a general formula given by Meeron¹⁸ and establishes rules for replacing moments by lower-order ones. The second part starts from a moment hierarchy given in the general from of Eq. (19), writes down the particular equations for all moments up to a given order N, i.e., replacing k, l, m, and n by numbers such that $k+l+m+n \leq N$, and truncates these equations with the help of the rules established in the first step. As we want to find a numerical solution, the equations finally are automatically converted into a FORTRAN subroutine which can directly be used in a Runge-Kutta implementation. Aside from saving a lot of boring work, these programs considerably reduce the probability of an error.



FIG. 2. As in Fig. 1, but for the solution of the moment hierarchy Eq. (19) which was truncated after the second order (Gaussian approximation).

As an illustration, we will now calculate the dynamical behavior of the photon numbers in the case of second-harmonic generation where only the fundamental mode is pumped, i.e., $F_1 \neq 0$ and $F_2 = 0$. The figures show the photon numbers in both fundamental and second-harmonic modes, $I_1 = \langle a_1^{\dagger}a_1 \rangle$ and $I_2 = \langle a_2^{\dagger}a_2 \rangle$, as a function of time. The initial state (t = 0) is the vacuum.

For comparison, we first repeated the simulations of Ref. 6 where this problem was treated using the positive P representation.⁵ In that approach one introduces extra space dimensions in order to obtain a Fokker-Planck equation with a positive semidefinite diffusion matrix, which can be transformed into an equivalent Langevin equation. The latter can now be solved by computer simulation. The result is shown in Fig. 1. One observes unphysical "spikes" which are due to single trajectories escaping far into the extra dimensions. It is impossible to get rid of these spikes by averaging over a larger number of trajectories. Explanations of this wrong behavior have



FIG. 3. As in Fig. 1, but here the moment hierarchy is truncated after the third order.

been attempted by several authors, 6,8,19 but until now no remedy could be found. So one must conclude that the positive *P* representation does not provide reliable results for the problem of second-harmonic generation with a large driving field.

In Fig. 2 where the solution was obtained using second-order truncation of the moment hierarchy Eq. (19), we find a smooth behavior. Although this represents some progress when compared to the simulation, the result is still not satisfactory because the moments do not become stationary. One sees oscillations which reflect the existence of a limit cycle in the classical dynamics of the problem.⁶ However, as we are looking at mean values, their effects should be smeared out in the course of time when approaching the stationary regime. This difficulty might be overcome by going to a higherorder truncation. The results of third order truncation are shown in Fig. 3. Here, the spurious oscillations have disappeared and the solution becomes stationary. So it seems that one needs the contributions of nonvanishing third-order cumulants to describe the dynamics of second-harmonic generation correctly. We find that the higher-order truncation scheme leads to qualitative features the Gaussian approximation fails to show.

VII. CONCLUSION

Those quantities that can be measured in experiments are the expectation values of quantum-mechanical operators. Usually, expectation values are calculated from the density operator ρ or from some discrete or continuous representation of ρ . However, there is a more direct way which consists in writing down the hierarchy of equations of motion for the moments themselves. As no solutions to the full, infinite moment hierarchy are known for most nonlinear problems, one has to truncate the hierarchy in some way. In this work, a truncation scheme based on cumulant expansions has been presented. The application of the scheme to the problem of second-harmonic generation shows that in some cases the extension of truncation to a higher order is needed and leads to new results. It has also been shown that only second-order cumulants depend on the operator ordering.

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