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# Numerical representation of quantum states in the positive-*P* and Wigner representations

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ABSTRACT

Numerical stochastic integration is a powerful tool for the investigation of quantum dynamics in interacting many-body systems. As with all numerical integration of differential equations, the initial conditions of the system being investigated must be specified. With application to quantum optics in mind, we show how various commonly considered quantum states can be numerically simulated by the use of widely available Gaussian and uniform random number generators. We note that the same methods can also be applied to computational studies of Bose–Einstein condensates, and give some examples of how this can be done.



## 1. Introduction

The theoretical study of non-equilibrium quantum many-body dynamics is a growing area, especially since the experimental achievement of trapped Bose–Einstein condensates. Many of the methods used for theoretically investigating condensates have been adapted from theoretical quantum optics [1], with varying degrees of success. One particular approximation technique that proved extremely successful in quantum optics is linearisation of the fluctuations about solutions of the classical equations of motion. This technique, if used appropriately, is a very powerful tool for the calculation of the steady-state spectra of intracavity parametric processes [2]. However, in a dynamically evolving system, or one operating near phase transitions or critical points, this method can give incorrect answers [3,4]. The validity of the approximation depends on three conditions. The first of these is that the solution of the classical equations is the same as the mean-field solution of the full quantum equations. The second and third are that the fluctuations about these solutions are in some sense small and that they can be represented as Gaussian, so that moments of higher than second order vanish. In the study of trapped Bose–Einstein condensates, the Hartree–Fock–Bogoliubov (HFB) method is a closely related approximation [5], and therefore needs to be used with the same care as the linearised fluctuation approximation in quantum optics.

When these conditions are not met, there are still a number of ways to proceed. In some very rare cases it may be possible to solve directly either a master equation for the density matrix, or even the Heisenberg equations of motion for the actual system operators. However, the most interesting quantum dynamics are not generally restricted to such cases. One set of methods which has been very successful is the phase-space representations originally used to develop stochastic differential equations in quantum optics [6]. These allow common classes of quantum Hamiltonians to be mapped via master and Fokker–Planck equations onto stochastic differential equations. In some cases the Fokker–Planck equation may be solved directly for a pseudoprobability distribution which then allows for the calculation of operator moments [1,7]. Once again, these cases are rare and can often only be solved in the steady-state regime. The method of choice if we wish to obtain dynamical quantum information is then to numerically integrate the stochastic equations of motion. As with any numerical analysis of differential equations, this then requires that the initial conditions be specified, as these can have marked effects on the subsequent dynamics, in both optical [8,9] and interacting atomic and molecular systems [10–16]. In what follows we will begin with a brief outline of the theory behind the phase-space representations and

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then show how to numerically simulate some of the more common and useful initial quantum states of optics and condensed atom physics, in both the positive-*P* [17] and Wigner representations [18].

## 2. Phase-space representations of the density matrix

Phase space techniques are a powerful tool to investigate the full quantum dynamics of interacting quantum systems in cases where it is impractical to solve either the Heisenberg equations of motion or the master (von Neumann) equation for the density matrix. Instead of working with operators or density matrices, they allow us to work directly with classical *c*-number variables, which are amenable to manipulation on available computers. Perhaps more importantly, the complexity of the computation scales with the number of interacting modes rather than with the size of the Hilbert space, which is often completely intractable. In fact, a single-mode quantum calculation has been performed using these methods for the order of $10^{23}$ interacting quanta [19], which would be completely out of the question using other methods. There are a number of phase-space representations, among them being the Wigner representation [18], the Glauber–Sudarshan *P* representation [20,21], the *Q* representation [22] (sometimes known as the Husimi representation), the complex *P* representation [17], and the *R* representation [20]. The most useful for numerical work are the positive-*P* and truncated Wigner representations [23], the latter being an approximation to the full Wigner representation.

### 2.1. Truncated Wigner equations

Historically, the first of these phase-space representations was the Wigner representation [18], which was formulated as a pseudoprobability function for the position and momentum of a particle. Mathematically, the quadrature phase amplitudes of quantum optics are completely equivalent to position and momentum, so that the Wigner function is a frequently used tool for describing nonclassical states of bosonic fields. Quantum mechanical expectation values for operator products expressed in symmetrical order are found naturally in the Wigner representation as classical averages of the corresponding Wigner variables. As an example, making the correspondence between the single-mode annihilation operator $\hat{a}$ and the complex Wigner variable $\alpha$, we find that

$$\overline{\alpha^*\alpha} = \frac{1}{2}\langle \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\rangle = N + \frac{1}{2}, \tag{1}$$

where $N$ is the number of quanta in the mode. Given a general Hamiltonian which is some combination of bosonic creation and annihilation operators, $H$, we find the von Neumann equation as

$$i\hbar\frac{d\rho}{dt} = [H,\rho], \tag{2}$$

from which the equation of motion for the Wigner function, $W$, is found using the correspondence rules,

$$\hat{a}\rho \leftrightarrow \left(\alpha + \frac{1}{2}\frac{\partial}{\partial\alpha^*}\right)W, \quad \hat{a}^\dagger\rho \leftrightarrow \left(\alpha^* - \frac{1}{2}\frac{\partial}{\partial\alpha}\right)W,$$
$$\rho\hat{a} \leftrightarrow \left(\alpha - \frac{1}{2}\frac{\partial}{\partial\alpha^*}\right)W, \quad \rho\hat{a}^\dagger \leftrightarrow \left(\alpha^* + \frac{1}{2}\frac{\partial}{\partial\alpha}\right)W. \tag{3}$$

Following the standard methods [24], as long as the equation found by the above procedure has no derivatives of higher than second order, it can be mapped onto a set of stochastic differential equations for the variables $\alpha$ and $\alpha^*$. Unfortunately, all interesting problems result in derivatives of third order or more and, although methods exist for mapping the resulting generalised Fokker–Planck equations onto stochastic difference equations [25], these are not very useful in practice. A common practice is to truncate the partial differential equation for the Wigner function at second order, often justified by claiming that the effect of these terms is small. This procedure may be formally justified by requiring the system modes to be highly occupied, and results in stochastic differential equations in what is known as the truncated Wigner representation. If there are no second order derivatives, the resulting equations are regular and quantum noise enters via the initial Wigner distribution for the variables. In optical problems, this then becomes functionally equivalent to stochastic electrodynamics [26] and has been shown to give misleading results in some cases [27,28]. This approximate method has also been used with some success in the study of Bose–Einstein condensates [29–32] and is closely related to "classical field methods", including the stochastic Gross–Pitaevski equation [33–36]. The appropriate initial states to use in the truncated Wigner equations are exactly the same as those that would be used in a full Wigner representation, with the approximations entering into the equations of motion.

### 2.2. Positive-P representation

The Glauber–Sudarshan *P* representation [20,21] is another representation of the density matrix in terms of coherent states and gives averages of the phase-space variables which are equivalent to normally-ordered operator expectation values,

$$\overline{(\alpha^*)^m\alpha^n} = \langle(\hat{a}^\dagger)^m\hat{a}^n\rangle. \tag{4}$$

As photodetectors naturally measure normally-ordered averages, this would at first glance seem to be an extremely useful representation. It does, however, have two serious drawbacks. The first is that it is difficult to represent any state which is "more quantum" than a coherent state, as these do not possess positive and analytic *P*-functions. Although a *P*-function can be written for any quantum state in terms of generalised functions [37], it is difficult to see how to sample these numerically. The second drawback arises when we consider the *P*-representation Fokker–Planck equation, found using the operator correspondences

$$\hat{a}\rho \leftrightarrow \alpha P, \quad \hat{a}^\dagger\rho \leftrightarrow \left(\alpha^* - \frac{\partial}{\partial\alpha}\right)P,$$
$$\rho\hat{a} \leftrightarrow \left(\alpha - \frac{\partial}{\partial\alpha^*}\right)P, \quad \rho\hat{a}^\dagger \leftrightarrow \alpha^* P. \tag{5}$$

It is readily seen that, for any interesting problem, the resulting Fokker–Planck equation will not have a positive-definite diffusion matrix and therefore will not be able to be mapped onto stochastic differential equations. The positive-*P* representation [17] was developed to circumvent this problem by using a doubled phase space. For Hamiltonians which lead to derivatives of no higher than second order, this results in a Fokker–Planck equation which always has a positive-definite diffusion matrix and therefore can always be mapped onto stochastic differential equations. The price which has to be paid is that, instead of having $\alpha$ and $\alpha^*$ as complex conjugate variables, the variables corresponding to this pair become independent. These are written in various ways, but in this article we will write the pair as $\alpha$ and $\alpha^+$, and the appropriate equations can be found by naively using the *P* representation correspondences of Eq. (5) and then substituting $\alpha^+$ for $\alpha^*$. The independence of the variables can cause serious stability problems with the numerical integration, but for problems where the integration converges, the positive-*P* representation is an extremely powerful theoretical tool [38]. As a final remark, we note that a method has been developed for mapping Hamiltonians which would give higher than second order derivatives in a generalised Fokker–Planck equation onto stochastic difference equations [39], which is useful for analysing