Optimization of the positive-*P* representation for the anharmonic oscillator

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We demonstrate how the freedom in the definition of the positive-*P* representation may be used to reduce stochastic sampling errors, using the single-mode anharmonic oscillator as an example. In the modeling of this system, which is well known for being problematic, we achieve an improvement of more than 20 orders of magnitude in the distribution of the trajectories.

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I. INTRODUCTION

The lack of numerical convergence of the positive-*P* representation [1] for undamped systems with a strong $\chi^{(3)}$ component is well known and is a severe problem for investigations of the quantum-dynamical properties of Bose-Einstein condensates (BEC) [2]. The problem is that individual stochastic trajectories can visit regions of the phase space where any computer loses its numerical accuracy. While the process of evaporative cooling by which a condensate is formed has been successfully modeled, the numerics quickly break down once condensation has been achieved [3]. Unless we wish to model processes for which the interesting physics happens over a very short time [4], stochastic integration of the condensate equations has not been a realistic option. Although at least two methods have been proposed and are under development in an attempt to solve this problem [5,6], general methods of taming the positive-*P* representation are yet to be developed.

The essence of phase-space techniques [7] is replacing *q*-number equations for operators by *c*-number equations for certain random *c*-number quantities, averages of which equal the operator averages. In this way, direct computer simulations of quantum systems become possible. From this perspective, any representation in phase space is a mapping of the quantum system in question onto a classical stochastic system. As has been pointed out recently by Plimak *et al.* [8], this mapping is anything but unique. What we demonstrate in this paper is that it is possible, using this freedom, to achieve an improvement of many orders of magnitude in the sampling error for the single-mode anharmonic oscillator case. This results in a dramatic reduction in sampling noise, changing things from ''computable in principle'' to ''computable in practice.''

Although our demonstration is based on the existence of analytical solutions to the positive-*P* equations for this particular system, this example is important in that it points to one avenue of investigation for further enquiry. What we are able to show is that the principle is valid. Generalization to systems where analytical solutions are not known, which is exactly where stochastic simulation is useful, is subject to further work.

II. GENERALIZED POSITIVE-*P* REPRESENTATION

Recently, an alternative field-theoretical approach to phase-space techniques has been proposed that allows the derivation of stochastic differential equations (SDEs) directly from a quantum Hamiltonian [8–10]. Its main advantage is that it makes the freedom involved in the derivation of quantum-classical mappings more manageable, allowing one to optimize the stochastics in the *c*-number equations.

For the purposes of demonstration we consider a single-mode bosonic quantum field with quartic interaction: the Kerr oscillator. It is described by the Hamiltonian

$$H=\omega_0\hat{a}^\dagger\hat{a}+\frac{\kappa}{2}\hat{a}^{\dagger 2}\hat{a}^2, \tag{1}$$

where $\hat{a}$ and $\hat{a}^\dagger$ are the usual pair of annihilation and creation operators, with commutation relation $[\hat{a},\hat{a}^\dagger]=1$. We use units such that $\hbar=1$. Following either the usual methods [7] or those outlined in Refs. [8–10], the following pair of coupled Itô SDEs can be obtained in a rotating frame:

$$i\partial_t a_1(t)=\kappa a_1^2(t)a_2^*(t)+\eta_1(t)a_1(t), \tag{2a}$$

$$i\partial_t a_2(t)=\kappa a_2^2(t)a_1^*(t)+\eta_2(t)a_2(t). \tag{2b}$$

The standard positive-*P* representation [1,7] is found by choosing the noises η_1,η_2 to be proportional to independent real standardized Gaussian noises, x_1,x_2,

$$\eta_k(t)=\sqrt{i\kappa}x_k(t),\quad \overline{x_k(t)x_l(t')}=\delta_{kl}\delta(t-t'),\quad k,l=1,2. \tag{3}$$

Stochastic averages over trajectories of the *c*-number variables equal the quantum operator expectation values. More precisely speaking, one finds the time-normally ordered averages of the Heisenberg operators, $\hat{a}(t),\hat{a}^\dagger(t)$, mapped onto stochastic averages of the random c-numbers, $a_1(t),a_2(t)$, as, for example,

$$\langle\hat{a}^\dagger(t')\hat{a}(t)\rangle=\overline{a_1(t)a_2^*(t')}. \tag{4}$$

Note that the time argument signifies that these are now Heisenberg operators, as opposed to the Schrödinger operators used in Eq. (1).

The positive-*P* equations for this system are notorious for numerical problems upon computer simulation. Some reasons for this difficulty are easy to understand. If we rewrite them as Stratonovich equations, which is equivalent to the replacement $a_{1,2}\to e^{-i\kappa t/2}a_{1,2}$, and also assume that $a_1(0)$

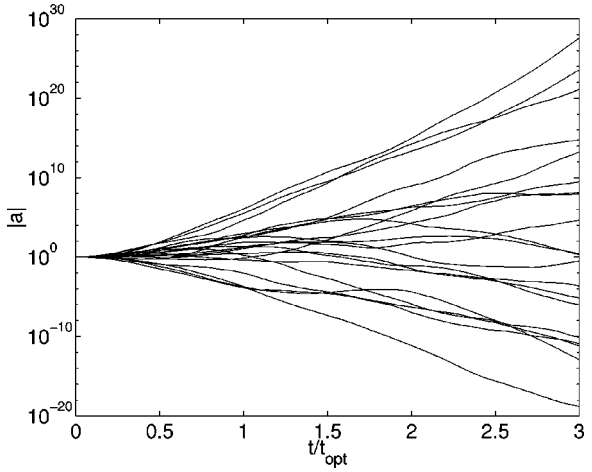

FIG. 1. A sample of 20 trajectories generated without noise optimization ($A=1$) in units of $\sqrt{N}$ for $N=10^4$ and $\kappa=10^{-2}$.

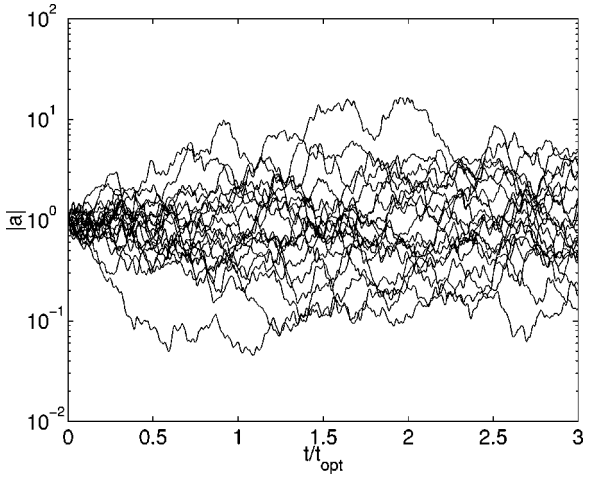

FIG. 2. A sample of 20 trajectories generated with noise optimization ($A=300$) in units of $\sqrt{N}$ for $N=10^4$ and $\kappa=10^{-2}$.

$=a_2(0)=a_0$, they can easily be solved analytically. Defining $\rho_{12}(t)=a_1(t)a_2^*(t)$, we may write the equation of motion,

$$i\partial_t\rho_{12}(t)=\eta_{12}(t)\rho_{12}(t), \tag{5}$$

where $\eta_{12}(t)=\eta_1(t)-\eta_2^*(t)$, so that

$$\rho_{12}(t)=N\exp\left[-i\int_0^t dt'\,\eta_{12}(t')\right], \tag{6}$$

where $N=|a_0|^2$ is the average number of quanta in the mode. Hence,

$$a_1(t)=a_0\exp\left[-i\kappa t/2-i\int_0^t dt'\,\eta_1(t')\right]\times\exp\left\{-iN\kappa\int_0^t dt'\exp\left[-i\int_0^{t'}dt''\,\eta_{12}(t'')\right]\right\}, \tag{7a}$$

$$a_2(t)=a_0\exp\left[-i\kappa t/2-i\int_0^t dt'\,\eta_2(t')\right]\times\exp\left\{-iN\kappa\int_0^t dt'\exp\left[i\int_0^{t'}dt''\,\eta_{12}^*(t'')\right]\right\}. \tag{7b}$$

One reason for the bad behavior of the positive-P representation now becomes evident. If $N\gg 1$, which is generally the case in physical systems, the exponent in the second factor can become very large even when the "small noise" condition, $\kappa t\ll 1$, holds.

The quantum-field-theoretical techniques of Refs. [8–10] expose a huge freedom that exists in choosing the noises η_1,η_2. Formally, only stochastic cumulants involving η_1 and η_2^* have to be fixed (for a definition of cumulants see, e.g., [11]). Cumulants mixing these with their complex conjugates may be chosen almost at will, with the only reservation being that they correspond to a positive probability. In general, the noises η_1 and η_2 are not bound to be Gaussian, nor even Markovian. In this paper we do not explore this freedom in full, confining our analysis to a pair of δ-correlated Gaussian noises. Of eight cumulants characterizing such a pair, the five that are essential for a correct relation to the quantum problem are fixed by

$$\overline{\eta_1(t)}=\overline{\eta_2(t)}=0,\quad \overline{\eta_1(t)\,\eta_2^*(t')}=0,$$
$$\overline{\eta_1(t)\,\eta_1(t')}=\overline{\eta_2(t)\,\eta_2(t')}=i\kappa\delta(t-t'). \tag{8}$$

The three inessential cumulants, $\overline{\eta_1(t)\,\eta_1^*(t')}$, $\overline{\eta_2(t)\,\eta_2^*(t')}$, and $\overline{\eta_1(t)\,\eta_2(t')}$, will be chosen so as to reduce the effect of the nonlinearity on the noise in the solutions (7).

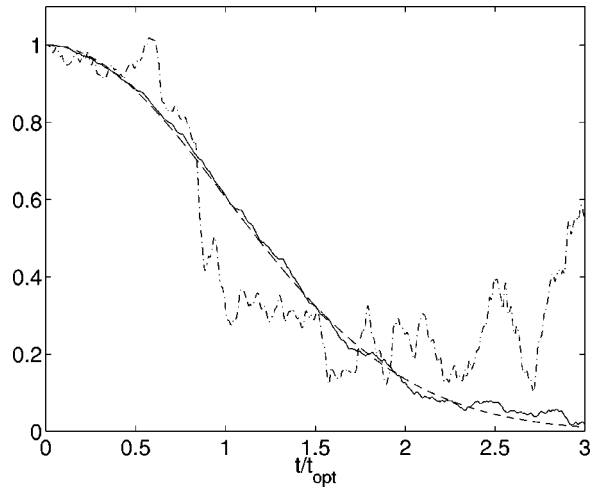

FIG. 3. Modulus of the correlation function (14), in units of N, found by simulating the noise-tuned positive-P equations ($A=300$) for $N=10^4$ and $\kappa=10^{-2}$. Results found with samples of 10^2 and 10^4 trajectories are plotted as, respectively, dash-dotted and solid lines; the analytical result (14) is plotted as a dashed line.

III. OPTIMIZATION OF THE POSITIVE P

Note, first of all, that the average $\overline{\eta_{12}(t)\eta_{12}^*(t')} = \overline{\eta_1(t)\eta_1^*(t')} + \overline{\eta_2(t)\eta_2^*(t')} - 2\Re\overline{\eta_1(t)\eta_2(t')}$ is inessential. However, it cannot be simply made zero. This would require $\eta_1(t) = \eta_2^*(t)$, which is incompatible with the essential averages. We therefore assume that $\overline{\eta_1(t)\eta_1^*(t')} = \overline{\eta_2(t)\eta_2^*(t')} = i\kappa A\delta(t-t')$, where $A \geqslant 1$ is a constant, and then use the remaining freedom in the average $\overline{\eta_1(t)\eta_2(t')}$ so as to minimize $\overline{\eta_{12}(t)\eta_{12}^*(t')}$. This results in

$$\eta_1(t) = \sqrt{i\kappa/2}[x_1(t)\sqrt{A+1} - ix_2(t)\sqrt{A-1}], \tag{9a}$$

$$\eta_2(t) = \sqrt{i\kappa/2}[x_2(t)\sqrt{A+1} - ix_1(t)\sqrt{A-1}], \tag{9b}$$

where x_1, x_2 are the pair of standardized real Gaussian noises introduced by Eq. (3). The usual positive-P representation follows with $A=1$.

Using Eq. (9) we find

$$\overline{\eta_{12}(t)\eta_{12}^*(t')} = 2\kappa(A - \sqrt{A^2-1}) \approx \frac{\kappa}{A}, \tag{10}$$

where the final estimate holds if $A \gg 1$. Hence if $A \to \infty$, the noise in the second factor in solutions (7) is suppressed, while the noise in the first factor is enhanced. If for $A=1$ the noise originating in the second factor dominates, then there must exist an optimal A which minimizes the total noise.

Assume that $A \gg 1$ and that an eased small noise condition, $\kappa t \ll A$, holds. Then,

$$\int_0^t dt' \exp\left[-i\int_0^{t'} dt''\eta_{12}(t'')\right] \approx t - i\int_0^t dt' \int_0^{t'} dt''\eta_{12}(t'')$$

$$= t + \mathcal{O}\left(\sqrt{\frac{\kappa t^3}{3A}}\right), \tag{11}$$

where we write $a = \mathcal{O}(b)$, implying that $\overline{|a|^2} = b^2$. Similarly,

$$\int_0^t dt'\,\eta_1(t') = \mathcal{O}(\sqrt{A\kappa t}). \tag{12}$$

By comparing these two estimates, we may find the optimization condition

$$\frac{N\kappa}{2}\sqrt{\frac{\kappa t^3}{3A}} \sim \sqrt{A\kappa t}, \tag{13}$$

resulting in $A \sim N\kappa t$. This corresponds to the contribution (11) to the noise being $\sqrt{N\kappa t}$ times suppressed. We should note that we have neglected correlations between Eqs. (12) and (11), so that our estimates are only correct within an order of magnitude.

These results can be viewed from a different perpective. Without optimization ($A=1$), the time for which the noise in Eq. (7) becomes large is estimated as $N(\kappa t_0)^{3/2} \sim 1$. With optimization, this becomes $N^{1/2}\kappa t_{\rm opt} \sim 1$, so that $t_{\rm opt}/t_0 \sim \sqrt{N\kappa t_0} \sim N^{1/6}$. This reflects an increase in the time interval over which one can expect simulations using Eqs. (2) to remain reasonably convergent. However, even with optimization the small noise condition is $N^{1/2}\kappa t_{\rm opt} \lesssim 1$, not $\kappa t_{\rm opt} \lesssim 1$. For $t \gg t_{\rm opt}$, the noise still grows exponentially.

The effect of this noise optimization is illustrated in Figs. 1, 2, and 3. The goal was to estimate the quantum average [also calculated analytically directly from Eq. (1)],

$$\langle \hat{a}^\dagger(t)\hat{a}(0)\rangle = \exp\{-i\kappa t/2 + N[\exp(-i\kappa t) - 1]\}, \tag{14}$$

using stochastic integration. In Fig. 1 a typical sample of 20 random trajectories is shown, which were generated without optimization ($A=1$) for the parameters $N=10^4$, $\kappa = 0.01$, over the time $t = 3t_{\rm opt} = 3$. The trajectories eventually span more than 40 orders of magnitude, so without optimization a sample of more than 10^{40} trajectories would be needed in order to suppress the sampling errors by brute force, and each trajectory would have to be generated to more than 40 decimal places to prevent loss of accuracy. Without optimization, stochastic integration of the correlation function (14) is not feasible. The trajectories in Fig. 2 were generated for the same set of parameters but with optimization ($A=300$). They span about two orders of magnitude, so that a sample of a hundred trajectories should suffice for a rough estimate of (14). In Fig. 3 we present the results of the Monte Carlo calculation of the modulus of Eq. (14), using samples of 10^2 and 10^4 noise-optimized trajectories. We see that averaging of as few as 100 trajectories gives an indication of the quantity sought, while averaging of 10^4 trajectories leads to a good result.

An interesting observation is that $t_{\rm opt}$ is of the order of the phase-correlation (collapse) time for the nonlinear oscillator. Whether this reflects any fundamental properties of quantum systems or is just a coincidence is subject to further investigation.

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