Quantum-field-theoretical approach to phase-space techniques: Generalizing the positive-*P* representation

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We present an introduction to phase-space techniques (PST) based on a quantum-field-theoretical (QFT) approach. In addition to bridging the gap between PST and QFT, our approach results in a number of generalizations of the PST. First, for problems where the usual PST do not result in a genuine Fokker-Planck equation (even after phase-space doubling) and hence fail to produce a stochastic differential equation (SDE), we show how the system in question may be approximated via stochastic difference equations (SΔE). Second, we show that introducing sources into the SDE's (or SΔE's) generalizes them to a full quantum nonlinear stochastic response problem (thus generalizing Kubo's linear reaction theory to a quantum nonlinear stochastic response theory). Third, we establish general relations linking quantum response properties of the system in question to averages of operator products ordered in a way different from time normal. This extends PST to a much wider assemblage of operator products than are usually considered in phase-space approaches. In all cases, our approach yields a very simple and straightforward way of deriving stochastic equations in phase space.

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I. INTRODUCTION

Most of the interesting nonlinear quantum systems are not amenable to theoretical analysis without making various approximations, which can lead to losing sight of some of the physics involved. A numerical treatment may then be the only valid option. For equilibrium systems, a variety of methods known under the name of quantum Monte Carlo have been devised. For real-time evolution, especially in the field of quantum optics, phase-space methods have been developed (for a review of phase-space techniques (PST) see, e.g., Ref. [1]). Stochastic simulations using stochastic differential equations (SDEs) in phase space have long been a successful computational tool in quantum stochastics [1,2], allowing for the numerical stochastic integration of systems for which analytical solution would be, at best, extremely difficult. More recently, these methods have also been extended into the field of Bose-Einstein condensation [3–7].

What we offer in this paper is a very simple and transparent way of directly linking quantum equations of motion to SDEs in phase space. Conventional phase-space techniques (PST) are based on the well-known duality between the Fokker-Planck equations (FPE) and Langevin equations or, more generally, SDE, which goes back as far as Einstein's and Langevin's theories of Brownian motion (see Risken's book [8] for a detailed discussion of the FPE and related issues). Our techniques do not rely on the existence of a Fokker-Planck equation for a suitable quasiprobability distribution and hence work for a much wider class of Hamiltonians (a version starting from a master equation will be presented elsewhere). We also show how PST may be generalized to scattering (response) problems.

The essence of PST is *mapping* of quantum problems onto *c*-number stochastic problems. A certain subset of operator averages having been chosen, one finds a *c*-number stochastic process involving *c*-number fields, such that the averages of the latter equal the corresponding quantum averages. (The reason why only a subset of quantum averages is mapped is the noncommutivity of *q*-number field operators. In PST, these chosen averages are singled out by requiring that quantum-field operators are ordered in a certain way. That is, any quantum-classical mapping is based on an *ordering* of operators.) For example, in the well-known positive-*P* representation [9] ($+P$, for brevity) one maps averages of *time-normally ordered* operator products onto averages of a stochastic process in a doubled phase space. An important feature of our techniques is that they only indicate the necessary conditions to be imposed on such a mapping and thus reveal the *freedom* associated with it. This makes our techniques useful in the search for generalizations of the $+P$ [10,11] or Wigner [12] representations in order to overcome certain mathematical problems and achieve better convergence (see, e.g., Ref. [13] for the discussion of problems associated with the conventional $+P$).

In this and subsequent papers, we will concern ourselves with the following three questions:

(a) Are averages other than time-normal amenable to the PST?

(b) Can the PST be generalized to scattering (response) problems?

(c) Can one devise a stochastic representation if the equation for the appropriate pseudoprobability distribution contains higher than second-order derivatives and hence is not a

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genuine Fokker-Planck equation?

These three questions are deeply interlinked. For example, if one chooses to work with Weyl's, or symmetric, operator ordering, the equation for the related Wigner pseudoprobability distribution, as a rule, is not a genuine FPE. We thus see an obvious link between questions (a) and (c). More importantly, we show that there exists a profound connection between questions (a) and (b). That such a connection must indeed exist is made immediately clear by closely considering Kubo's famous formula for the linear response function [14]. Using as an example a nonlinear quantum oscillator, the latter is expressed by the average commutator,

$$R(t-t')=-i\hbar^{-1}\theta(t-t')\langle[\hat{\mathrm{a}}(t),\hat{\mathrm{a}}^{\dagger}(t')]\rangle, \tag{1}$$

where $\hat{\mathrm{a}}(t),\hat{\mathrm{a}}^{\dagger}(t)$ are the oscillator annihilation and creation operators in the Heisenberg picture. The commutator is a combination of two terms, $\langle[\hat{\mathrm{a}}(t),\hat{\mathrm{a}}^{\dagger}(t')]\rangle=\langle\hat{\mathrm{a}}(t)\hat{\mathrm{a}}^{\dagger}(t')\rangle-\langle\hat{\mathrm{a}}^{\dagger}(t')\hat{\mathrm{a}}(t)\rangle$, of which the first is anti-time-normally ordered and the second is time-normally ordered. Furthermore, Eq. (1) may be inverted [15,16] resulting in

$$\langle\hat{\mathrm{a}}(t)\hat{\mathrm{a}}^{\dagger}(t')\rangle=\langle\hat{\mathrm{a}}^{\dagger}(t')\hat{\mathrm{a}}(t)\rangle+i\hbar[R(t-t')-R^{*}(t'-t)]. \tag{2}$$

An antinormally-ordered average is thus expressed as a combination of the corresponding normally-ordered average and linear response functions.

This relation between the non-normally ordered averages and response turns out to be fundamental. We show below that Kubo's formula for the linear response function may be generalized to an arbitrary quantum nonlinear stochastic response function. Namely, any such function is expressed as a finite combination of averages of double-time-ordered operator products (known, e.g., from the Perel-Keldysh diagram approach [17]). On the other hand, any double-time-ordered average can be expressed as a finite combination of response functions. The implications of this result for the quantum measurement problem are yet to be understood. From our perspective, it eliminates (b) as a separate question, while an answer to (a) proves to be unexpectedly simple: the response formulation of a quantum system is achieved by including sources into the $+P$ equations. [This also applies to various generalizations of $+P$ emerging in response to questions (a) and (c).] Dropping the sources recovers the $+P$ equations known in PST; physically, this corresponds to considering only radiation problems. (Note that external sources are commonly present in quantum-optical problems as pump terms. The difference between the radiation and response formulations is whether the pump is, respectively, fixed or arbitrarily variable.)

As to (c), it would seem at first glance that an affirmative answer is prohibited by Pawula's theorem [8,18]. This theorem states, loosely speaking, that Langevin equations may only be written for those systems for which the equation for the probability distribution is a genuine Fokker-Planck equation. This certainly prohibits an *exact* mapping of a quantum problem on a *c*-number problem described by an SDE. The necessary opening appears if we agree to have only an *approximate* mapping and consider stochastic *difference* equations (SΔEs) in discretized time. As numerical simulation on a discrete time grid is often the only possible exact treatment for highly nonlinear systems, the development of SΔEs, although these have no continous time limit, is, for all practical purposes, sufficient (and does not violate Pawula's theorem as this only applies in the continuous time limit). The question as to whether a stochastic process in a certain generalized mathematical sense can be defined corresponding to our methods is a subject for futher investigation.

This paper is structured as follows. Using the quantum oscillator with Kerr nonlinearity as a demonstrative example, in Sec. II we reiterate a derivation of the Keldysh diagram series [17], resulting in a closed perturbative relation for the double-time-ordered averages. (More precisely speaking, we derive a *generating expression* [19] for the Keldysh series. However, we do not expand this generating expression in a power series, which would result in an actual diagram series [19], nor do we introduce any diagram notation as such. This also applies to other types of diagram series mentioned below.) We discuss in detail causal regularization [19] of the propagator, which is necessary in order to make our relations unambiguous. In Sec. III, we investigate the *causal structure* of the closed perturbative relation found in Sec. II, recasting it as a generating expression for a Wyld-type series [20], otherwise termed *causal* series [19,21,22]. We then show that this Wyld series is a formal solution to a full nonlinear quantum-stochastic response problem, generalising Kubo's linear reaction approach [14]. Examples of formulas for stochastic response functions are given in the Appendix. In Sec. IV, we show that generating expressions for causal series also emerge as formal solutions to *c*-number stochastic problems [19]. We then develop techniques based on the Hubbard-Stratonovich transformation (HST) [23] which allows for a constructive mapping of quantum nonlinear response problems onto classical nonlinear stochastic response problems. We discuss how multiple HST's may be used in deriving SΔE's for quantum systems for which the usual methods would result in a generalized FPE with higher-order derivatives [24,25] thus failing to produce an SDE. This yields strikingly simple and powerful techniques for obtaining stochastic representations of quantum problems. Perhaps the most important property of these techniques is that they can be formulated using simple recipes and then used without any reference to the advanced methods employed in their derivation. The utility of our methods is demonstrated in Sec. V. We start by reformulating our results recipe style, the way they should be applied in calculations, then illustrate them by the examples of the Kerr oscillator, optical parametric oscillator and triply degenerate four-wave mixing.

II. QUANTUM-FIELD THEORY OF THE KERR OSCILLATOR

A. The model

The techniques we introduce in this paper are applicable to any Hamiltonians which have a polynomial form in the

field operators. We also assume that the Hamiltonian can be divided into a quadratic part, called the free Hamiltonian, and the remainder, termed the interaction Hamiltonian; this allows one to introduce, in the usual manner, Schrödinger, Heisenberg, and interaction-picture field operators. However, this requirement may always be satisfied by subtracting a suitable quadratic term from the Hamiltonian, and declaring the remainder as being the ''interaction'' part (cf. the way a Higgs-type phase transition in an anharmonic oscillator was treated in Ref. [21]).

This generality notwithstanding, our techniques may be effectively demonstrated for a 1D oscillator (as is usual in quantum-field theory). We therefore consider a nonlinear quantum oscillator with the Hamiltonian

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_{\rm int}=\omega\hat{a}^\dagger\hat{a}+\frac{\kappa}{2}\hat{a}^{\dagger 2}\hat{a}^2, \tag{3}$$

using units such that $\hbar=1$. In Eq. (3), $\hat{a}^\dagger$ and $\hat{a}$ are the pair of creation and annihilation operators with commutator $[\hat{a},\hat{a}^\dagger]=1$, which play the role of Schrödinger-picture field operators for this system. The field operators in the interaction picture are simply

$$\hat{a}(t)=e^{-i\omega t}\hat{a},\ \hat{a}^\dagger(t)=e^{i\omega t}\hat{a}^\dagger, \tag{4}$$

while Heisenberg picture operators will be denoted in roman font as $\hat{\mathrm{a}}^\dagger(t)$ and $\hat{\mathrm{a}}(t)$.

B. Time orderings of operators

We start by reiterating the definitions of *time-ordered* operator products. Time ordering of field operators sorts these from right to left in the order of *increasing* time arguments, e.g. [with $\theta(t)$ being the Heaviside function],

$$T_+\hat{\mathrm{a}}(t')\hat{\mathrm{a}}^\dagger(t)=\hat{\mathrm{a}}^\dagger(t)\hat{\mathrm{a}}(t')\,\theta(t-t')+\hat{\mathrm{a}}(t')\hat{\mathrm{a}}^\dagger(t)\,\theta(t'-t). \tag{5}$$

For equal times, we specify the time ordering as normal ordering (which places all creation operators on the left of annihilation operators). That is,

$$T_+\hat{\mathrm{a}}(t)\hat{\mathrm{a}}^\dagger(t)=T_+\hat{\mathrm{a}}^\dagger(t)\hat{\mathrm{a}}(t)=\hat{\mathrm{a}}^\dagger(t)\hat{\mathrm{a}}(t). \tag{6}$$

We also specify reverse time ordering T_- which places operators in the order of *decreasing* time arguments. Formally, it may be defined as the conjugate of T_+:

$$T_-\hat{P}=[T_+(\hat{P}^\dagger)]^\dagger, \tag{7}$$

where $\hat{P}$ is a product of field operators. Then, e.g.,

$$T_-\hat{\mathrm{a}}(t')\hat{\mathrm{a}}^\dagger(t)=\hat{\mathrm{a}}^\dagger(t)\hat{\mathrm{a}}(t')\,\theta(t'-t)+\hat{\mathrm{a}}(t')\hat{\mathrm{a}}^\dagger(t)\,\theta(t-t'). \tag{8}$$

For equal times, T_- also becomes normal ordering. Finally, double-time ordering is the combination of the T_+ and T_--orderings,

$$T_-\hat{P}_-T_+\hat{P}_+, \tag{9}$$

where $\hat{P}_-$ and $\hat{P}_+$ are operator products.

To avoid the excessive use of brackets in formulas, we imply that the T_+-ordering symbol applies to all operators on its right. The same holds for the T_--ordering symbol if used alone. However, in double-time-ordered expressions T_- acts on operators between itself and T_+. So, in (9), T_+ acts on $\hat{P}_+$ while T_- acts on $\hat{P}_-$. In order to emphasise or explicitly delineate the range of applicability of an ordering symbol, brackets are placed around the whole ordered expression including the symbol, as in Eq. (7) above and Eqs. (20), (22), and (23) below.

C. Closed perturbative relations for quantum-field averages

For all practical purposes, the quantities of interest are operator expectation values rather than the operators themselves. For reasons which will become clear below, we consider averages of double-time-ordered operator products. A characteristic functional of these is defined as

$$\Xi(\zeta_-,\zeta_+,\zeta_-^\dagger,\zeta_+^\dagger)=\left\langle T_-\exp\int dt(\zeta_-\hat{\mathrm{a}}^\dagger+\zeta_-^\dagger\hat{\mathrm{a}})\times T_+\exp\int dt(\zeta_+\hat{\mathrm{a}}^\dagger+\zeta_+^\dagger\hat{\mathrm{a}})\right\rangle. \tag{10}$$

The angle brackets used here define an averaging over the Heisenberg ρ matrix of the quantum field (or over the field's initial state, which is the same thing):

$$\langle\cdots\rangle=\mathrm{Tr}\hat{\rho}(\cdots). \tag{11}$$

The functional (10) depends on four arbitrary *c*-number functions, $\zeta_-(t),\zeta_+(t),\zeta_-^\dagger(t),\zeta_+^\dagger(t)$; for brevity, we have omitted the time arguments on the rhs of Eq. (10). (Note that, for operators, † is Hermitian conjugation, whereas for the *c*-number functions it is merely a notation distinguishing two different sets of these. This applies to all other sets of conjugated *c*-numbers introduced later in the paper.)

Our immediate goal is to formulate a closed perturbative relation for the characteristic functional (10). We will closely follow the way in which Feynman diagram techniques were derived in textbooks dating back to 1950s and 1960s [26]. In the pre-path-integral era, a standard derivation leading to Feynman diagrams included three major steps:

(i) Introduce the interaction picture and express time-ordered products of Heisenberg field operators via those of the interaction-picture operators.

(ii) Use Wick's theorem so as to reorder time-ordered products normally.

(iii) Perform the averaging over the initial-field-state assumed to be vacuum; since averaging of any normally ordered product over vacuum yields zero, this results in a *c*-number representation for the quantum averages.

The result is the closed perturbation relation that we are seeking. Expanding it in a power series would yield an actual

diagram series. However, we will leave it ''intact'' for later use in the derivation of quantum-classical mappings.

An example of such a derivation starting from T_+ ordered averages may be found in Ref. [27]. Its success however depends on the field being initially in a vacuum state. Physically, this is too strong a restriction, so we have to generalize the techniques developed in Ref. [27] so as to cover nonvacuum initial states. When working with such states, it is convenient to characterize the initial state of the oscillator by the corresponding P distribution,

$$P(\alpha)=\frac{1}{\pi^2}\int d^2\eta\langle e^{\eta(\hat{a}^\dagger-\alpha^*)-\eta^*(\hat{a}-\alpha)-|\eta|^2/2}\rangle,$$

$$\hat{\rho}=\int d^2\alpha P(\alpha)|\alpha\rangle\langle\alpha|, \tag{12}$$

where $|\alpha\rangle$ is the well-known coherent state. For any normally ordered operator expression we then have

$$\langle{:}X(\hat{a}^\dagger(t),\hat{a}(t)){:}\rangle=\int d^2\alpha P(\alpha)\langle\alpha|{:}X(\hat{a}^\dagger(t),\hat{a}(t)){:}|\alpha\rangle$$

$$=\int d^2\alpha P(\alpha)X(\alpha^*(t),\alpha(t)), \tag{13}$$

where $\alpha(t)=\alpha e^{-i\omega t}$ is the coherent amplitude of the interaction-picture field operator, $\hat{a}(t)|\alpha\rangle=\alpha(t)|\alpha\rangle$. The latter relation allows one to perform the averaging as required by step (iii) of the aforementioned schedule.

Step (ii) of this schedule also needs an amendment. It is easy to see that, given nonvacuum initial field states, closed formulas for time-ordered averages can no longer be derived. The minimal set of operator averages for which closed perturbation relations exist is that of double-time-ordered averages. We thus need a modification of Wick's theorem so as to include double-time ordering. This modification is in fact well known, leading to the Perel-Keldysh diagram techniques [17]. We shall discuss it in some detail, taking the opportunity to introduce quantities and formulas which will be used later.

Wick's theorem states that ''a time-ordered product of interaction-picture field operators equals the sum of all possible normally ordered operator products, obtained by replacing pairs of operators in the initial product by corresponding contractions (including the term without contractions).'' For the oscillator we have only one nonzero contraction, namely,

$$T_+\hat{a}(t')\hat{a}^\dagger(t)-{:}\hat{a}^\dagger(t)\hat{a}(t'){:}$$

$$=\langle 0|T_+\hat{a}^\dagger(t)\hat{a}(t')|0\rangle$$

$$=\theta(t'-t)e^{-i\omega(t'-t)}\equiv iG(t'-t), \tag{14}$$

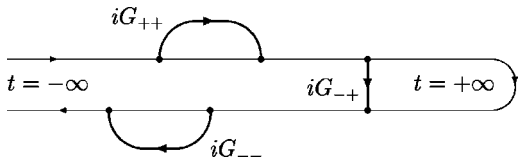

FIG. 1. The Schwinger-Perel-Keldysh C contour (thin lines) and the three contractions contributing to Δ_C (thick lines), cf. Eq. (19). The arrows on contractions are from creation to annihilation, cf. Eq. (16). For G_{++} and G_{--}, the time order of ends corresponds to these being nonzero.

where $G(t)$ is a retarded Green's function of the free Schrödinger equation,

$$\left(i\frac{\partial}{\partial t}-\omega\right)G(t)=\delta(t). \tag{15}$$

It may be verified that the proof of Wick's theorem [26] is based only on the linear ordering of the time axis; consequently Wick's theorem may be generalized to operators defined formally on any linearly ordered set. This clearly applies to the double-time ordering, Eq. (9), which may alternatively be introduced as an ordering on the so-called C contour [17]. The C contour (see Fig. 1) first travels from $t=-\infty$ to $t=+\infty$ (direct branch) and then back to $t=-\infty$ (reverse branch). Assigning an operator a C-contour index ''+'' or ''−'' is equivalent to placing it, respectively, under the T_+ or T_- ordering in Eq. (9). For the T_C ordering, operator contraction becomes a matrix with respect to the C-contour indices $(\alpha,\beta=+,-)$,

$$iG_{\alpha\beta}(t'-t)=\langle 0|T_C\hat{a}_\alpha(t')\hat{a}^\dagger_\beta(t)|0\rangle. \tag{16}$$

The three nonzero components of $G_{\alpha\beta}$ (also shown schematically in Fig. 1) are conveniently expressed in terms of $G(t)$ introduced in Eq. (14):

$$G_{++}(t)=G(t),$$

$$G_{--}(t)=-G^*(-t),$$

$$G_{-+}(t)=G(t)-G^*(-t). \tag{17}$$

For our purposes, it is convenient to use a closed functional form of Wick's theorem. As was first noticed by Hori [28], the pattern of products with contractions required by Wick's theorem is exactly that produced by a certain functional differential operator; this also remains the case after Wick's theorem is generalized to the double time ordering [29]. The functional (Hori's) form of Wick's theorem as applied to the double time ordering is

$$T_-\hat{P}_-T_+\hat{P}_+={:}[e^{\Delta_C}(\hat{P}_-|_{\hat{a}\to a_-;\hat{a}^\dagger\to a_-^\dagger}\hat{P}_+|_{\hat{a}\to a_+;\hat{a}^\dagger\to a_+^\dagger})]|_{a_-,a_+\to\hat{a};a_-^\dagger,a_+^\dagger\to\hat{a}^\dagger}{:}. \tag{18}$$

Here, $\hat{P}_-$ and $\hat{P}_+$ are arbitrary operator products, $a_\pm(t), a_\pm^\dagger(t)$ are four independent c-number functions, and Δ_C is a quadratic form of functional derivatives:

$$\Delta_C = \int dt dt' \left[iG_{++}(t'-t)\frac{\delta^2}{\delta a_+(t')\delta a_+^\dagger(t)} + iG_{--}(t'-t) \times \frac{\delta^2}{\delta a_-(t')\delta a_-^\dagger(t)} + iG_{-+}(t'-t)\frac{\delta^2}{\delta a_-(t')\delta a_+^\dagger(t)} \right]. \tag{19}$$

Note that Eqs. (18) and (19) have been formulated so as to eliminate the concept of the C contour from any further considerations.

Consider now step (i) of the aforementioned derivation schedule. As is shown in many textbooks on quantum-field theory (QFT) (see, e.g., Ref. [26]), a time-ordered product of Heisenberg operators, $\mathcal{A}(t), \ldots, \mathcal{B}(t')$, may be expressed as

$$T_+\mathcal{A}(t)\cdots\mathcal{B}(t') = \mathcal{S}^\dagger[T_+\mathcal{S}A(t)\cdots B(t')], \tag{20}$$

where $A(t), \ldots, B(t')$, are the same operators in the interaction picture and $\mathcal{S}$ is the S matrix. In our demonstrative model,

$$\mathcal{S} = T_+\exp\int dt\left[-\frac{i\kappa}{2}\hat{a}^{\dagger 2}(t)\hat{a}^2(t)\right], \tag{21}$$

so that [cf. Eq. (10)]

$$T_+\exp\int dt(\zeta\hat{a}^\dagger + \zeta^\dagger\hat{a}) = \mathcal{S}^\dagger\left[T_+\exp\int dt\left(\zeta\hat{a}^\dagger + \zeta^\dagger\hat{a} - \frac{i\kappa}{2}\hat{a}^{\dagger 2}\hat{a}^2\right)\right]. \tag{22}$$

This formula was used in Ref. [27]. Amending it to the case of double-time ordering is straightforward. Conjugating (22),

$$T_-\exp\int dt(\zeta\hat{a}^\dagger + \zeta^\dagger\hat{a}) = \left[T_-\exp\int dt\left(\zeta\hat{a}^\dagger + \zeta^\dagger\hat{a} + \frac{i\kappa}{2}\hat{a}^{\dagger 2}\hat{a}^2\right)\right]\mathcal{S}, \tag{23}$$

then multiplying Eqs. (22) and (23), we find

$$T_-\exp\int dt(\zeta_-\hat{a}^\dagger + \zeta_-^\dagger\hat{a})T_+\exp\int dt(\zeta_+\hat{a}^\dagger + \zeta_+^\dagger\hat{a}) = T_-\exp\int dt\left(\zeta_-\hat{a}^\dagger + \zeta_-^\dagger\hat{a} + \frac{i\kappa}{2}\hat{a}^{\dagger 2}\hat{a}^2\right) \times T_+\exp\int dt\left(\zeta_+\hat{a}^\dagger + \zeta_+^\dagger\hat{a} - \frac{i\kappa}{2}\hat{a}^{\dagger 2}\hat{a}^2\right). \tag{24}$$

Importantly, the factors $\mathcal{S}$ and $\mathcal{S}^\dagger$ outside the orderings have canceled each other, resulting in a genuine double-time-ordered structure on the rhs of Eq. (24).

Finally, combining Eqs. (24) and (18) and then applying relation (13) yields

$$\Xi(\zeta_-,\zeta_+,\zeta_-^\dagger,\zeta_+^\dagger) = \int d^2\alpha P(\alpha)\left\{ \exp(\Delta_C)\exp\int dt\left[\zeta_- a_-^\dagger + \zeta_-^\dagger a_- + \zeta_+ a_+^\dagger + \zeta_+^\dagger a_+ + \frac{i\kappa}{2}(a_-^{\dagger 2}a_-^2 - a_+^{\dagger 2}a_+^2)\right]\Big|_{a\to\alpha}\right\}, \tag{25}$$

where $a\to\alpha$ is a short hand for the substitution, $a_+(t) = a_-(t) = \alpha(t), a_+^\dagger(t) = a_-^\dagger(t) = \alpha^*(t)$. A more pedagogical approach may be found in our e-print Ref. [29] (see, also Refs. [15,21]).

D. Causal regularization

Wick's theorem requires that no contractions should occur between operators with equal time arguments. (This is simply because the time ordering was specified for equal times as normal ordering.) A convenient way of enforcing this caveat is a *causal regularization* of $G(t)$. To this end, we shall assume that $G(t)$ is smoothed while still preserving its causal nature: $G(t)=0$ for $t<0$. For example, one can replace, $G(t)\to(1-e^{-\Gamma t})G(t)$, where Γ is a large constant (a reader versed in QFT would immediately recognize this as a nonrelativistic single-mode version of the Pauli-Villars regularization [26]). This makes $G(t)$ a continuous function, for which $G(0)=0$ holds unambiguously, so that a contraction between any pair of operators with equal time arguments is always zero.

For the double-time ordering, a regularized matrix of contractions is defined as per Eq. (17). The T_- ordering also being specified for equal time as normal ordering, the "no contractions between same-time operators" caveat of Wick's theorem applies equally to operators under the T_- ordering. It is then enforced through the equation relating $G_{--}(t)$ to $G(t)$ and the causal regularization of $G(t)$. At the same time, through the equation relating $G_{-+}(t)$ to $G(t)$, the regularization also modifies $G_{-+}(t)$, unnecessarily "burning a hole" in it in the vicinity of $t=0$. We have to make sure that this modification of $G_{-+}(t)$ does not lead to incorrect results. The fact that weird results may indeed follow is demonstrated by, e.g., a "proof" that $\hat{a}$ and $\hat{a}^\dagger$ commute. With regularization, $G_{-+}(0)=0$, and we "obtain,"

$$\hat{a}\hat{a}^\dagger = T_C\hat{a}_-(t)\hat{a}_+^\dagger(t) = \hat{a}^\dagger(t)\hat{a}(t) + iG_{-+}(0) = \hat{a}^\dagger\hat{a}. \tag{26}$$

The flaw in this "proof" is that all quantities we deal with should be regarded as generalized functions (distributions) and not pointwise functions. This is especially true under regularization. "Holes" in continuous functions which emerge due to regularization should be simply ignored

(smeared out). We would only expect problems associated with the ''holes'' if they were overlapping with sufficiently strong singularities, δ functions or worse, whereas the worst type of singularity that we may expect to occur is a step function. The ''hole'' in $G_{-+}(t)$ is thus of no material consequence.

III. SIGNAL PROPAGATION BY MEANS OF INTERACTING BOSONIC FIELDS

Our next goal is to investigate the *causal structure* of Eqs. (25). The concept of causality is introduced via the contraction $iG(t)$, which, according to Eq. (15), is, up to a phase, exactly the retarded Green's function of the free Schrödinger equation. Following this, we are able to define the *input and output* of a quantum system. We then show that, physically, the input and output thus introduced correspond to a generalization of Kubo's linear reaction approach [14] to a full nonlinear quantum-stochastic response problem.

A. Causal variables

Consider in more detail the differential quadratic form in Eq. (25). Making use of relations (17), and utilizing the notation

$$\frac{\delta}{\delta a} G \frac{\delta}{\delta a^\dagger} = \int dt dt' G(t'-t) \frac{\delta^2}{\delta a(t') \delta a^\dagger(t)}, \tag{27}$$

we find

$$\Delta_C = i\left(\frac{\delta}{\delta a_+} + \frac{\delta}{\delta a_-}\right) G \frac{\delta}{\delta a_+^\dagger} - i\left(\frac{\delta}{\delta a_+^\dagger} + \frac{\delta}{\delta a_-^\dagger}\right) G^* \frac{\delta}{\delta a_-}. \tag{28}$$

We now change the functional variables, $a_\pm(t), a_\pm^\dagger(t) \rightarrow a(t), a^\dagger(t), \xi(t), \xi^\dagger(t)$, in order to obtain

$$\Delta_C = \frac{\delta}{\delta a} G \frac{\delta}{\delta \xi^\dagger} + \frac{\delta}{\delta a^\dagger} G^* \frac{\delta}{\delta \xi}. \tag{29}$$

That is,

$$\frac{\delta}{\delta \xi^\dagger(t)} = i \frac{\delta}{\delta a_+^\dagger(t)},$$

$$\frac{\delta}{\delta \xi(t)} = -i \frac{\delta}{\delta a_-(t)},$$

$$\frac{\delta}{\delta a^\dagger(t)} = \frac{\delta}{\delta a_+^\dagger(t)} + \frac{\delta}{\delta a_-^\dagger(t)},$$

$$\frac{\delta}{\delta a(t)} = \frac{\delta}{\delta a_+(t)} + \frac{\delta}{\delta a_-(t)}. \tag{30}$$

These relations determine the new variables up to arbitrary functions which we chose to be zero:

$$a_+(t) = a(t), \quad a_+^\dagger(t) = a^\dagger(t) + i\xi^\dagger(t),$$

$$a_-(t) = a(t) - i\xi(t), \quad a_-^\dagger(t) = a^\dagger(t). \tag{31}$$

Consider now the integrand in the second exponent in Eq. (25): (again omitting time arguments for brevity)

$$\zeta_- a_-^\dagger + \zeta_-^\dagger a_- + \zeta_+ a_+^\dagger + \zeta_+^\dagger a_+ = (\zeta_- + \zeta_+) a^\dagger + (\zeta_-^\dagger + \zeta_+^\dagger) a - i\xi\zeta_-^\dagger + i\xi^\dagger \zeta_+. \tag{32}$$

This clearly suggests another substitution, this time in the functional Ξ itself,

$$\Xi(\zeta_-, \zeta_+, \zeta_-^\dagger, \zeta_+^\dagger) \equiv \Phi(\zeta, \zeta^\dagger, \sigma, \sigma^\dagger), \tag{33}$$

where

$$\zeta(t) = \zeta_-(t) + \zeta_+(t), \quad \zeta^\dagger(t) = \zeta_-^\dagger(t) + \zeta_+^\dagger(t),$$

$$\sigma(t) = +i\zeta_+(t), \quad \sigma^\dagger(t) = -i\zeta_-^\dagger(t), \tag{34}$$

so that

$$\zeta_+(t) = -i\sigma(t), \quad \zeta_+^\dagger(t) = \zeta^\dagger(t) - i\sigma^\dagger(t),$$

$$\zeta_-(t) = \zeta(t) + i\sigma(t), \quad \zeta_-^\dagger(t) = i\sigma^\dagger(t). \tag{35}$$

In the *causal variables* [37] thus introduced, Eq. (25) becomes

$$\Phi(\zeta, \zeta^\dagger, \sigma, \sigma^\dagger) = \int d^2\alpha P(\alpha) \times \left\{ \left[\exp\left(\frac{\delta}{\delta a} G \frac{\delta}{\delta \xi^\dagger} + \frac{\delta}{\delta a^\dagger} G^* \frac{\delta}{\delta \xi} \right) \times \exp \int dt [\zeta a^\dagger + \zeta^\dagger a + \xi\sigma^\dagger + \xi^\dagger \sigma + S_{\rm int}(\xi, \xi^\dagger, a, a^\dagger)] \right] \Big|_{a=\alpha, a^\dagger = \alpha^*, \xi = \xi^\dagger = 0} \right\}, \tag{36}$$

where

$$S_{\rm int}(\xi, \xi^\dagger, a, a^\dagger) = \kappa(\xi a^{\dagger 2} a + \xi^\dagger a^2 a^\dagger) + \frac{i\kappa}{2}(\xi^{\dagger 2} a^2 - \xi^2 a^{\dagger 2}). \tag{37}$$

(Unlike in Ref. [29], $S_{\rm int}$ here is a pointwise function, not a functional.)

It should be stressed that Eq. (36) is universal, while all details of the problem enter through $S_{\rm int}$. In general $S_{\rm int}$ is found as

$$S_{\rm int}(\xi, \xi^\dagger, a, a^\dagger) = ih(a^\dagger, a - i\xi) - ih(a^\dagger + i\xi^\dagger, a), \tag{38}$$

where h is the normally ordered representation of the interaction Hamiltonian

$$\mathcal{H}_{\rm int} = :h(\hat{a}^\dagger, \hat{a}):. \tag{39}$$

Generalization of Eq. (36) to multimode problems (see Sec. V) is also straightforward.

B. Quantum nonlinear reaction problem

To gain more insight into the causal variables, we now introduce a variable pump term into the interaction Hamiltonian, which then reads (in the interaction picture)

$$\tilde{H}_{\rm int}(t)=H_{\rm int}(t)+s(t)\hat{a}^{\dagger}(t)+s^{*}(t)\hat{a}(t). \tag{40}$$

The *external source* $s(t)$ is a given c-number function. Note that we mark all quantities defined in the presence of the source with a tilde (the interaction picture operators are not changed and so bear no tilde). With the source,

$$\tilde{S}_{\rm int}=S_{\rm int}+\xi s^{*}+\xi^{\dagger}s. \tag{41}$$

Moving $\xi s^{*}+\xi^{\dagger}s$ to the second exponent in Eq. (36) results in the identity

$$\tilde{\Phi}(\zeta,\zeta^{\dagger},\sigma,\sigma^{\dagger})=\Phi(\zeta,\zeta^{\dagger},\sigma+s,\sigma^{\dagger}+s^{*}). \tag{42}$$

In this way, the physical information contained in the dependence of $\Phi(\zeta,\zeta^{\dagger},\sigma,\sigma^{\dagger})$ on the σ's is the system's reaction to an external perturbation. (Physically, this means that quantum statistical averages contain much more information than classical statistical averages, covering also scattering experiments performed with the quantum system in question.) The variables $\sigma,\sigma^{\dagger}$ define an input to the system, while $\zeta,\zeta^{\dagger}$ define an output. A natural question then is if we can assign some physical meaning to these concepts. To start with, consider the formal meaning of the output. Assuming the source to be arbitrary, the full physical information about the system is obtainable from

$$\tilde{\Phi}(\zeta,\zeta^{\dagger},0,0)=\Phi(\zeta,\zeta^{\dagger},s,s^{*}). \tag{43}$$

In turn, making use of Eq. (10) we get

$$\tilde{\Phi}(\zeta,\zeta^{\dagger},0,0)=\langle T_{-}\exp(\zeta^{\dagger}\hat{\rm a})T_{+}\exp(\hat{\zeta}\hat{\rm a}^{\dagger})\rangle. \tag{44}$$

This is nothing but a characteristic functional of Glauber's renowned time-normal averages of the Heisenberg field operator in the presence of the source [30]. The source terms in the Hamiltonian are also quite recognizable; they appear in Kubo's linear reaction theory [14]. Introducing causal variables is thus equivalent to a *nonlinear-reaction* reformulation of a quantum system. In the Appendix, we show how stochastic nonlinear response functions of a quantum system may be formulated generalizing Kubo's linear reaction approach. All these functions exhibit natural causality properties, justifying the term *causal variables* [37].

It should be stressed that, unlike the linear reaction theory, the nonlinear reaction theory depends explicitly on which quantities are to be ''measured.'' Causal variables as introduced by Eqs. (35) and the response theory outlined in the Appendix correspond to ''measuring'' time-normal averages of the field operators. Were the ''measured'' quantitities to be defined differently, the quantum reaction theory would have been reformulated accordingly. ''Measuring'' symmetric averages will be considered in a later paper.

Returning to the question of whether the formal reaction formulation corresponds to any physics, we see that both the input and output are associated with the concept of quantum back-action evasion. (That absence of detector back action on the source is a prerequisite for the measuring of time-normal field averages is shown, e.g., in Refs. [15,31].) Thus, under macroscopic conditions, the input-output formulation corresponds to a *light-scattering* experiment performed with the quantum system in question. Under microscopic conditions, the input and output remain formal concepts.

IV. QUANTUM EXPECTATION VALUES AS CLASSICAL STOCHASTIC AVERAGES

A. Classical stochastic response problem

Relation (36) gives a formal solution to the quantum response problem formulated in terms of time-normal averages. It is instructive to compare this relation with a solution to a classical stochastic response problem. To this end, consider a c-number stochastic field $a(t)$, which obeys an integral equation

$$a(t)=\alpha(t)+\int dt' G(t-t')\sigma_{\rm tot}(t'), \tag{45}$$

where $\alpha(t)$ is the in field and $\sigma_{\rm tot}(t)$ is the field source. For the purposes of this paragraph, the kernel $G(t)$ is assumed to be regular and retarded, $G(t)=0,t\leqslant 0$, and otherwise arbitrary. We assume that the in field $\alpha(t)$ is also arbitrary. [This allows one to regularize $G(t)$ without changing $\alpha(t)$.] The full field source $\sigma_{\rm tot}(t)$ consists of two parts,

$$\sigma_{\rm tot}(t)=\sigma(t)+\sigma'(t). \tag{46}$$

The *external* source $\sigma(t)$ is regarded as given, while the *random source* $\sigma'(t)$ depends on the field. That is, the random source describes the field's effective self-action (which originates physically, e.g., from interaction with a medium). As a random quantity $\sigma'(t)$ is fully characterized by a probability distribution, conditional on the field at the same time t:

$$\Pi(\sigma'(t)|a(t)). \tag{47}$$

Formally resolving the self-action problem results in a probability distribution over the random source $\sigma'(t)$ conditional on the in-field $\alpha(t)$ and the external source $\sigma(t)$. This is found by substituting Eq. (45) for $a(t)$,

$$\Pi(\sigma'|\alpha+G(\sigma+\sigma')), \tag{48}$$

where we have introduced a short-hand notation $\alpha+G(\sigma+\sigma')$ for the rhs of (45), and once more omitted time arguments. Most importantly, Eq. (48) does not contain a vicious cycle because of the assumed regular-and-retarded nature of $G(t)$: $\sigma'(t)$ depends on $\sigma'(t')$ only for $t'<t$.

Consider now the statistical properties of the field. With the self-action resolved, these are also conditional on the

in-field $\alpha(t)$ and the external source $\sigma(t)$. For the characteristic functional of multitime stochastic field averages we find [with $\zeta(t)$ being an arbitrary function]

$$\begin{aligned}\Sigma(\zeta|\alpha,\sigma)&=\overline{\exp\left(\int dt\zeta(t)a(t)\right)}\\&=\overline{\exp\int dt\zeta[\alpha+G(\sigma+\sigma')]}\\&=\left\{\prod_t\int d^2\sigma'\Pi(\sigma'|\alpha+G(\sigma+\sigma'))\right\}\\&\quad\times\exp\int dt\zeta[\alpha+G(\sigma+\sigma')]\\&=\int D^\infty\sigma'\Pi^\infty(\sigma'|\alpha+G(\sigma+\sigma'))\\&\quad\times\exp\int dt\zeta[\alpha+G(\sigma+\sigma')].\end{aligned}\tag{49}$$

The upper bar here denotes an averaging over the statistics of σ', which is afterwards explicitly rewritten as a trajectorial (functional) integral; the *functional* probability distribution Π^∞ is a product of distributions (48) over all times. Then, first, we pull $G(\sigma+\sigma')$ out of $\Pi^\infty(\sigma'|\alpha+G[\sigma+\sigma'])$ by applying a functional shift operator

$$\Pi^\infty(\sigma'|\alpha+G(\sigma+\sigma'))=\mathrm{e}^{(\delta/\delta\alpha)G(\sigma+\sigma')}\Pi^\infty(\sigma'|\alpha).\tag{50}$$

We use here a condensed notation similar to Eq. (27). Second, we pull all factors except Π^∞ out of the functional integral, resulting in [with $\xi(t)$ being another arbitrary function]

$$\begin{aligned}\Sigma(\zeta|\alpha,\sigma)&=\int D^\infty\sigma'\exp\int dt\zeta\alpha\\&\quad\times\exp\left(\zeta+\frac{\delta}{\delta\alpha}\right)G(\sigma+\sigma')\Pi^\infty(\sigma'|\alpha)\\&=\exp\int dt\zeta\alpha\exp\left(\zeta+\frac{\delta}{\delta\alpha}\right)G\left(\sigma+\frac{\delta}{\delta\xi}\right)\\&\quad\times\int D^\infty\sigma'\exp\int dt\xi\sigma'\Pi^\infty(\sigma'|\alpha)|_{\xi=0}\\&=\exp\int dt\zeta\alpha\exp\left(\zeta+\frac{\delta}{\delta\alpha}\right)G\left(\sigma+\frac{\delta}{\delta\xi}\right)\\&\quad\times\exp\int dtS(\xi|\alpha)|_{\xi=0}.\end{aligned}\tag{51}$$

We have introduced a characteristic function of *cumulants* of the random source at time t conditional on the full field,

$$S(\xi(t)|a(t))=\ln\int d^2\sigma'(t)e^{\xi(t)\sigma'(t)}\Pi(\sigma'(t)|a(t)).\tag{52}$$

After further algebra, which is made easier by use of the following form of the rule of product differentiation,

$$\begin{aligned}&\mathbf{\Phi}\left(\frac{\delta}{\delta\varphi}\right)\mathbf{\Phi}_1(\varphi)\mathbf{\Phi}_2(\varphi)\\&\quad=\mathbf{\Phi}\left(\frac{\delta}{\delta\varphi_1}+\frac{\delta}{\delta\varphi_2}\right)\mathbf{\Phi}_1(\varphi_1)\mathbf{\Phi}_2(\varphi_2)|_{\varphi_1,\varphi_2=\varphi},\end{aligned}\tag{53}$$

where $\varphi(t),\varphi_1(t),\varphi_2(t)$ are c-number functions and $\mathbf{\Phi}(\varphi)$, $\mathbf{\Phi}_1(\varphi),\mathbf{\Phi}_2(\varphi)$ are functionals of such functions, we arrive at

$$\begin{aligned}\Sigma(\zeta|\alpha,\sigma)=&\left\{\exp\left(\frac{\delta}{\delta a}G\frac{\delta}{\delta\xi}\right)\right.\\&\left.\times\exp\int dt[\zeta a+\xi\sigma+S(\xi|a)]\right\}\Big|_{\xi=0,a=\alpha}.\end{aligned}\tag{54}$$

B. Hubbard-Stratonovich transformations: Introducing noise sources constructively

1. Second-order noises: Stochastic differential equations

Disregarding the averaging over the pseudodistribution, Eq. (36) looks very much like a generalization of Eq. (54) to a pair of random fields. It is then only natural to use this similarity in order to construct a classical stochastic problem, of which the averages would equal the quantum averages. This leads us to consider the following problem: assume the function $S(\xi|a)$ is known. Can we explicitly construct a stochastic differential equation (SDE) to which it corresponds?

An unconditionally affirmative answer to this question exists only if S has the form

$$S(\xi|a)=\xi\sigma_{\mathrm{reg}}(a)+\xi^2\varphi_2(a),\tag{55}$$

where $\sigma_{\mathrm{reg}}(a)$ and $\varphi_2(a)$ are some functions. If $\varphi_2(a)=0$, $S(\xi|a)=\xi\sigma_{\mathrm{reg}}(a)$ is equivalent to $\Pi(\sigma'|a)=\delta(\sigma'-\sigma_{\mathrm{reg}}(a))$. In turn, this means that the source σ_{tot} in Eq. (45) is nonstochastic,

$$\sigma_{\mathrm{tot}}(t)=\sigma(t)+\sigma_{\mathrm{reg}}(a(t)).\tag{56}$$

Thus the linear (in ξ) part of $S(\xi|a)$ corresponds to a regular evolution; $\sigma_{\mathrm{reg}}(a)$ is nothing but a drift term. The quadratic part of S may be dealt with by using a Hubbard-Stratonovich transformation [23]. For our purposes, however, it is convenient always to regard time as discretized; t is then a discrete variable enumerating the time slices, each of size dt (with the values of t corresponding to the beginnings of the increments). Consider a standardized discretized real Kronecker-correlated Gaussian noise, $\chi(t)$,

$$\overline{\chi(t)}=0,\quad\overline{\chi(t)\chi(t')}=\delta_{tt'},\tag{57}$$

where $\delta_{tt'}$ is the Kronecker symbol ($\delta_{tt'}=1$ if $t=t'$ and zero otherwise). We then "stochastically linearize" $S(\xi|a)$, independently in each time slice:

$$\overline{\exp\{dt[\xi\sigma_{\rm reg}(a)+\xi^2\varphi_2(a)]\}} = \exp\left\{ dt\xi\left[\sigma_{\rm reg}(a)+\frac{\chi}{\sqrt{dt}}\sqrt{2\varphi_2(a)}\right]\right\}, \quad (58)$$

where the upper bar means averaging over the statistics of the χ's. Assuming that the averaging may be commuted with the differential operation in Eq. (54), we recover a (discretized) stochastic integral equation (45) with

$$\sigma_{\rm tot}(t)=\sigma(t)+\sigma_{\rm reg}(a(t))+\frac{\chi(t)}{\sqrt{dt}}\sqrt{2\varphi_2(a(t))}. \quad (59)$$

In the continuous limit, $dt\to 0$, $\chi(t)/\sqrt{dt}$ becomes the derivative of a Wiener process [32], and we find ourselves within the conventional theory of SDEs. On removing the regularization of the kernel G, we obtain an Itô SDE for the field, $a(t)$, [cf. Eq. (15)]

$$ida(t)=[\omega+\sigma_{\rm reg}(a(t))]dt+\sqrt{2\varphi_2(a(t))}dW(t). \quad (60)$$

The fact that Itô calculus should be chosen is due to the causal regularization of $G(t)$, which makes sources at time t independent of fields at the same time, which is exactly the characteristic property of Itô calculus.

2. Higher-order noises: Stochastic difference equations

We now assume that $S(\xi|a)$ also contains a cubic term,

$$S_3(\xi|a)=\xi^3\varphi_3(a). \quad (61)$$

With time discretized, it is very easy to "stochastically linearize" this expression by employing a combination of real and complex Hubbard-Stratonovich transformations. Let $\eta(t)$ be a standardized discretized complex Kronecker-correlated Gaussian noise:

$$\overline{\eta(t)}=0, \quad \overline{\eta(t)\eta(t')}=0, \quad \overline{\eta^*(t)\eta(t')}=\delta_{tt'}. \quad (62)$$

Such a noise may be constructed as a combination of two independent real noises, $\eta(t)=[\chi'(t)+i\chi''(t)]/\sqrt{2}$. The real noise is useful for "halving powers" (x being any quantity uncorrelated with χ),

$$\exp(x^2)=\overline{\exp(\chi x\sqrt{2})}, \quad (63)$$

whereas the complex noise allows one to factorize arbitrary products, (with x,y any quantities uncorrelated with η)

$$\exp(xy)=\overline{\exp(x\eta+y\eta^*)}. \quad (64)$$

The cubic contribution is then "stochastically linearized" in two steps (with χ and η independent):

$$\exp[dt\xi^3\varphi_3(a)]=\overline{\exp[dt(\xi\eta p+\xi^2\eta^* q)]} = \overline{\exp[dt\xi(\eta p+\chi\sqrt{2q\eta^*/dt})]}, \quad (65)$$

where p,q are uncorrelated with η,χ and obey the condition

$$pq=\frac{\varphi_3(a)}{dt}. \quad (66)$$

This yields the following contribution to σ':

$$\sigma_3'=\eta p+\chi\sqrt{2q\eta^*/dt}, \quad (67)$$

where p,q are subject to Eq. (66) and otherwise may be chosen arbitrarily. It is easy to see that we cannot make this contribution scale as $1/\sqrt{dt}$, which is a prerequisite for a continuous limit. Indeed, let p scale as $1/dt^s$, where s is some number. The second term in Eq. (67) then scales as $1/dt^{1-s/2}$. The least singular scaling of σ_3' is achieved when both terms scale equally, as $1/dt^{2/3}$.

This way, if $S(\xi|a)$ is a polynomial of a higher than second order in ξ, it does not correspond to any continuous time process (this is the content of Pawula's theorem [18]). In this case, Eq. (54) can only be *approximated* as a characteristic functional of averages of a process in discretized time,

$$ida(t)=(\omega a+\sigma_{\rm reg}+\sigma_3'+\cdots)dt. \quad (68)$$

Unlike in Eq. (60), here $da(t)$ stands for a finite difference, $da(t)=a(t+dt)-a(t)$, and the ellipsis denotes other stochastic contributions.

C. Mathematical subtleties

We will now discuss briefly some of the formal mathematical details which were not investigated in depth in the above considerations. First, Eq. (36) was derived by perturbative means. It is not immediately clear if it makes sense as a nonperturbative relation. The same applies to the formal solution of the classical stochastic response problem, Eq. (54). Our approach, which is based on the formal identity between (36) and (54), is thus, strictly speaking, no more than a conjecture. It is justified in practice by the agreement we observe with the known results of the conventional phase-space approaches, which are based on a more solid mathematical foundation. Outside this scope, a more rigorous derivation of our results remains subject to further work. It should however be noted that, due to time discretization and the causal regularization of the retarded Green's function, perturbative expansions of both Eq. (36) and Eq. (54) contain only a finite number of terms and are thus guaranteed to be convergent. (This implies a finite time interval over which these expansions are written and does not generalize to an arbitrary polynomial interaction Hamiltonian; nor does it directly generalize to relativistic problems.) Although not serving as a formal mathematical proof, this certainly makes our results more plausible.

Second, our derivation of Eq. (60) implied commutivity of the averaging and the differential operation in Eq. (54). This assumption corresponds to that of vanishing boundary terms in the standard derivation via the Fokker-Planck equation [1]. A full discussion of this problem is far outside the scope of the present paper, so we will content ourselves with one observation. In Ref. [21], an imaginary-time version of these techniques was applied to the Kerr oscillator described by Hamiltonian of Eq. (3). The corresponding imaginary-

time SDE was found to be linear, allowing for an exact solution for the stochastic measure. The latter was found to be a genuine convergent measure only for $\kappa<2\omega$. It was shown, however, that the results may be extended into the region $\kappa>2\omega$ (including $\omega<0$) by properly redefining the measure (which in turn may be shown to correspond to an analytical extension of the results over ω [33]). This example demonstrates how the problem of boundary terms may manifest itself in our approach, and how it can be tackled.

Third, the discretized process we find for the case of higher-order noises does not have a continuous time limit. Our assumption is that this limit exists for physical averages, i.e., those corresponding to quantum-field averages. Some arguments in favor of this follow from the aforementioned observation that the perturbation expansion of Eq. (54) contains only a finite number of terms, in other words, it is simply a polynomial. Considering, for instance, the example of Eq. (61), it means that any average of the field $a(t)$ [cf. Eq. (68)] is expressed as a polynomial containing only multiple sums of the products of the function $\varphi_3(a(t))$. This results in a closed Bogoliubov-Born-Green type chain of equations for the averages of $a(t)$, whereas ''nonphysical'' averages [i.e., those mixing $a(t)$ with $a^*(t)$] never occur. A more careful analysis shows that the multiple sums already have a continuous time limit as integrals, resulting in a genuine Bogoliubov-Born-Green chain. It does not prove, however, that a solution to this chain exists (which is another way in which the problem of boundary terms can manifest itself).

It should be noted that, for systems with higher-order noises decribed by SΔEs, the sampling noise grows as the time-grid spacing decreases. This is in contrast to the properties of the Wiener process, where sampling noise is independent of the grid spacing for a given sample size. In practice, however, this distinction between Wiener and higher-order noises is quantitative rather than qualitative. What matters for numerics is not errors for a given sample size, but for a given computational time. From this point of view, differences between Eqs. (60) and (68) (say) are anything but dramatic. Numerics always require time discretization, so that Eq. (60) always has to be approximated as a SΔE. Furthermore, with the computational time fixed, sampling noise for the Wiener process also diverges in the limit $dt\to 0$. The sampling noise for higher-order noises diverges faster, but, as already noted, this difference is quantitative rather than qualitative.

To conclude this discussion we note that numerical stochastic integration is essentially a type of computational experiment. One needs *criteria* of convergence rather than a proof of it. In the cases where we were able to compare the results found using SΔEs with those found using other methods, (see, e.g., Ref. [34], where a ''+W'' SΔE corresponding to the full Wigner representation was simulated) we always encountered the following dilemma. Either the integration converged to a verifiable result, or the failure of the method due to sampling errors and(or) numerical instabilities was obvious. Thus mere convergence of the method appears to be an indication of its reliability. This is consistent with the strategy normally used in $+P$ simulations (and also with the dilemma of the convergent vs divergent measure observed in Ref. [21], discussed three paragraphs above).

V. SUMMARY AND EXAMPLES

A. Technical summary

Although the derivation of our techniques is rather involved, from the practical viewpoint they boil down to a fairly small collection of simple recipes. We will now formulate the results generalized to an n-mode case. For an n-mode system, Schrödinger-picture annihilation and creation operators are vectors with respect to the mode index,

$$\hat{\boldsymbol{a}}=\{\hat{a}_k\},\quad \hat{\boldsymbol{a}}^\dagger=\{\hat{a}_k^\dagger\},\quad k=1,\ldots,n, \tag{69}$$

as are the interaction-picture field operators,

$$\hat{\boldsymbol{a}}(t)=\{\hat{a}_k(t)\},\quad \hat{\boldsymbol{a}}^\dagger(t)=\{\hat{a}_k^\dagger(t)\},\quad k=1,\ldots,n. \tag{70}$$

The system Hamiltonian consists, as usual, of the free and interaction Hamiltonians (implying the interaction picture)

$$\mathcal{H}(t)=\mathcal{H}_0(t)+\mathcal{H}_{\rm int}(t). \tag{71}$$

The free Hamiltonian is

$$\mathcal{H}_0(t)=\hat{\boldsymbol{a}}^\dagger(t)H\hat{\boldsymbol{a}}(t), \tag{72}$$

where $H=\{H_{kk'}\}$, $k,k'=1,\ldots,n$, is a Hermitian matrix in the mode indices. The free Schrödinger equation thus reads

$$i\frac{d\hat{\boldsymbol{a}}(t)}{dt}=H\hat{\boldsymbol{a}}(t). \tag{73}$$

The interaction Hamiltonian is defined in normally ordered form,

$$\hat{\mathcal{H}}_{\rm int}(t)=:h(\hat{\boldsymbol{a}}(t),\hat{\boldsymbol{a}}^\dagger(t)):+\boldsymbol{s}^*(t)\hat{\boldsymbol{a}}(t)+\boldsymbol{s}(t)\hat{\boldsymbol{a}}^\dagger(t), \tag{74}$$

where $\boldsymbol{s}(t)=\{s_k(t)\}$, $k=1,\ldots,n$, is the vector of c-number external sources. The sources are only important if one is interested in a nonlinear-reaction formulation of a quantum system and(or) averages which are other than time-normally ordered.

For simplicity, we only list here the results pertaining to time-normally ordered averages in the presence of the sources; the full assemblage of double-time-ordered averages is accessible via Eqs. (10), (33), (42), and (43). The phase-space description of the quantum system is based on the generic system of $2\times n$ equations,

$$\begin{aligned} i\frac{d\boldsymbol{a}(t)}{dt}&=H\boldsymbol{a}(t)+\boldsymbol{s}(t)+\boldsymbol{\sigma}'(t),\\ -i\frac{d\boldsymbol{a}^\dagger(t)}{dt}&=H\boldsymbol{a}^\dagger(t)+\boldsymbol{s}^*(t)+\boldsymbol{\sigma}'^\dagger(t), \end{aligned} \tag{75}$$

for $2\times n$ c-number random fields,

$$\boldsymbol{a}(t)=\{a_k(t)\},\quad \boldsymbol{a}^\dagger(t)=\{a_k^\dagger(t)\},\quad k=1,\ldots,n. \quad (76)$$

The quantum-classical mapping rules are as in the positive-P representation: replace operators by the c numbers, $\hat{\mathrm{a}}\to\boldsymbol{a}$, $\hat{\mathrm{a}}^\dagger\to\boldsymbol{a}^\dagger$, and the quantum averaging by the statistical averaging associated with the statistics of the random sources $\boldsymbol{\sigma}'$, $\boldsymbol{\sigma}'^\dagger$, e.g.,

$$\langle T_-\hat{\mathrm{a}}_1^\dagger(t_1)\hat{\mathrm{a}}_2^\dagger(t_2)T_+\hat{\mathrm{a}}_3(t_3)\hat{\mathrm{a}}_4^\dagger(t_4)\rangle = \overline{a_1^\dagger(t_1)a_2^\dagger(t_2)a_3(t_3)a_4^\dagger(t_4)}, \quad (77)$$

etc.

All relations listed so far are universal. The physics which, in the quantum problem is in the interaction Hamiltonian, in the phase-space representation enters via the random sources, $\boldsymbol{\sigma}'(t),\boldsymbol{\sigma}'^\dagger(t)$. The nontrivial part of the mapping rules concerns how the latter are found from the former. It reads: first, calculate S_{int} as

$$S_{\mathrm{int}}(\boldsymbol{\xi},\boldsymbol{\xi}^\dagger,\boldsymbol{a},\boldsymbol{a}^\dagger)=ih(\boldsymbol{a}^\dagger,\boldsymbol{a}-i\boldsymbol{\xi})-ih(\boldsymbol{a}^\dagger+i\boldsymbol{\xi}^\dagger,\boldsymbol{a}) =ih(\boldsymbol{a}^\dagger,\boldsymbol{a}-i\boldsymbol{\xi})+(\text{conjugate}), \quad (78)$$

where conjugation acts as a formal Hermitian transformation [i.e., it interchanges quantities with and without dagger, $\boldsymbol{a}(t)\leftrightarrow\boldsymbol{a}^\dagger(t)$, $\boldsymbol{\xi}(t)\leftrightarrow\boldsymbol{\xi}^\dagger(t)$, and complex conjugates other c numbers]. Second, ''stochastically linearize'' S_{int} using a suitable set of Hubbard-Stratonovich transformations,

$$\exp[dtS_{\mathrm{int}}(\boldsymbol{\xi},\boldsymbol{\xi}^\dagger,\boldsymbol{a},\boldsymbol{a}^\dagger)]=\overline{\exp[dt(\boldsymbol{\xi}\boldsymbol{\sigma}'^\dagger+\boldsymbol{\xi}^\dagger\boldsymbol{\sigma}')]}. \quad (79)$$

(Note that terms without ξ's in S_{int} always cancel.) The σ''s thus obtained are exactly those to be substituted in Eqs. (75). This completes their derivation. If S_{int} is at most quadratic in ξ's, Eqs. (75) are a system of genuine Itô stochastic differential equations. Otherwise they can only be interpreted as difference equations over a finite time step dt.

We complete this section by introducing a shorthand notation for the real, Eq. (63), and complex, Eq. (64), Hubbard-Stratonovich transformations, respectively,

$$x^2\overset{\chi}{\to}x\chi\sqrt{2},\quad xy\overset{\eta}{\Rightarrow}x\eta+y\eta^*. \quad (80)$$

These relations imply the definition of the corresponding noises as standardized Gaussian Kronecker-correlated noises (respectively, real and complex ones), cf. Eqs. (57) and (62). They allow one to directly process S_{int} into the σ''s while avoiding most of the bookkeeping.

B. Quantum reaction of the Kerr oscillator

We now return to our demonstration system. Using the short-hand notation, Eq. (80), S_{int} given by Eq. (37) is processed as

$$dtS_{\mathrm{int}}(\xi,\xi^\dagger,a,a^\dagger)=dt\kappa\xi a^{\dagger 2}a+dt\frac{i\kappa}{2}\xi^{\dagger 2}a^2 +(\text{conjugate}) \overset{\chi,\chi^\dagger}{\to} dt\xi^\dagger(\kappa a^2a^\dagger+\sqrt{i\kappa/dt}\chi a) +(\text{conjugate}), \quad (81)$$

where we have introduced two real Gaussian noises, $\chi(t)$ and $\chi^\dagger(t)$ (the latter being found in the conjugate term). This completes the derivation of the Itô SDEs for the classical fields which read

$$i\frac{da(t)}{dt}=s(t)+\kappa a^2(t')a^\dagger(t')+\sqrt{i\kappa/dt}\chi(t')a(t'),$$

$$-i\frac{da^\dagger(t)}{dt}=s^*(t)+\kappa a^{\dagger 2}(t')a(t')+\sqrt{-i\kappa/dt}\chi^\dagger(t')a^\dagger(t'). \quad (82)$$

As was explained above, the fact that Itô calculus should be chosen is due to the causal regularization of $G(t)$, which makes the fields independent of the sources at the same time moment.

Without the external sources (i.e., with $s=0$), equations such as Eq. (82) are well known in quantum optics under the name of the positive-P representation. In that form, they allow one to calculate time-normal averages of the field operators, describing *radiation* properties of the system. With the sources included, they cover the full quantum-stochastic nonlinear *reaction* problem. They also become applicable to a much wider assemblage of operator averages, cf. Eqs. (10), (33), (42), and (43).

C. Degenerate OPO

We shall now illustrate the simplicity of the general recipe in a multimode case by deriving the positive-P equations for a degenerate optical parametric oscillator (OPO). The degenerate OPO consists of two coupled oscillators described by the Hamiltonian

$$\mathcal{H}=\omega\hat{a}_1\hat{a}_1^\dagger+2\omega\hat{a}_2\hat{a}_2^\dagger+\frac{i\kappa}{2}[\hat{a}_1^{\dagger 2}\hat{a}_2-\hat{a}_1^2\hat{a}_2^\dagger]. \quad (83)$$

Then,

$$
\begin{aligned}
S_{\mathrm{int}}(\boldsymbol{\xi},\boldsymbol{\xi}^{\dagger},\boldsymbol{a},\boldsymbol{a}^{\dagger}) &= i\frac{i\kappa}{2}[a_1^{\dagger 2}(a_2 - i\xi_2) - (a_1 - i\xi_1)^2 a_2^{\dagger}] \\
&\quad + (\text{conjugate}) \\
&= -i\kappa\xi_1 a_1 a_2^{\dagger} + i\frac{\kappa}{2}\xi_2 a_1^{\dagger 2} - \frac{\kappa}{2}\xi_1^2 a_2^{\dagger} \\
&\quad + (\text{conjugate}) \\
&\overset{\chi,\chi^{\dagger}}{\rightarrow} + i\xi_1^{\dagger}(\kappa a_1^{\dagger} a_2 + \chi\sqrt{\kappa a_2}) \\
&\quad - i\xi_2^{\dagger}\frac{\kappa}{2}a_1^2 - i\xi_1(\kappa a_1 a_2^{\dagger} + \chi^{\dagger}\sqrt{\kappa a_2^{\dagger}}) \\
&\quad + i\xi_2\frac{\kappa}{2}a_1^{\dagger 2}, \qquad (84)
\end{aligned}
$$

where $\chi(t),\chi^{\dagger}(t)$ are a pair of independent real δ-correlated Gaussian noises. The positive-P representation equations for the OPO, generalized to the response problem, then read

$$
\begin{aligned}
\frac{da_1(t)}{dt} &= -i\sigma_1(t) + \kappa a_1^{\dagger}(t)a_2(t) + \chi(t)\sqrt{\kappa a_2(t)}, \\
\frac{da_1^{\dagger}(t)}{dt} &= +i\sigma_1^{\dagger}(t) + \kappa a_1(t)a_2^{\dagger}(t) + \chi^{\dagger}(t)\sqrt{\kappa a_2^{\dagger}(t)}, \qquad (85) \\
\frac{da_2(t)}{dt} &= -i\sigma_2(t) - \frac{\kappa}{2}a_1^2(t), \\
\frac{da_2^{\dagger}(t)}{dt} &= +i\sigma_2^{\dagger}(t) - \frac{\kappa}{2}a_1^{\dagger 2}(t).
\end{aligned}
$$

This derivation is strikingly simple and straightforward, and compares very favorably to the common derivation based on phase-space techniques [2] [not to mention that Eqs. (85) allow for a much deeper insight].

D. Triply degenerate four-wave mixing: Stochastic difference equations

As an illustrative example of a multimode system which requires the stochastic difference treatment, we will consider here the system of triply degenerate four-wave mixing in a nonlinear medium, where three of the waves have frequency ω and the fourth has frequency 3ω [24]. In our derivation we will make the approximation that only two modes are important, so as to demonstrate our method in the most simple way possible. These processes can then be described by the interaction Hamiltonian

$$
\mathcal{H}(z) = \frac{i\hbar\kappa}{3}[\hat{a}^{\dagger 3}\hat{b} - \hat{a}^3\hat{b}^{\dagger}], \qquad (86)
$$

where $\hat{a}(z)$ and $\hat{b}(z)$ are the annihilation operators for quanta at frequencies ω and 3ω, respectively, at position z inside the nonlinear medium, and κ represents the effective couping between the modes. Note that we are assuming a trivial relationship between propagation time and position here.

Assuming that z is a discrete variable changing in finite steps of dz, we write

$$
\begin{aligned}
dzS_{\mathrm{int}} &= dz\left[\xi_1^{\dagger}\kappa\alpha^{\dagger 2}\beta + \xi_1^{\dagger 2}\kappa\alpha^{\dagger}\beta + \xi_1^{\dagger 3}\frac{\kappa}{3}\beta + \xi_2^{\dagger}\left(-\frac{\kappa}{3}\alpha^3\right)\right] \\
&\quad + (\text{conjugate}), \qquad (87)
\end{aligned}
$$

where the c-number variables $(\alpha,\alpha^{\dagger}\beta,\beta^{\dagger})$ are equivalent in the $+P$ sense to the operators $(\hat{a},\hat{a}^{\dagger},\hat{b},\hat{b}^{\dagger})$. This completes the first step of the derivation. The deterministic terms in the resulting equations of motion are immediately obvious, being those to first order in the ξ's in Eq. (87). The noise terms are readily found using real and complex Hubbard-Stratonovich transformations, respectively. In the short-hand of Eq. (80), applying a real HST to the quadratic term in Eq. (87) yields

$$
dz\xi_1^{\dagger 2}\kappa\alpha^{\dagger}\beta \overset{\chi_1}{\rightarrow} \xi_1^{\dagger}\chi_1\sqrt{2\kappa\alpha^{\dagger}\beta dz}. \qquad (88)
$$

The cubic term in S_{int}, $dz\xi_1^{\dagger 3}\kappa\beta/3$, is also simply taken care of, by applying a complex HST followed by a real one,

$$
dz\xi_1^{\dagger 3}\frac{\kappa\beta}{3} \overset{\eta}{\Rightarrow} dz\xi_1^{\dagger 2}\frac{p}{2}\eta + \xi_1^{\dagger}q\eta^* \overset{\chi_2}{\rightarrow} \xi_1^{\dagger}(\chi_2\sqrt{p\eta dz} + q\eta^*). \qquad (89)
$$

After formal conjugation, we obtain the set of coupled SΔEs,

$$
\begin{aligned}
d\alpha &= \kappa\alpha^{\dagger 2}\beta dz + \chi_1\sqrt{2\kappa\alpha^{\dagger}\beta dz} + \chi_2\sqrt{p\eta dz} + q\eta^*, \\
d\alpha^{\dagger} &= \kappa\alpha^2\beta^{\dagger}dz + \chi_1^{\dagger}\sqrt{2\kappa\alpha\beta^{\dagger}dz} + \chi_2^{\dagger}\sqrt{p^{\dagger}\eta^{\dagger}dz} + q^{\dagger}\eta^{\dagger *}, \qquad (90) \\
d\beta &= -\frac{\kappa}{3}\alpha^3 dz, \\
d\beta^{\dagger} &= -\frac{\kappa}{3}\alpha^{\dagger 3}dz,
\end{aligned}
$$

with the p's and q's constrained by the conditions

$$
pq = \frac{2\kappa\beta}{3}, \quad p^{\dagger}q^{\dagger} = \frac{2\kappa\beta^{\dagger}}{3} \qquad (91)
$$

due to our choice of complex transformations, but otherwise arbitrary. Equations (90) contain four real $(\chi_1,\chi_2,\chi_1^\dagger,\chi_2^\dagger)$ and two complex $(\eta,\eta^\dagger)$ Gaussian noises, which are all $\delta_{zz'}$ (Kronecker) correlated. We note here that Eq. (90) without the third-order noises has a natural continuous limit identical to positive-*P* equations obtained via the usual methods, but that the derivation is much shorter. For situations with noises of less than third order, this method of finding the equations is almost trivial as compared to proceeding via the master and Fokker-Planck equations. We note here that equations with third-order noises have previously been introduced for intracavity third harmonic generation [35,36], but without full details of the derivation and without stating that the equations could not be understood as genuine stochastic differential equations.

VI. CONCLUSION

Over recent years the technique of stochastic integration has proven to be a very powerful tool for the computation of operator expectation values in dynamical quantum systems, especially in the field of quantum optics. Its exact application, however, has necessarily been limited to systems possessing Hamiltonians which can be mapped onto genuine Fokker-Planck equations. Even in these cases, the derivation of the appropriate stochastic differential equations can be a time consuming process. For processes which result in a time evolution equation with derivatives of higher than second order, there is no mapping onto stochastic differential equations.

We have used the techniques of quantum-field theory to develop a powerful method for the mapping of operator Hamiltonians onto stochastic equations in a positive-*P* representation, which can include the full nonlinear stochastic response problem. Instead of taking the usual phase-space route from operator Hamiltonian via a master equation and an FPE to *c*-number equations [1,2], we show how stochastic representations may be derived by directly linking operator Heisenberg equations of motion to *c*-number Langevin equations. For Hamiltonians which are no more than quadratic in either annihilation or creation operators, we find the appropriate positive-*P* stochastic differential equations after no more than a few lines of algebra. For systems of higher order, we find SΔEs in a discretized version of Itô calculus, which although we cannot define a continuous limit as SDEs, we can simulate numerically. Our approach thus has two main advantages. First, the use of real Hubbard-Stratonovich transformations provides a quick and effective method to find stochastic differential equations, while inherent in the method is a freedom in the choice of noise terms which can be used to dramatically decrease the sampling errors [10] which are often a problem with stochastic integration. Second, the use of real and complex transformations allows for the extension of stochastic simulation to a much wider class of problems than can be considered using the conventional approach.

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APPENDIX: QUANTUM NONLINEAR STOCHASTIC RESPONSE THEORY

In terms of quantum averages, Eq. (43) reads

$$\begin{aligned}\langle T_-\exp(\zeta^\dagger\hat{\hat{a}})T_+\exp(\zeta\hat{\hat{a}}^\dagger)\rangle &= \Big\langle T_-\exp\int dt[(\zeta+is)\hat{a}^\dagger+is^*\hat{a}] \\ &\quad\times T_+\exp\int dt[(\zeta^\dagger-is^*)\hat{a}-is\hat{a}^\dagger]\Big\rangle, \quad \text{(A1)}\end{aligned}$$

where we have used the definition of the causal variables, Eqs. (35), for the special case $\sigma(t)=\sigma^{\dagger *}(t)=s(t)$. From (A1), we immediately find

$$\begin{aligned}\langle T_-\hat{\hat{a}}^\dagger(t_1')\cdots\hat{\hat{a}}^\dagger(t_n')T_+\hat{\hat{a}}(t_1)\cdots\hat{\hat{a}}(t_m)\rangle &= \Big\langle T_-\hat{a}^\dagger(t_1')\cdots\hat{a}^\dagger(t_n') \\ &\quad\times\exp\Big[i\int dt(s\hat{a}^\dagger+s^*\hat{a})\Big]T_+\hat{a}(t_1)\cdots\hat{a}(t_m) \\ &\quad\times\exp\Big[-i\int dt(s\hat{a}^\dagger+s^*\hat{a})\Big]\Big\rangle. \quad \text{(A2)}\end{aligned}$$

This relation allows one to find various quantum nonlinear stochastic response functions of the system. So, for the linear response, we recover Kubo's relation

$$\left.\frac{\delta\langle\hat{\hat{a}}(t)\rangle}{\delta s(t')}\right|_{s=0}=\left.\frac{\delta\Big\langle T_-\exp\Big[i\int dt''(s\hat{a}^\dagger+s^*\hat{a})\Big]T_+\hat{a}(t)\exp\Big[-i\int dt''(s\hat{a}^\dagger+s^*\hat{a})\Big]\Big\rangle}{\delta s(t')}\right|_{s=0}=i\langle\hat{a}^\dagger(t')\hat{a}(t)\rangle-i\langle T_+\hat{a}^\dagger(t')\hat{a}(t)\rangle$$
$$=-i\theta(t-t')\langle[\hat{a}(t),\hat{a}^\dagger(t')]\rangle. \quad \text{(A3)}$$

For the anomalous linear response

$$\left.\frac{\delta\langle\hat{\tilde{a}}^{\dagger}(t)\rangle}{\delta s(t')}\right|_{s=0} = i\langle T_{-}\hat{a}^{\dagger}(t)\hat{a}^{\dagger}(t')\rangle - i\langle\hat{a}^{\dagger}(t)\hat{a}^{\dagger}(t')\rangle$$
$$= -i\,\theta(t-t')\langle[\hat{a}^{\dagger}(t),\hat{a}^{\dagger}(t')]\rangle, \qquad \text{(A4)}$$

again as expected. (This is certainly zero for the Hamiltonian (3), but can be nonzero for systems like the OPO. Importantly, relation (A2) does not depend on the nonlinear interaction.) Nonlinear response functions are found by multiple differentiations. A simple example of a stochastic response function is (average field intensity vs source amplitude)

$$\left.\frac{\delta\langle\hat{\tilde{a}}^{\dagger}(t)\hat{\tilde{a}}(t')\rangle}{\delta s(t'')}\right|_{s=0} = i\langle[T_{-}\hat{a}^{\dagger}(t)\hat{a}^{\dagger}(t'')]\hat{a}(t')\rangle$$
$$-i\langle\hat{a}^{\dagger}(t)[T_{+}\hat{a}^{\dagger}(t'')\hat{a}(t')]\rangle$$
$$= i\,\theta(t-t'')\langle\hat{a}^{\dagger}(t'')\hat{a}^{\dagger}(t)\hat{a}(t')\rangle$$
$$-i\,\theta(t'-t'')\langle\hat{a}^{\dagger}(t)\hat{a}(t')\hat{a}^{\dagger}(t'')\rangle$$
$$+i[\,\theta(t''-t)-\theta(t''-t')]$$
$$\times\langle\hat{a}^{\dagger}(t)\hat{a}^{\dagger}(t'')\hat{a}(t')\rangle, \qquad \text{(A5)}$$

and so on.

Note that the final expression in Eq. (A5) is explicitly causal, as certainly are Eqs. (A3) and (A4). A formal proof of causality in the representation of causal variables may be found in Ref. [15].

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