N-boson time-dependent problem: A reformulation with stochastic wave functions

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We present a numerically tractable method to solve exactly the evolution of a N boson system with binary interactions. The density operator of the system ρ is obtained as the stochastic average of particular operators $|\Psi_1\rangle\langle\Psi_2|$ of the system. The states $|\Psi_{1,2}\rangle$ are either Fock states $|N:\phi_{1,2}\rangle$ or coherent states $|\mathrm{coh}:\phi_{1,2}\rangle$ with each particle in the state $\phi_{1,2}(x)$. We determine the conditions on the evolution of $\phi_{1,2}$, which involves a stochastic element, under which we recover the exact evolution of ρ. We discuss various possible implementations of these conditions. The well known positive P representation arises as a particular case of the coherent state ansatz. We treat numerically two examples: a two-mode system and a one-dimensional harmonically confined gas. These examples, together with an analytical estimate of the noise, show that the Fock state ansatz is the most promising one in terms of precision and stability of the numerical solution.

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I. INTRODUCTION

Since the experimental realization of the first atomic gaseous Bose-Einstein condensates a few years ago [1–4], the physics of dilute Bose gases has been considered with a renewed interest. One fascinating aspect of these new systems is the possibility to accumulate in a single quantum state a large fraction of the atoms confined in a trap.

At very low temperature, a simple theoretical description of the dynamics of these systems is obtained by neglecting the uncondensed atoms, and by considering the wave function of the condensate, which obeys a Schrödinger equation with a nonlinear term originating from the mean-field interactions between the atoms. Such an approach neglects two- and more-particle correlations and is valid under a weak-interaction condition which is usually stated in terms of the density n and the scattering length a of the gas as $(na^3)^{1/2} \ll 1$. Current gaseous condensates satisfy such a condition. Nevertheless effects beyond the Gross-Pitaevskii equation may be considered at zero temperature; also finite temperature phenomena are not accounted for by the pure state mean field approach.

More complex theories have been developed in order to cope with effects beyond the Gross-Pitaevskii equation: Bogoliubov's approach takes into account the next term in the $(na^3)^{1/2}$ expansion [5,6]. Also quantum kinetic theories have been developed to study the formation of the condensate and to include the effect of the noncondensed particles [7–9]. Unfortunately the corresponding calculations are quite heavy for 3D nonhomogeneous systems such as trapped gases, and this constitutes a first limitation to the use of these methods. Also approximations used in some of the existing mean field theories are not under rigorous control, making it difficult to assess their domain of validity (for a review see, e.g., [10]). Therefore a computational scheme capable to provide exact results can have a great importance both from a purely theoretical point of view and for a quantitative analysis of experimental data.

When the Bose gas is at thermal equilibrium such an exact numerical calculation of the properties of the gas is available, using the quantum Monte Carlo techniques, based on Feynman path integral formulation of quantum mechanics [11,12]. The aim of this paper is to present an alternative exact and numerically tractable solution to the problem of the interacting Bose gas, a method not restricted to the case of thermal equilibrium but which allows for the study of the dynamics of the gas. The method is based on a stochastic evolution of Hartree states, in which all atoms have the same wave function, these Hartree states being either Fock states (fixed number of atoms) or coherent states. As a particular case of this solution with coherent states, we recover the stochastic scheme corresponding to the evolution of the density operator of the system in the positive P representation [13–15]. This scheme, which has been applied already to study the dynamics of Bose-Einstein condensates in [16,17], is known to lead to strong unstability problems, which fortunately do not show up for other implementations of the present method.

The outline of the paper is the following: In Sec. II, we present the stochastic formulation of the evolution of these Hartree states which, after average over the stochastic component, leads to the exact evolution. Section III is devoted to the presentation of two particular schemes implementing this stochastic formulation. We first present a ''simple'' scheme, which minimizes the statistical spread of the calculated N-atom density matrix. We also investigate a more elaborate scheme in which the trace of the calculated density matrix remains strictly constant in the evolution. With this constraint, we recover for coherent states the known stochastic simulation associated with the positive P representation [16]. Finally we investigate in Secs. IV and V two examples, a two-mode model system and a one-dimensional Bose gas, respectively. These examples illustrate the accuracy and the limitations of the method. Generally speaking we find that the ''simple'' scheme simulations are only limited by the computation power: the number of realizations needed for a good statistical accuracy increases exponentially with time for the simulation with Fock states. On the contrary the simulations with constant trace are subject to divergences of

the norms of the stochastic wave functions in finite time, a phenomenon already known for coherent states in the context of the positive P representation [13,18].

II. STOCHASTIC FORMULATION OF THE N-BOSON PROBLEM USING HARTREE FUNCTIONS

A. Model considered in this paper

The Hamiltonian of the trapped interacting Bose gas under examination can be written in terms of the Bose field operator $\hat{\Psi}(x)$ as

$$\mathcal{H}=\int dx\,\hat{\Psi}^{\dagger}(x)h_0\hat{\Psi}(x)+\tfrac{1}{2}\int\int dx\,dx'\,\hat{\Psi}^{\dagger}(x)\hat{\Psi}^{\dagger}(x') \times V(x-x')\hat{\Psi}(x')\hat{\Psi}(x), \tag{1}$$

where x is the set of spatial coordinates of a particle, $h_0=-(\hbar^2/2m)\nabla^2+V_{\rm ext}(x)$ is the single particle Hamiltonian in the external confining potential $V_{\rm ext}$ and where interactions are assumed to occur via a two-body potential $V(x-x')$.

In practice we consider the dilute gas and the low temperature regimes, which correspond respectively to $n|a|^3 \ll 1$ and $|a|\ll\lambda$ for a three-dimensional problem ($\lambda=h/(2\pi m k_B T)^{1/2}$ is the thermal de Broglie wavelength). The true interaction potential can then be replaced by a simpler model potential leading to the same scattering length a provided that the range b of this model potential is much smaller than the healing length $\xi=(8\pi n a)^{-1/2}$ and than λ [5,6]. This ensures that the physical results do not depend on b. For simplicity we will use here repulsive Gaussian potentials corresponding to a positive scattering length $a>0$.

B. A stochastic Hartree ansatz with Fock states

From a mathematical point of view, the exact evolution of the N-body density matrix ρ can be obtained from the Hamiltonian (1) using the quantum-mechanical equation of motion

$$\dot{\rho}(t)=\frac{1}{i\hbar}[\mathcal{H},\rho(t)], \tag{2}$$

but any concrete calculation is impracticable even for moderate particle numbers N, due to the multi-mode nature of the problem leading to a huge dimensionality of the N-body Hilbert space.

For this reason approximate theories have been developed in order to get useful results at least in some specific ranges of parameters; the simplest one is the so-called mean-field theory, in which the N-particle density matrix is approximated by a Fock state Hartree ansatz

$$\rho(t)=|N:\phi(t)\rangle\langle N:\phi(t)|, \tag{3}$$

where $|N:\phi\rangle$ represents the state with N particles all in the same mode (or single-particle state) ϕ. The evolution of the normalized *condensate wave function* ϕ is determined using either a factorization approximation in the evolution equation for the field operator [6] or a variational procedure [19]. The result is the well-known mean-field equation

$$i\hbar\frac{\partial\phi(x)}{\partial t}=\left(-\frac{\hbar^2\nabla^2}{2m}+V_{\rm ext}(x)\right)\phi(x)+(N-1) \times\left(\int dx'\,V(x-x')|\phi(x')|^2\right)\phi(x). \tag{4}$$

For an interaction potential $V(x-x')$ modeled by a contact term $g\,\delta(x-x')$ (where $g=4\pi\hbar^2 a/m$ in a three-dimensional problem) it reduces to the Gross-Pitaevskii equation commonly used to analyze the dynamics of pure Bose-Einstein condensed gases.

A first attempt to improve the accuracy of the Hartree ansatz (3) is to allow for a stochastic contribution dB in the evolution of the macroscopic wave function ϕ:

$$\phi(t+dt)=\phi(t)+F\,dt+dB. \tag{5}$$

In all this paper the noise dB is treated in the standard Ito formalism [20] so that it has a zero mean $\overline{dB}=0$ and $dB^2\propto dt$; a deterministic contribution is given by the ''force'' term $F dt$. In this framework, the N-body density matrix would result from the stochastic mean over noise or, in other terms, from a mean over the time dependent probability distribution $\mathcal{P}_t(\phi)$ in the functional space of the wave functions ϕ:

$$\rho(t)\overset{?}{=}\langle|N:\phi(t)\rangle\langle N:\phi(t)|\rangle_{\rm stoch}=\int\mathcal{D}\phi\,\mathcal{P}_t(\phi)|N:\phi\rangle\langle N:\phi|. \tag{6}$$

An immediate advantage of this prescription over the pure state ansatz Eq. (3) is that it could deal with finite temperature problems [21]. However as shown in Sec. II E, the simple generalization Eq. (5) of the Gross-Pitaevskii equation cannot lead to an exact solution of the N-body problem [22]. Therefore we have to enlarge the family of dyadics over which we expand the density operator; more precisely we use Hartree dyadics in which the wave functions in the bra and in the ket are different:

$$\sigma(t)=|N:\phi_1(t)\rangle\langle N:\phi_2(t)|. \tag{7}$$

The two wave functions $\phi_1(x)$ and $\phi_2(x)$ are assumed to evolve according to Ito stochastic differential equations:

$$\phi_\alpha(t+dt)=\phi_\alpha(t)+F_\alpha\,dt+dB_\alpha\quad(\alpha=1,2). \tag{8}$$

The expansion Eq. (6) is then replaced by

$$\rho(t)=\langle|N:\phi_1(t)\rangle\langle N:\phi_2(t)|\rangle_{\rm stoch} =\int\int\mathcal{D}\phi_1\,\mathcal{D}\phi_2\,\mathcal{P}_t(\phi_1,\phi_2)|N:\phi_1\rangle\langle N:\phi_2|. \tag{9}$$

We will see in the following that within this extended Hartree ansatz one can find a stochastic evolution for $\phi_{1,2}$ reproducing the exact time evolution.

Actual calculations (see Secs. IV and V) will be performed with a Monte Carlo technique, in which the evolution of the probability distribution $\mathcal{P}$ is simulated by a large but finite number $\mathcal{N}$ of independent realizations $\phi_{1,2}^{(i)}(t)$, i

$=1,\ldots,\mathcal{N}$. At any time the (approximate) density matrix ρ is given by the mean over such an ensemble of wave functions:

$$\rho(t)\simeq\frac{1}{\mathcal{N}}\sum_{i=1}^{\mathcal{N}}|N:\phi_1^{(i)}(t)\rangle\langle N:\phi_2^{(i)}(t)|. \tag{10}$$

The expectation value of any operator $\hat{O}$ is thus expressed by

$$\langle\hat{O}\rangle\simeq\frac{1}{\mathcal{N}}\sum_{i=1}^{\mathcal{N}}\langle N:\phi_2^{(i)}(t)|\hat{O}|N:\phi_1^{(i)}(t)\rangle. \tag{11}$$

For an Hermitian operator one can equivalently consider only the real part of this expression since the imaginary part is vanishingly small in the large $\mathcal{N}$ limit.

Consider as an example the one-particle density matrix of the gas, usually defined as

$$\rho^{(1)}(x,x')=\langle\hat{\Psi}^\dagger(x')\hat{\Psi}(x)\rangle. \tag{12}$$

Inserting in this expression our form of the complete density matrix (10), we obtain the simple result

$$\rho^{(1)}(x,x')=N\langle\phi_1(x)\phi_2^*(x')\langle\phi_2|\phi_1\rangle^{N-1}\rangle_{\text{stoch}}, \tag{13}$$

from which it is easy to obtain the spatial density $n(x)=\rho^{(1)}(x,x)$ and the correlation function $g^{(1)}(x,x')=\rho^{(1)}(x,x')/(n(x)n(x'))^{1/2}$. Also, the condensate fraction can be obtained from the largest eigenvalue of $\rho^{(1)}(x,x')$.

1. Remarks

(1) The desired stochastic evolution, which has to satisfy $\mathrm{Tr}[\rho]=1$, cannot preserve the normalization of $\phi_{1,2}$ to unity; we can write indeed

$$\mathrm{Tr}[\rho(t)]=\langle\langle\phi_2(t)|\phi_1(t)\rangle^N\rangle_{\text{stoch}}=1, \tag{14}$$

which for $|\phi_1\rangle\neq|\phi_2\rangle$ imposes $||\phi_1||\ ||\phi_2||>1$ for some realizations.

(2) The expansion Eq. (9) is always possible with a positive distribution function $\mathcal{P}_t(\phi_1,\phi_2)$. We prove this statement by showing that a general density operator ρ can be written as in Eq. (10) in the limit $\mathcal{N}\to+\infty$. Using the identity

$$\mathrm{Id}_N=\lim_{\mathcal{M}\to+\infty}\frac{1}{\mathcal{M}}\sum_{j=1}^{\mathcal{M}}|N:\psi^{(j)}\rangle\langle N:\psi^{(j)}|, \tag{15}$$

where the functions $\psi^{(j)}$ have a uniform distribution over the unit sphere in the functional space, we obtain

$$\rho=\lim_{\mathcal{M}\to+\infty}\frac{1}{\mathcal{M}^2}\sum_{j_1,j_2=1}^{\mathcal{M}}|N:\psi^{(j_1)}\rangle\times\langle N:\psi^{(j_2)}|\langle N:\psi^{(j_1)}|\rho|N:\psi^{(j_2)}\rangle. \tag{16}$$

This expression is not yet in the form of Eq. (10) since the matrix elements $\langle N:\psi^{(j_1)}|\rho|N:\psi^{(j_2)}\rangle$ are complex. Fortunately we can always write this matrix element as the $2N$th power of the complex number $\xi_{(j_1,j_2)}$. It is then sufficient to set $\phi_1^{(j_1,j_2)}=\psi^{(j_1)}\xi_{(j_1,j_2)}$ and $\phi_2^{(j_1,j_2)}=\psi^{(j_2)}\xi^*_{(j_1,j_2)}$, to put $\mathcal{N}=\mathcal{M}^2$ and to reindex (j_1,j_2) as a single index i, in order to recover the expansion Eq. (10). Note that this expansion is not unique and does not have the pretension to be the most efficient one. For instance if the system is initially in a Hartree state $|N:\phi_0\rangle$, such a procedure is clearly not needed since one has just to set $\phi_1^{(i)}(t=0)=\phi_2^{(i)}(t=0)=\phi_0$. This will be the case of the numerical examples in Secs. IV and V.

C. Stochastic evolution of a Fock state Hartree dyadic

In this subsection we calculate the stochastic time evolution during an infinitesimal time interval dt of the dyadic $\sigma(t)$ given in Eq. (7). This will be used later in a comparison with the exact master equation.

After dt, the dyadic σ has evolved into

$$\sigma(t+dt)=|N:\phi_1+d\phi_1\rangle\langle N:\phi_2+d\phi_2|, \tag{17}$$

where $d\phi_1$ and $d\phi_2$, defined according to Eq. (8), contain both the deterministic contribution $F_\alpha dt$ and the stochastic one dB_α. Splitting each contribution into a longitudinal and an orthogonal component with respect to ϕ_α and isolating a Gross-Pitaevskii term in the deterministic contribution, we can write

$$dB_\alpha(x)=\phi_\alpha(x)\,d\gamma_\alpha+dB_\alpha^\perp(x), \tag{18}$$

$$F_\alpha(x)=F_\alpha^{GP}(x)+\lambda_\alpha\phi_\alpha(x)+F_\alpha^\perp(x). \tag{19}$$

Our choice of the Gross-Pitaevskii term is the following one:

$$F_\alpha^{GP}(x)=\frac{1}{i\hbar}\left[h_0+\frac{(N-1)}{\|\phi_\alpha\|^2}\int dx'\,V(x-x')|\phi_\alpha(x')|^2\right]\times\phi_\alpha(x)-\frac{1}{i\hbar}\left[\frac{(N-1)}{2}\frac{\langle\phi_\alpha\phi_\alpha|V|\phi_\alpha\phi_\alpha\rangle}{\|\phi_\alpha\|^4}\right]\phi_\alpha(x). \tag{20}$$

The first term gives the standard Gross-Pitaevskii evolution, including the kinetic term, the potential energy of the trap and the mean-field interaction energy; the second term, which arises naturally because we are considering Fock states (rather than coherent states as commonly done) takes into account the difference between the total mean-field energy per particle of the condensate and its chemical potential μ [23].

We split the field operator in its longitudinal and transverse components, keeping in mind that the wave functions ϕ_α are not of unit norm:

$$\hat{\Psi}^\dagger(x)=\frac{\phi_\alpha^*(x)}{\|\phi_\alpha\|^2}\hat{a}^\dagger_{\phi_\alpha}+\delta\hat{\Psi}^\dagger_\alpha(x), \tag{21}$$

with

$$\hat{a}^\dagger_{\phi_\alpha}=\int dx\,\phi_\alpha(x)\hat{\Psi}^\dagger(x). \tag{22}$$

The relevant bosonic commutation relations then read

$$[\hat{a}_{\phi_\alpha},\hat{a}^\dagger_{\phi_\alpha}]=\|\phi_\alpha\|^2 \quad \text{and} \quad [\hat{a}_{\phi_\alpha},\delta\hat{\Psi}^\dagger_\alpha(x)]=0. \tag{23}$$

We will also need the projector $\mathcal{Q}_\alpha$ onto the subspace orthogonal to ϕ_α:

$$\mathcal{Q}^{(x)}_\alpha[\psi(x,x',\dots)]=\psi(x,x',\dots)-\frac{\phi_\alpha(x)}{||\phi_\alpha||^2}\int dy\ \phi^*_\alpha(y) \times\psi(y,x',\dots). \tag{24}$$

This projector arises in the calculation as we have introduced a component of the field operator orthogonal to ϕ_α. Using $\int dx\ \phi_\alpha(x)\ \delta\hat{\Psi}^\dagger_\alpha(x)=0$ we shall transform integrals involving $\delta\hat{\Psi}^\dagger_\alpha(x)$ as follows:

$$\int dx\ \psi(x,x',\dots)\delta\hat{\Psi}^\dagger_\alpha(x) = \int dx\ \mathcal{Q}^{(x)}_\alpha[\psi(x,x',\dots)]\delta\hat{\Psi}^\dagger_\alpha(x). \tag{25}$$

Inserting these definitions in Eq. (17) the expression for σ at time $t+dt$ can be written as

$$\begin{aligned}\sigma(t+dt)-\sigma(t)=&S^{(0)}_1|N:\phi_1\rangle\langle N:\phi_2|+\text{e.c.}+\int dx\ S^{(1)}_1(x)\,\delta\hat{\Psi}^\dagger_1(x)|N-1:\phi_1\rangle\langle N:\phi_2|+\text{e.c.}\\ &+\int\int dx\,dx'\ S^{(2)}_1(x,x')\,\delta\hat{\Psi}^\dagger_1(x)\,\delta\hat{\Psi}^\dagger_1(x')|N-2:\phi_1\rangle\langle N:\phi_2|+\text{e.c.}\\ &+\int\int dx\,dx'\ S^{(1,1)}(x,x')\,\delta\hat{\Psi}^\dagger_1(x)|N-1:\phi_1\rangle\langle N-1:\phi_2|\,\delta\hat{\Psi}_2(x'),\end{aligned} \tag{26}$$

where the notation e.c. stands for the *exchanged* and *conjugate* of a quantity, that is the complex conjugate of the quantity after having exchanged the indices 1 and 2. The explicit expressions for the $S^{(i)}_\alpha$ are

$$S^{(0)}_1=N\frac{\langle\phi_1|F^{GP}_1\rangle}{\|\phi_1\|^2}dt+N\lambda_1\,dt+N d\gamma_1+\frac{N(N-1)}{2}d\gamma_1^2+\frac{N^2}{2}d\gamma_1\,d\gamma_2^*, \tag{27}$$

$$S^{(1)}_1(x)=\sqrt{N}\{\mathcal{Q}^{(x)}_1[F^{GP}_1(x)]dt+F^\perp_1(x)dt+dB^\perp_1(x)+(N-1)d\gamma_1\,dB^\perp_1(x)+N\,dB^\perp_1(x)d\gamma_2^*\}, \tag{28}$$

$$S^{(2)}_1(x,x')=\frac{\sqrt{N(N-1)}}{2}dB^\perp_1(x)dB^\perp_1(x'), \tag{29}$$

$$S^{(1,1)}(x,x')=N dB^\perp_1(x)dB^{\perp *}_2(x'). \tag{30}$$

Analogous expressions for $S^{(0)}_2$, $S^{(1)}_2$, $S^{(2)}_2$ are obtained by exchanging the subscripts 1 and 2. In the next subsection, we evaluate the exact evolution of the same dyadic during a time interval dt, so that we can determine the constraints on the force and noise terms entering into these equations.

D. Exact evolution of a Fock state Hartree dyadic

To make the stochastic scheme described in the previous sections equivalent to the exact dynamics as it is given by Eq. (1), the final result of the previous subsection, Eqs. (26)–(30), has to be compared with the exact evolution of the density matrix $\sigma(t)$. Consider a dyadic $\sigma=|N:\phi_1\rangle\langle N:\phi_2|$ at time t; according to the equation of motion (2), and using the fact that the state $|N:\phi_\alpha\rangle$ is a vacuum state for the operator $\delta\hat{\Psi}_\alpha(x)$, we find that the dyadic has evolved after an infinitesimal time step dt into

$$\begin{aligned}\sigma(t+dt)=\sigma(t)+\frac{dt}{i\hbar}(\mathcal{H}\sigma(t)-\sigma(t)\mathcal{H})=\sigma(t)+E^{(0)}_1|N:\phi_1\rangle\langle N:\phi_2|+\text{e.c.}+\int dx\,E^{(1)}_1(x)\,\delta\hat{\Psi}^\dagger_1(x)|N-1:\phi_1\rangle\langle N:\phi_2|+\text{e.c.}\\ +\int\int dx\,dx'\,E^{(2)}_1(x,x')\,\delta\hat{\Psi}^\dagger_1(x)\,\delta\hat{\Psi}^\dagger_1(x')|N-2:\phi_1\rangle\langle N:\phi_2|+\text{e.c.},\end{aligned} \tag{31}$$

where the $E^{(i)}_\alpha$ are given by

$$E^{(0)}_1=\frac{N\,dt}{i\hbar}\left[\frac{\langle\phi_1|h_0|\phi_1\rangle}{\|\phi_1\|^2}+\frac{(N-1)}{2}\frac{\langle\phi_1\phi_1|V|\phi_1\phi_1\rangle}{\|\phi_1\|^4}\right], \tag{32}$$

$$E_1^{(1)}(x)=\frac{dt\sqrt{N}}{i\hbar}\mathcal{Q}_1^{(x)}\left[\left(h_0+\frac{(N-1)}{\|\phi_1\|^2}\int dx'\,V(x-x')|\phi_1(x')|^2\right)\phi_1(x)\right], \tag{33}$$

$$E_1^{(2)}(x,x')=\frac{dt\sqrt{N(N-1)}}{2i\hbar}\mathcal{Q}_1^{(x)}\mathcal{Q}_1^{(x')}[V(x-x')\phi_1(x)\phi_1(x')]. \tag{34}$$

Analogous expressions for $E_2^{(0)}$, $E_2^{(1)}$, $E_2^{(2)}$ are obtained by exchanging the subscripts 1 and 2.

E. Validity conditions for the stochastic Fock state Hartree ansatz

The similarity of the structures of Eqs. (26) and (31) suggests the possibility of a stochastic scheme equivalent to the exact evolution: to achieve this, it is necessary to find out specific forms of deterministic (19) and stochastic (18) terms for which the mean values of the $S_\alpha^{(i)}$ equal the $E_\alpha^{(i)}$:

$$\overline{S_1^{(0)}+S_2^{(0)*}}=E_1^{(0)}+E_2^{(0)*}, \tag{35}$$

$$\overline{S_\alpha^{(1)}(x)}=E_\alpha^{(1)}(x), \tag{36}$$

$$\overline{S_\alpha^{(2)}(x,x')}=E_\alpha^{(2)}(x,x'), \tag{37}$$

$$\overline{S^{(1,1)}(x,x')}=0. \tag{38}$$

From the last equation (38), it follows immediately why independent bras and kets are needed in the ansatz (7): in the case $\phi_1=\phi_2=\phi$ such a condition would in fact lead to a vanishing orthogonal noise and finally to the impossibility of satisfying Eq. (37).

In terms of the different components, these conditions can be rewritten as

$$(\lambda_1+\lambda_2^*)dt+\frac{(N-1)}{2}[d\gamma_1^2+d\gamma_2^{2*}]+Nd\gamma_1 d\gamma_2^*=0, \tag{39}$$

$$F_1^\perp(x)dt+(N-1)dB_1^\perp(x)\,d\gamma_1+NdB_1^\perp(x)\,d\gamma_2^*=0, \tag{40}$$

$$F_2^\perp(x)dt+(N-1)dB_2^\perp(x)\,d\gamma_2+NdB_2^\perp(x)\,d\gamma_1^*=0, \tag{41}$$

$$dB_\alpha^\perp(x)dB_\alpha^\perp(x')=\frac{dt}{i\hbar}\mathcal{Q}_\alpha^x\mathcal{Q}_\alpha^{x'}[V(x-x')\phi_\alpha(x)\phi_\alpha(x')], \tag{42}$$

$$dB_1^\perp(x)dB_2^{\perp *}(x')=0. \tag{43}$$

As we shall discuss in detail in Sec. III, several different stochastic schemes can be found satisfying Eqs. (39)–(43); each of them gives an evolution identical in average to the exact one, but the statistical properties can be very different.

F. A stochastic Hartree ansatz with coherent states

Up to now we have worked out the case of a Fock state ansatz $|N:\phi_1\rangle\langle N:\phi_2|$. Actually coherent states rather than Fock states are generally used, both in quantum optics and in condensed matter physics. We now show that our stochastic procedure also applies with a coherent state ansatz of the form

$$\sigma(t)=\Pi(t)|\mathrm{coh}:\phi_1\rangle\langle\mathrm{coh}:\phi_2|, \tag{44}$$

with

$$|\mathrm{coh}:\phi_\alpha\rangle=\exp\left(\overline{N}^{1/2}\int dx\,\phi_\alpha(x)\hat{\Psi}^\dagger(x)\right)|\mathrm{vac}\rangle, \tag{45}$$

where $\overline{N}$ is the mean number of particles. We have included here a prefactor $\Pi(t)$ which was absent in the case of the Fock state ansatz (7); in the Fock state case indeed such a prefactor could be reincluded into the definition of ϕ_1 and ϕ_2. The wave functions $\phi_\alpha(x)$ and the prefactor factor Π evolve according to Ito stochastic differential equations

$$d\phi_\alpha=F_\alpha dt+dB_\alpha,$$

$$d\Pi=f\,dt+db. \tag{46}$$

Splitting the field operator as

$$\hat{\Psi}(x)=\overline{N}^{1/2}\phi_\alpha(x)+\delta\hat{\Psi}_\alpha(x) \tag{47}$$

and using

$$\delta\hat{\Psi}_\alpha(x)|\mathrm{coh}:\phi_\alpha\rangle=0, \tag{48}$$

we find that the equivalence of the stochastic scheme and the exact evolution translates into the following set of conditions:

$$f=0, \tag{49}$$

$$F_1(x)dt+\frac{1}{\Pi}db\,dB_1(x)=\frac{dt}{i\hbar}h_0\phi_1(x), \tag{50}$$

$$F_2(x)dt+\frac{1}{\Pi^*}db^*\,dB_2(x)=\frac{dt}{i\hbar}h_0\phi_2(x), \tag{51}$$

$$dB_\alpha(x)dB_\alpha(x')=\frac{dt}{i\hbar}V(x-x')\phi_\alpha(x)\phi_\alpha(x'), \tag{52}$$

$$dB_1(x)dB_2^*(x')=0. \tag{53}$$

As we shall see in Sec. III, such conditions are satisfied by several stochastic schemes. Very remarkably, the stochastic evolution deduced from the positive P representation [24] arises naturally as one of them.

Within this coherent state ansatz the one-particle density matrix is evaluated using

$$\rho^{(1)}(x,x') = \overline{N}\langle \phi_1(x)\phi_2^*(x')\Pi(t)\exp(\overline{N}\langle\phi_2|\phi_1\rangle)\rangle_{\text{stoch}}. \tag{54}$$

In a practical implementation of the simulation it turns out to be numerically more efficient to represent $\Pi(t)$ as the exponential of some quantity

$$\Pi(t) = e^{\overline{N}S(t)} \tag{55}$$

and to evolve $S(t)$ according to the stochastic equation

$$dS = \frac{db}{\overline{N}\Pi} - \frac{\partial/db}{\overline{\partial N}\Pi} \tag{56}$$

III. PARTICULAR IMPLEMENTATIONS OF THE STOCHASTIC APPROACH

In the previous section we have derived the conditions that a stochastic scheme has to satisfy in order to recover the exact evolution given by the Hamiltonian (1); in the case of the Fock state ansatz (7), we get the system (39)–(43), while in the case of the coherent state ansatz (44) we get the conditions (49)–(53). As the number of these equations is actually smaller than the number of unknown functions there is by no mean uniqueness of the solutions, that is of the simulation schemes. We need a strategy to identify interesting solutions.

We therefore start this section by considering various indicators of the statistical error of the simulation (Sec. III A) which can be used as guidelines in the search for simulation schemes. These indicators are defined as variances of relevant quantities which are conserved in the exact evolution but which may fluctuate in the simulation. We show that these indicators are nondecreasing functions of time; attempts to minimize the time derivative of a specific indicator will lead to particular implementations of the general stochastic method, such as the *simple* scheme (Sec. III B) and the *constant trace* scheme (Sec. III C).

A. Growth of the statistical errors

The first indicator that we consider measures the squared deviation of the stochastic operator $\sigma(t)$ from the exact density operator $\rho(t)$:

$$\begin{aligned}\Delta(t) &= \langle \mathrm{Tr}[(\sigma^\dagger(t)-\rho(t))(\sigma(t)-\rho(t))]\rangle_{\text{stoch}} \\ &= \langle \mathrm{Tr}[\sigma^\dagger(t)\sigma(t)]\rangle_{\text{stoch}} - \mathrm{Tr}[\rho(t)^2].\end{aligned} \tag{57}$$

We now show that $\Delta(t)$ is a nondecreasing function of time. When the stochastic scheme satisfies the validity conditions derived in the previous section, we can write the stochastic equation for σ as

$$d\sigma = \frac{dt}{i\hbar}[\mathcal{H},\sigma] + d\sigma_s, \tag{58}$$

where $d\sigma_s$ is a zero-mean noise term linear in dB_α (and db for the coherent state simulation). In the case of simulation with Fock states it is given by

$$\begin{aligned}d\sigma_s = N^{1/2}\Big\{ &\int dx\, dB_1(x)\hat{\Psi}^\dagger(x)|N-1:\phi_1\rangle\langle N:\phi_2| \\ &+ \int dx\, dB_2^*(x)|N:\phi_1\rangle\langle N-1:\phi_2|\hat{\Psi}(x)\Big\}.\end{aligned} \tag{59}$$

In the case of simulation with coherent states it is given by

$$\begin{aligned}d\sigma_s = db|\mathrm{coh}:\phi_1\rangle\langle\mathrm{coh}:\phi_2| + \overline{N}^{1/2}\Pi\Big\{ &\int dx\, dB_1(x) \\ &\times\hat{\Psi}^\dagger(x)|\mathrm{coh}:\phi_1\rangle\langle\mathrm{coh}:\phi_2| + \int dx\, dB_2^*(x) \\ &\times|\mathrm{coh}:\phi_1\rangle\langle\mathrm{coh}:\phi_2|\hat{\Psi}(x)\Big\}.\end{aligned} \tag{60}$$

We calculate the variation of Δ during dt, replacing σ by $\sigma+d\sigma$ in Eq. (57) and keeping terms up to order dt. Using the invariance of the trace in a cyclic permutation and averaging over all possible realizations, we finally obtain

$$d\Delta = \langle \mathrm{Tr}[d\sigma_s^\dagger d\sigma_s]\rangle_{\text{stoch}}, \tag{61}$$

which is a positive quantity. Minimization of this quantity is the subject of Sec. III B. Physically $d\Delta \geqslant 0$ means that the impurity of the stochastic density operator σ always increases in average, while the exact density operator has a constant purity $\mathrm{Tr}[\rho^2]$.

The second kind of indicator that we consider measures the statistical error on constants of motion of the exact evolution. Consider a time independent operator X commuting with the Hamiltonian. The stochastic evolution leads to a statistical error on the expectation value of X with a variance given by the ensemble average

$$\begin{aligned}\Delta_X(t) &= \langle|\mathrm{Tr}[X\sigma(t)]-\mathrm{Tr}[X\rho(t)]|^2\rangle_{\text{stoch}} \\ &= \langle|\mathrm{Tr}[X\sigma(t)]|^2\rangle_{\text{stoch}} - |\mathrm{Tr}[X\rho(t)]|^2.\end{aligned} \tag{62}$$

From Eq. (58) we obtain the variation after a time step dt of the expectation value of X along a stochastic trajectory:

$$d(\mathrm{Tr}[X\sigma]) = \frac{dt}{i\hbar}\mathrm{Tr}(X[\mathcal{H},\sigma]) + \mathrm{Tr}[Xd\sigma_s]. \tag{63}$$

Using the invariance of the trace under cyclic permutation and the commutation relation $[\mathcal{H},X]=0$ we find that the first term in the right-hand side of Eq. (63) vanishes so that

$$d\Delta_X = \langle \mathrm{Tr}[X d\sigma_s]\mathrm{Tr}[X^\dagger d\sigma_s^\dagger]\rangle_{\mathrm{stoch}}, \tag{64}$$

a quantity which is always non-negative.

Using expression (64) one can ''design'' simulations preserving exactly the conserved quantity, the constraint to meet being $\mathrm{Tr}[X d\sigma_s]=0$: for instance in the Fock state simulation, one first chooses the transverse noises $dB_\alpha^\perp$ satisfying Eqs. (42) and (43); then one simply has to take for the longitudinal noise of ϕ_1

$$d\gamma_1 = -\frac{1}{\sqrt{N}}(\langle N:\phi_2|X|N:\phi_1\rangle)^{-1}\int dx\, dB_1^\perp(x) \times \langle N:\phi_2|X\,\delta\hat{\Psi}_1^\dagger(x)|N-1:\phi_1\rangle \tag{65}$$

and a similar expression for $d\gamma_2$; finally the force terms F_α are adjusted in order to satisfy Eqs. (39)–(41). As natural examples of conserved quantities one can choose $X=1$ or $X=\mathcal{H}$; the former case is discussed in detail in Sec. III C.

B. The *simple* schemes

These schemes are characterized by the minimization of the incremental variation of the statistical spread of the N-particle density matrix $\sigma(t)$, a spread that we have already quantified in Eq. (57) by $\Delta(t)$. To be more specific we assume that we have evolved a dyadic up to time t, and we look for the noise terms that minimize the increase of $\mathrm{Tr}[\sigma^\dagger\sigma]$ between t and $t+dt$.

1. Simulation with Fock states

In the case of the Fock state ansatz, we calculate explicitly the variation of $\mathrm{Tr}[\sigma^\dagger\sigma]$ from Eq. (59) and we get

$$\frac{d\,\mathrm{Tr}[\sigma^\dagger\sigma]}{N\,\mathrm{Tr}[\sigma^\dagger\sigma]} = N(d\gamma_1+d\gamma_2^*)(d\gamma_1^*+d\gamma_2) + \sum_{\alpha=1,2}||\phi_\alpha||^{-2} \times \int dx\, dB_\alpha^\perp(x) dB_\alpha^{\perp *}(x) + [d\gamma_1 + d\gamma_2^* + \mathrm{c.c.}]. \tag{66}$$

We now look for the noise terms $d\gamma_\alpha$ and $dB_\alpha^\perp$ minimizing this quantity subject to the constraints Eqs. (39)–(43).

We first note that we can choose $d\gamma_1=d\gamma_2=0$ without affecting the transverse noises, as shown by Eqs. (39)–(43): the correlation function of the transverse noises do not involve the $d\gamma_\alpha$, and we can accommodate for any choice of $d\gamma_\alpha$ by defining appropriately the force terms $F_\alpha^\perp, \lambda_\alpha$. In the particular case defining our simple scheme we take all these force terms equal to zero so that the force terms F_α coincide with the mean field forces defined in Eq. (20):

$$F_\alpha(x) \equiv F_\alpha^{GP}(x). \tag{67}$$

Note that the choice of vanishing $d\gamma$'s immediately leads to a vanishing noise term in Eq. (66).

Secondly the terms involving the transverse noise in Eq. (66) are bounded from below: As the modulus of a mean is less than or equal to the mean of the modulus, we have

$$|dB_\alpha^\perp(x) dB_\alpha^\perp(x)| \leqslant dB_\alpha^\perp(x) dB_\alpha^{\perp *}(x), \tag{68}$$

with the left-hand side of this inequality fully determined by condition Eq. (42).

For the remaining part of the present section (Sec. III B) we assume that the interaction potential $V(x)$ has a positive Fourier transform

$$\tilde{V}(k) \geqslant 0 \quad \text{for all } k, \tag{69}$$

where the Fourier transform of $V(x)$ is defined as

$$\tilde{V}(k) = \int dx\, V(x) e^{-ikx}. \tag{70}$$

In Sec. V, we will choose a repulsive Gaussian interaction potential, which satisfies the condition Eq. (69). Note that as a consequence of Eq. (69) and of the inverse Fourier transform formula the model interaction potential is maximal and positive in $x=0$:

$$V(0) \geqslant |V(x)| \quad \text{for all } x. \tag{71}$$

Under the assumption Eq. (69) we have found for the transverse noise a choice which fulfills Eqs. (42) and (43) and which saturates the inequality Eq. (68). We first discretize the Fourier space with an arbitrarily small wave vector step dk and we set

$$dB_\alpha^\perp(x) = \left(\frac{dt}{i\hbar}\right)^{1/2} \mathcal{Q}_\alpha^{(x)} \times \left[\phi_\alpha(x)\sum_k \frac{\sqrt{dk}}{(2\pi)^{d/2}}(\tilde{V}(k))^{1/2} e^{ikx} e^{i\theta_\alpha(k)}\right], \tag{72}$$

where d is the dimension of position space. The phases θ_α have the following statistical property:

$$\overline{e^{i\theta_\alpha(k)} e^{i\theta_\alpha(k')}} = \delta_{k,-k'} \tag{73}$$

and θ_1, θ_2 are uncorrelated. In practice for half of the k-space (e.g., $k_z>0$) $\theta_\alpha(k)$ is randomly chosen between 0 and 2π; for the remaining k's we take $\theta_\alpha(-k) = -\theta_\alpha(k)$. One can then check that this choice for the transverse noise reproduces the correlation function Eqs. (42) and (43).

We show now that the implementation (72) saturates the inequality Eq. (68), so that it leads to the minimal possible value for $d\,\mathrm{Tr}[\sigma^\dagger\sigma]$ within the validity constraints of the stochastic approach. We calculate explicitly the right-hand side of Eq. (68):

$$= dB_\alpha^\perp(x) dB_\alpha^{\perp *}(x)$$

$$= \frac{dt}{\hbar} (\mathcal{Q}_\alpha^{(x)*} \mathcal{Q}_\alpha^{(x')} [V(x-x') \phi_\alpha^*(x) \phi_\alpha(x')])_{x=x'}$$

$$= \frac{dt}{\hbar} |\phi_\alpha(x)|^2 \left[V(0) - 2 \int dy \frac{|\phi_\alpha(y)|^2}{||\phi_\alpha||^2} V(x-y) + \frac{\langle \phi_\alpha, \phi_\alpha | V | \phi_\alpha, \phi_\alpha \rangle}{||\phi_\alpha||^4} \right], \quad (74)$$

where $\mathcal{Q}_\alpha^*$ projects onto the subspace orthogonal to ϕ_α^* and where we have used the positivity of the Fourier transform $\tilde{V}$ of the model interaction potential. The left-hand side of Eq. (68) is calculated using Eq. (42):

$$dB_\alpha^\perp(x)^2 = \frac{dt}{i\hbar} \phi_\alpha^2(x) \left[V(0) - 2 \int dy \frac{|\phi_\alpha(y)|^2}{||\phi_\alpha||^2} V(x-y) + \frac{\langle \phi_\alpha, \phi_\alpha | V | \phi_\alpha, \phi_\alpha \rangle}{||\phi_\alpha||^4} \right]. \quad (75)$$

As the expressions between square brackets in Eqs. (75) and (74) are real positive we deduce the equality in Eq. (68).

We can now calculate explicitly the variation of $\mathrm{Tr}[\sigma^\dagger \sigma]$ by integrating Eq. (74) over x:

$$\frac{d\,\mathrm{Tr}[\sigma^\dagger \sigma]}{N\,\mathrm{Tr}[\sigma^\dagger \sigma]} = \frac{dt}{\hbar} \left[2V(0) - \sum_{\alpha=1,2} \frac{\langle \phi_\alpha, \phi_\alpha | V | \phi_\alpha, \phi_\alpha \rangle}{||\phi_\alpha||^4} \right]. \quad (76)$$

This expression is particularly useful since it allows one to derive an upper bound on the increase of $\mathrm{Tr}[\sigma^\dagger \sigma]$: as we assume here a positive Fourier transform of the potential $V(x-x')$, the matrix element $\langle \phi_\alpha, \phi_\alpha | V | \phi_\alpha, \phi_\alpha \rangle$ is also positive so that the right-hand side of Eq. (76) is smaller than $2V(0)dt/\hbar$. After time integration we obtain

$$\mathrm{Tr}[\sigma^\dagger \sigma](t) \leqslant \mathrm{Tr}[\sigma^\dagger \sigma](0) e^{2NV(0)t/\hbar}. \quad (77)$$

An important consequence of this inequality is that none of the solutions of the stochastic equations of this scheme explode *in finite time*.

Using Eq. (57) and the fact that the trace of the squared density operator ρ^2 is a constant under Hamiltonian evolution we can deduce an upper bound on the squared statistical error $\Delta(t)$:

$$\Delta(t) + \mathrm{Tr}[\rho^2] \leqslant [\Delta(0) + \mathrm{Tr}[\rho^2]] e^{2NV(0)t/\hbar}. \quad (78)$$

Note that it involves the model dependent quantity $V(0)$ and not only the physical parameters of the problem such as the chemical potential or the scattering length. It may be therefore important to adjust the model interaction potential $V(x-x')$ in order to minimize the growth of the statistical error for given physical parameters.

To summarize the proposed simple scheme has several noticeable properties. The deterministic force acting on the ϕ_α's is simply the mean field contribution, so that the whole correction to the mean field evolution is provided by the transverse noises $dB_\alpha^\perp$. Also the evolutions of the two states ϕ_α are totally independent from each other.

2. Simulation with coherent states

In the case of the coherent state ansatz, an explicit calculation of $d\,\mathrm{Tr}[\sigma^\dagger \sigma]$ from Eq. (60) gives

$$\frac{d\,\mathrm{Tr}[\sigma^\dagger \sigma]}{\mathrm{Tr}[\sigma^\dagger \sigma]} = \left| \frac{db}{\Pi} + \overline{N} \int dx\, dB_1(x) \phi_1^*(x) + dB_2^*(x) \phi_2(x) \right|^2 + \overline{N} \sum_{\alpha=1,2} \int dx\, dB_\alpha(x) dB_\alpha^*(x) + \left[\frac{db}{\Pi} + \overline{N} \int dx\, dB_1(x) \phi_1^*(x) + dB_2^*(x) \phi_2(x) + \mathrm{c.c} \right], \quad (79)$$

where $|dz|^2$ stands for $dz\, dz^*$ in the Ito sense.

We now proceed to the minimization of the increment of $\mathrm{Tr}[\sigma^\dagger \sigma]$ within the coherent state ansatz along the same lines as the previous subsection. First we optimize the noise db on the normalization factor Π:

$$db = -\overline{N} \Pi \left(\int dx\, dB_1(x) \phi_1^*(x) + dB_2^*(x) \phi_2(x) \right). \quad (80)$$

This choice leads to a vanishing noise term in Eq. (79). We insert this expression for db in the validity conditions Eq. (50) and Eq. (51) and we obtain

$$F_\alpha(x) = \frac{1}{i\hbar} \left[h_0 + \overline{N} \int dx'\, V(x-x') |\phi_\alpha(x')|^2 \right] \phi_\alpha(x). \quad (81)$$

Finally if the model interaction potential has a positive Fourier transform [cf. Eq. (69)] minimization of the contribution of the noise terms dB_α with the constraint Eq. (52) is achieved with the choice

$$dB_\alpha(x) = \left(\frac{dt}{i\hbar} \right)^{1/2} \phi_\alpha(x) \sum_k \frac{\sqrt{dk}}{(2\pi)^{d/2}} (\tilde{V}(k))^{1/2} e^{ikx} e^{i\theta_\alpha(k)}, \quad (82)$$

where the phases $\theta_\alpha(k)$ are randomly generated as in Eq. (73).

The first equation (81) fixes the deterministic evolution to the usual mean-field equation (4). We note here that the mean-field term in Eq. (81) does not contain the normalization of the spatial density $\overline{N} |\phi_\alpha(x')|^2$ by $||\phi_\alpha||^2$, a feature present in the Fock state simulation [see Eq. (20)]. This is a disadvantage of the coherent state simulation since this normalization factor appearing in the Fock state simulation has a regularizing effect: the norms $||\phi_\alpha||$ may indeed deviate significantly from unity in the stochastic evolution. The second

equation (82) determines the stochastic noise on the wave functions in a way very similar to the Fock state case (72). In particular the evolutions of ϕ_1 and ϕ_2 are still uncorrelated. The only difference is the disappearance of the projector $\mathcal{Q}_\alpha$ in the expression of the noise, which leads to an increased noise with respect to the simulation with Fock states.

As in the Fock state case, the deterministic evolution of the present scheme has a Gross-Pitaevski form and thus conserves the norms $||\phi_{1,2}||$. This condition, together with the upper bound $\zeta_{1,2} \leqslant V(0)dt||\phi_{1,2}||^2/\hbar$ on the eigenvalues $\zeta_{1,2}$ of the noise covariance operator $dB_\alpha(x)dB_\alpha^*(x')$, can be used to prove that the stochastic equations possess a finite, *non-exploding* solution valid for all times (see [25] in Sec. IV E).

As in the previous subsection we now estimate the squared error Δ. We calculate the variation of $\mathrm{Tr}[\sigma^\dagger\sigma]$ for the choice of noise Eq. (82):

$$\frac{1}{\mathrm{Tr}[\sigma^\dagger\sigma]}\frac{d\,\mathrm{Tr}[\sigma^\dagger\sigma]}{dt}=\frac{\overline{N}V(0)}{\hbar}\sum_{\alpha=1,2}||\phi_\alpha||^2. \tag{83}$$

The average over all stochastic realizations of the norm squared of the wave functions can be calculated exactly:

$$\langle||\phi_\alpha||^2\rangle_{\mathrm{stoch}}(t)=e^{tV(0)/\hbar}\langle||\phi_\alpha||^2\rangle_{\mathrm{stoch}}(0). \tag{84}$$

This leads to a remarkable identity on the trace of $\sigma^\dagger\sigma$:

$$\langle \ln \mathrm{Tr}[\sigma^\dagger\sigma]\rangle_{\mathrm{stoch}}(t)=\langle \ln \mathrm{Tr}[\sigma^\dagger\sigma]\rangle_{\mathrm{stoch}}(0)+\overline{N}(e^{tV(0)/\hbar}-1)\times\left\langle\sum_{\alpha=1,2}||\phi_\alpha||^2\right\rangle_{\mathrm{stoch}}(0). \tag{85}$$

Using finally the concavity of the logarithmic function, leading to the logarithm of a mean being larger than the mean of the logarithm we obtain a lower bound on the squared error Δ on the N-body density matrix:

$$\Delta(t)+\mathrm{Tr}[\rho^2]\geqslant A\exp[2B\overline{N}(e^{tV(0)/\hbar}-1)], \tag{86}$$

where we have introduced the constant quantities

$$A=\exp[\langle \ln \mathrm{Tr}[\sigma^\dagger\sigma]\rangle_{\mathrm{stoch}}(0)], \tag{87}$$

$$B=\frac{1}{2}\left\langle\sum_{\alpha=1,2}||\phi_\alpha||^2\right\rangle_{\mathrm{stoch}}(0). \tag{88}$$

We recall that a vanishing $V(0)$ would correspond here to an identically vanishing interaction potential $V(x)$, according to Eq. (71).

C. The *constant trace* schemes

We have given the expression of the one-body density matrix $\rho^{(1)}$ in terms of $\phi_\alpha(x)$ for the simulation with Fock states Eq. (13). This expressions shows that $\rho^{(1)}$ is very sensitive in the large N limit to fluctuations of $\langle\phi_2|\phi_1\rangle$. The same remark applies to two-body observables. In order to improve the statistical properties of the simulation one can consider the possibility of a simulation scheme with $\langle\phi_2|\phi_1\rangle=1$ at any time. This actually corresponds to a conserved trace of each single dyadic $\sigma(t)$. This possibility is analyzed in Sec. III C 1; it is extended to the coherent state simulation in Sec. III C 2, leading to the well-known positive *P*-representation formalism.

1. Simulation with Fock states

Within the Fock state ansatz, the conservation of the trace of the dyadic $\mathrm{Tr}[\sigma]$ can be achieved by (i) choosing the transverse noises $dB_\alpha^\perp$ according to the formula Eq. (72) and (ii) using the expression Eq. (65) for the longitudinal noise with $X=1$. Point (ii) gives

$$d\gamma_1=-\langle\phi_2|\phi_1\rangle^{-1}\int dx\,\phi_2^*(x)dB_1^\perp(x). \tag{89}$$

The force terms λ_α and F_α are fixed by the conditions (39)–(41):

$$\lambda_1\,dt=-\frac{N-1}{2}\langle\phi_2|\phi_1\rangle^{-2}\int dx\,dx'\,\phi_2^*(x)\times\phi_2^*(x')dB_1^\perp(x)dB_1^\perp(x') \tag{90}$$

and

$$F_1^\perp(x)dt=(N-1)\langle\phi_2|\phi_1\rangle^{-1}\times\int dx'\,\phi_2^*(x')dB_1^\perp(x')dB_1^\perp(x). \tag{91}$$

The expressions for $d\gamma_2,\lambda_2$ and $F_2^\perp(x)$ are obtained by exchanging the indices 1 and 2 in these results.

2. Simulation with coherent states

In the case of the coherent state ansatz, the value of $d\sigma_s$, which is the zero-mean noise term entering the variation of the dyadic σ during a time step dt, is given in Eq. (60). The requirement of a constant trace $\mathrm{Tr}[\sigma]=\Pi e^{\overline{N}\langle\phi_2|\phi_1\rangle}$ leads to the following condition on the noise terms:

$$db+\overline{N}\Pi\int dx(\phi_2^*(x)dB_1(x)+dB_2^*(x)\phi_1(x))=0. \tag{92}$$

We choose the noise terms dB_α as in Eq. (82). The remaining parameters F_α are now unambiguously determined by Eqs. (50) and (51):

$$F_1(x)=\frac{1}{i\hbar}\left[h_0+\overline{N}\int dx'\,\phi_2^*(x')V(x-x')\phi_1(x')\right]\phi_1(x), \tag{93}$$

$$F_2(x)=\frac{1}{i\hbar}\left[h_0+\overline{N}\int dx'\,\phi_1^*(x')V(x-x')\phi_2(x')\right]\phi_2(x). \tag{94}$$

This scheme exactly recovers the stochastic evolution in the positive *P* representation, which was originally obtained with a different mathematical procedure [24].

IV. STOCHASTIC VERSUS EXACT APPROACH FOR A TWO-MODE MODEL

In order to test the convergence of the stochastic schemes developed in the preceding section we now apply this method to a simple two-mode model for which the exact solution of the N-body Schrödinger equation can also be obtained by a direct numerical integration. This allows (i) to check that the stochastic methods when averaged over many realizations give the correct result indeed, and (ii) to determine the statistical error for each of the four implementations of the stochastic approach (''constant trace'' vs ''simple,'' Fock vs coherent states).

The toy-model that we consider is motivated by the dynamics of two self-interacting condensates coherently coupled one to the other, as it is the case for two condensates separated by a barrier [26] (Josephson-type coupling) or for condensates in two different internal states coupled by an electromagnetic field [27] (Rabi-type coupling). In this model we restrict the expansion of the atomic field operator to two orthogonal modes,

$$\hat{\psi}(x) = \hat{a}\, u_a(x) + \hat{b}\, u_b(x). \tag{95}$$

The Hamiltonian Eq. (1) takes the simple form

$$\mathcal{H} = \frac{\hbar\Omega}{2}(\hat{a}^\dagger\hat{b} + \hat{b}^\dagger\hat{a}) + \hbar\kappa(\hat{a}^{\dagger 2}\hat{a}^2 + \hat{b}^{\dagger 2}\hat{b}^2), \tag{96}$$

where $\hat{a},\hat{b}$ annihilate a particle in modes u_a and u_b, κ characterizes the strength of the atomic interactions inside each condensate and Ω is the Rabi coupling amplitude between the two condensates. Here we have restricted for simplicity to the case where (i) the condensates have identical interaction properties, (ii) the interactions between atoms in different wells are negligible, and (iii) the Rabi coupling is resonant. The most general two-mode case could be treated along the same lines.

The direct numerical solution of the Schrödinger equation is performed in a basis of Fock states $|n_a, n_b\rangle$ with $n_{a,b}$ particles in modes u_a, u_b. The numerical integration is simplified by the fact that $n_a + n_b$ is a quantity conserved by the Hamiltonian evolution. We start with a state in which all atoms are in mode u_b, either in a Fock state $|n_a = 0, n_b = N\rangle$ (for the Fock state simulations) or in a coherent state $\propto \exp(N^{1/2}\hat{b}^\dagger)|0,0\rangle$ (for the coherent state simulations). We watch the time evolution of the mean fraction of particles in mode u_a, $p_a \equiv \langle \hat{a}^\dagger\hat{a}\rangle/N$.

Mean-field theory (the Gross-Pitaevskii equation), valid in the limit $N \gg 1$ with a fixed $\kappa N/\Omega$ [28], predicts periodic oscillations of $\langle \hat{a}^\dagger\hat{a}\rangle/N$; the peak-to-peak amplitude of the oscillations is equal to unity if $\kappa N/\Omega < 1$, and is smaller than one otherwise [29]. In the exact solution the oscillations are no longer periodic due to emergence of incommensurable frequencies in the spectrum of H.

In the simulation method we evolve sets of two complex numbers representing the amplitudes of the functions $\phi_1(x)$ and $\phi_2(x)$ on the modes $u_{a,b}(x)$ (plus the Π coefficient in the coherent state case). The results are presented in Fig. 1

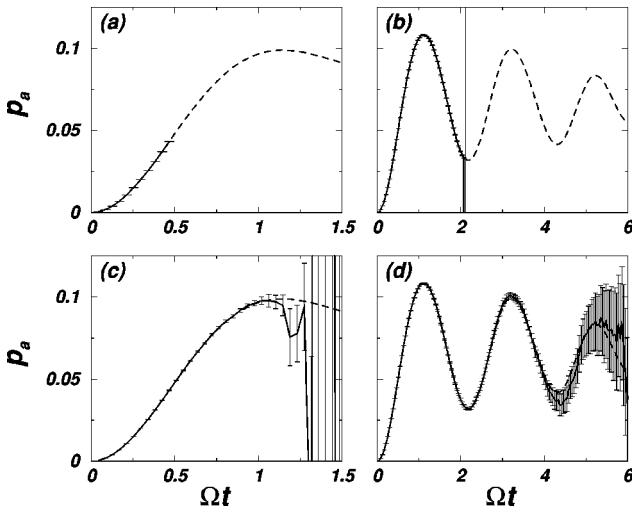

FIG. 1. In the two-mode model mean fraction of atoms in the mode u_a as function of time, obtained with (a) the positive P representation, (b) the Fock state simulation with constant trace, (c) the simple simulation with coherent states, and (d) the simple simulation with Fock states. The solid line represents the average over $\mathcal{N} = 2\times 10^5$ simulations, with corresponding error bars. The dashed line is the direct numerical solution of the Schrödinger equation. The number of atoms is $N = 17$, initially all in mode u_b. The interaction constant is $\kappa = 0.1\Omega$. The time step used in the numerical stochastic calculation is $\Omega dt = 10^{-3}$. The calculations in (a) and (b) have been stopped after the divergence of one realization.

for $N = 17$ particles and $\kappa/\Omega = 0.1$, together with the result of the direct integration of the Schrödinger equation.

The first row in the figure concerns the constant trace simulations. Figure 1(a) shows results of the simulation based on the positive P representation, that is the constant trace simulation with coherent states. As well known [13,18] this scheme leads to divergences of the norm $||\phi_1||\,||\phi_2||$ for some realizations of the simulation. We have cut the plot in Fig. 1 at the first divergence, a procedure shown to be justified for the positive P representation in [13,18]. The same type of divergences occurs in the constant trace simulation with Fock states [Fig. 1(b)], and we heuristically cut the divergencies with the same procedure. Note however that the characteristic time for the first divergence to occur is somewhat longer. We have checked for these constant trace simulations that the probability distribution of $||\phi_1||\,||\phi_2||$ broadens with time, eventually getting a power law tail. The corresponding exponent α decreases in time below the critical value $\alpha_{\rm crit} = 3$ for which the variance of $||\phi_1||\,||\phi_2||$ becomes infinite. This scenario is identical to the one found with the positive P representation [13,18].

The simple simulation schemes plotted on the second row of Fig. 1 provide results which are at all time in agreement with the direct integration within the error bars. Contrarily to the constant trace schemes we do not observe finite time divergences in the simple schemes. For a given evolution time we have checked that the error bars scale as $1/\sqrt{\mathcal{N}}$ where $\mathcal{N}$ is the number of stochastic realizations. For a given $\mathcal{N}$ we found that the error bars increase quasiexponentially with time.

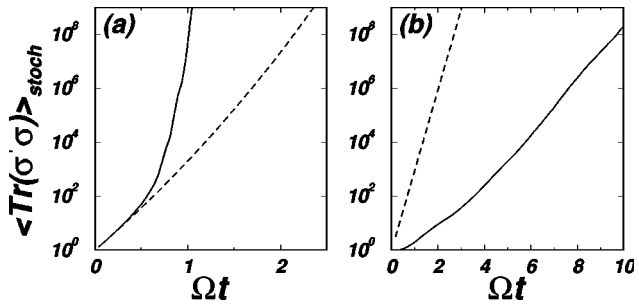

FIG. 2. Statistical error on the *N*-body density matrix for the two-mode model: (a) ''simple'' scheme with coherent states and (b) ''simple'' scheme with Fock states. The solid line is the numerical result of the simulations. The dashed lines in (a) and (b) correspond respectively to the lower and upper bounds, Eq. (86) and Eq. (78). The parameters are the same as in Fig. 1.

The noise in the simple simulation schemes is investigated in more detail in Fig. 2 which shows the error estimator $\langle \mathrm{Tr}[\sigma^{\dagger}\sigma]\rangle_{\mathrm{stoch}}$ as function of time, for coherent states in Fig. 2(a) and for Fock states in Fig. 2(b). The coherent state result confirms the prediction Eq. (86). The Fock state result is found to be notably smaller than the upper bound Eq. (78). This is due to the fact that the terms proportional to $\langle \phi_\alpha, \phi_\alpha | V | \phi_\alpha, \phi_\alpha \rangle$ in Eq. (76) are not negligible as compared to the term $V(0)$. We have checked these conclusions for various values of N and κ/Ω.

For a large number of particles it is known [30] that the oscillations of $\langle \hat{a}^{\dagger}\hat{a}\rangle$ experience a collapse followed by revivals. These revivals are purely quantum phenomena for the field dynamics and they cannot be obtained in classical field approximation such as the Gross-Pitaevskii equation. We expect to see a precursor of this phenomenon even for the small number of particles $N=17$. As the simple scheme simulation with Fock states is the most efficient of the four schemes for the investigation of the long time limit, we have pushed it to the time at which a ''revival'' can be seen, as shown in Fig. 3. This figure is obtained with $\mathcal{N}=10^8$ simulations.

V. STOCHASTIC APPROACH FOR A ONE-DIMENSIONAL BOSE GAS

The interacting Bose gas is in general a multimode problem, and the simulation schemes may have in this case a behavior different from the one in a few-mode model such as in Sec. IV. We have therefore investigated a model for a one-dimensional Bose gas. The atoms are confined in a harmonic trap with an oscillation frequency ω. They experience binary interactions with a Gaussian interaction potential of strength g and range b:

$$V(x-x') = \frac{g}{(2\pi)^{1/2} b} \exp[-(x-x')^2/(2b^2)]. \quad (97)$$

At time $t=0$ all the atoms are in the same normalized state ϕ solution of the time independent Gross-Pitaevskii equation

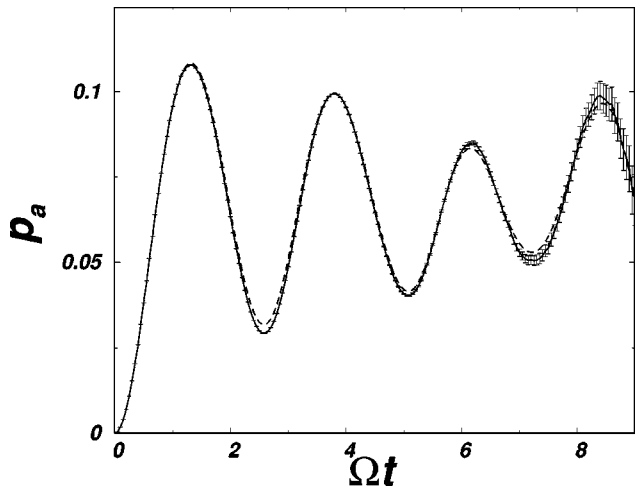

FIG. 3. Fraction of atoms in mode u_a in the two-mode model, for the parameters of Fig. 1. The dashed line is the direct numerical solution of the Schrödinger equation. The solid line with error bars is the result of the ''simple'' scheme simulation with Fock states with $\mathcal{N}=10^8$ realizations. To keep a reasonable computation time with such a large value of $\mathcal{N}$ we have increased the time step in the numerical stochastic integration by a factor 25 with respect to Fig. 1. This explains the small systematic deviation of the simulation result from the exact result visible for example at time $\Omega t=2.6$. The quantum phenomenon of collapse and revival of the oscillation amplitude clearly apparent on the exact result is well reproduced by the simulation.

$$\mu\phi(x) = -\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \phi(x) + (N-1) \times \int dx'\, V(x-x') |\phi(x')|^2 \phi(x). \quad (98)$$

At time $t=0^+$ the trap frequency is suddenly increased by a factor two, which induces a breathing of the cloud [31–33].

This expected breathing is well reproduced by the numerical simulations. The mean squared spatial width R^2 of the cloud as function of time is obtained by taking $\hat{O} = \Sigma_{k=1}^{N} \hat{x}_k^2/N$ in Eq. (11) where $\hat{x}_k$ is the position operator of the kth particle. The quantity R^2 is shown in Fig. 4 for the simulation schemes with Fock states. One recovers the key feature of the constant trace simulation, that is a divergence of the norm $||\phi_1||\,||\phi_2||$ in finite time for some realizations. Before the occurrence of the first divergence the stochastic variance of the size squared of the cloud, defined as

$$\mathrm{var}(R^2)_{\mathrm{stoch}} = \frac{1}{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} [R_i^2(t) - R^2(t)]^2, \quad \text{with}$$

$$R_i^2(t) = \mathrm{Re}[\langle N{:}\,\phi_2^{(i)}(t) | \hat{O} | N{:}\,\phi_1^{(i)}(t)\rangle], \quad (99)$$

is notably smaller in the constant trace scheme than in the simple scheme, as shown in Fig. 5(a). This contrast between the two schemes for the statistical error on one-body observables was absent in the two-mode model of Sec. IV.

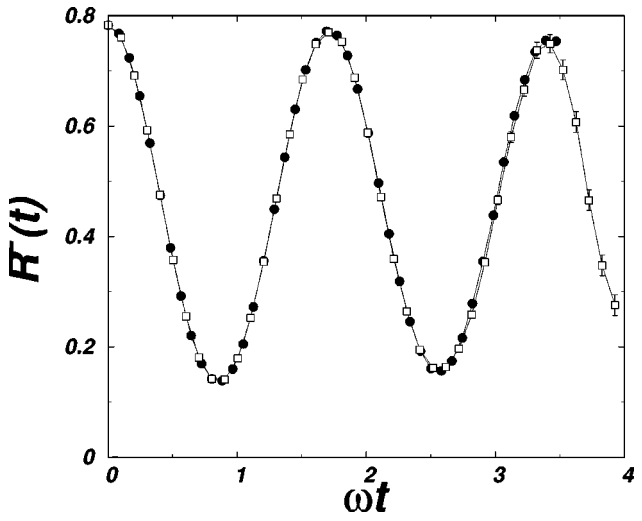

FIG. 4. Mean squared spatial width R^2 of a harmonically confined cloud of $N=10$ atoms as a function of time. The breathing of the cloud is induced by an abrupt change of the trap frequency from ω to 2ω. The width R is measured in units of the harmonic oscillator length $a_{\rm ho}=(\hbar/(m\omega))^{1/2}$. The interaction potential is chosen such that $b=0.5a_{\rm ho}$ and $g=0.4\hbar\omega a_{\rm ho}$ leading to a chemical potential $\mu=1.7\hbar\omega$ in the Gross-Pitaevskii equation (98). The calculation is performed on a spatial grid with 32 points ranging from $-6a_{\rm ho}$ to $+6a_{\rm ho}$ (with periodic boundary conditions). ●: Constant trace simulation with $\mathcal{N}=1000$ realizations. For $\omega t>3.5$ a divergence has occured for one of the realizations and the calculation has been stopped. □: Simple scheme simulation with $\mathcal{N}=40\,000$ realizations.

We have also investigated the noise on the N-body density matrix characterized by $\langle {\rm Tr}[\sigma^\dagger\sigma]\rangle_{\rm stoch}$ [see Fig. 5(b)]. As expected this error indicator is smaller with the simple scheme. For this simple scheme it varies quasi exponentially with time with an exponent $\gamma\simeq 4\omega$, which is smaller by a factor roughly 2 than the one of the upper bound Eq. (78). This difference is due to the fact that the range b of the interaction potential is chosen here of the same order as the size R of the cloud so that the terms $\langle\phi_\alpha,\phi_\alpha|V|\phi_\alpha,\phi_\alpha\rangle$ neglected in the derivation of the upper bound are actually significant. We have checked for various ranges b much smaller than R that γ then approaches the upper bound $2NV(0)/\hbar$.

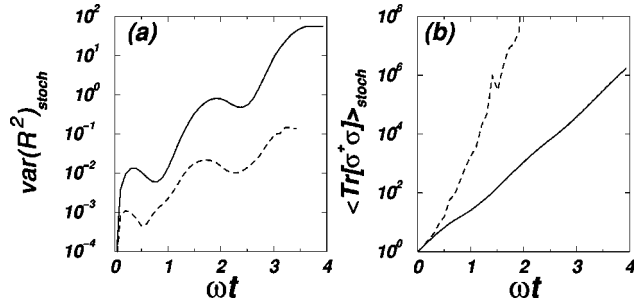

FIG. 5. For the one-dimensional Bose gas in the conditions of Fig. 4, (a) stochastic variance of the size squared of the cloud and (b) noise on the N-body density matrix. Solid lines: simple scheme with Fock states. Dashed lines: constant trace scheme with Fock states.

VI. CONCLUSION AND PERSPECTIVES

In this paper we have investigated a general method to solve exactly the N-body problem in the bosonic case. The principle of the approach is to add to the usual mean-field Gross-Pitaevskii equation a fluctuating term. We have determined the general conditions ensuring that the average over all possible realizations of this stochastic equation reproduces the exact N-body Schrödinger equation.

This idea already received a particular implementation in quantum optics, in the frame of the positive P representation. We recover here the scheme based on the positive P representation as a particular case of a simulation evolving coherent states of the bosonic field with the constraint that the trace of the density operator should remain exactly equal to unity for each single realization. This provides a simple derivation of the stochastic evolution within this representation alternative to the usual one [24] based on analyticity properties.

Among the many possible implementations of the general stochastic approach we have also investigated schemes evolving Fock states (that is number states) rather than coherent states. This is well suited to situations where the total number of particles is conserved. In particular we have identified a scheme preserving exactly the trace of the density operator which is for number states the counterpart of the one based on the positive P representation.

Schemes with constant trace are subject to divergence of the norm of some realizations in finite time. This effect, already known in the context of the positive P representation [13,18], makes these schemes difficult to use.

In order to overcome this divergence problem we have investigated schemes in which the condition on the trace is relaxed. We have chosen instead to minimize the statistical spread on the N-body density matrix, which gave rise to the ''simple'' schemes, either with coherent states or Fock states. In this case the N-body density operator is obtained as a stochastic average of dyadics such as $|{\rm coh}:\overline{N}^{1/2}\phi_1\rangle\langle{\rm coh}:\overline{N}^{1/2}\phi_2|$ or $|N:\phi_1\rangle\langle N:\phi_2|$, where the evolutions of ϕ_1 and ϕ_2 are fully decoupled. The deterministic parts are given by Gross-Pitaevskii equations, which preserves the norm of $\phi_{1,2}$, contrarily to the case of constant trace schemes. The decoupling between the evolutions of ϕ_1 and ϕ_2 allows a reinterpretation of our representation of the N-body density operator. If the initial density operator is given by $\rho(t=0)=|N:\phi_0\rangle\langle N:\phi_0|$ it will be given at time t by

$$\rho(t)=|\Psi(t)\rangle\langle\Psi(t)|, \tag{100}$$

with the N-particle state vector

$$|\Psi(t)\rangle=\lim_{\mathcal{N}\to\infty}\frac{1}{\mathcal{N}}\sum_{j=1}^{\mathcal{N}}|N:\phi^{(j)}(t)\rangle. \tag{101}$$

In this expression $\phi^{(j)}$ are stochastic realizations with the initial condition $\phi^{(j)}(t=0)=\phi_0$.

The ''simple'' schemes have much better stability properties than the constant trace schemes: differently from the

case of constant trace schemes, the deterministic evolution of the ''simple'' schemes has a Gross-Pitaevskii form and thus conserves the norms $||\phi_{1,2}||$. Furthermore we have shown that the corresponding stochastic equations possess a finite, *nonexploding* solution for all times.

We have numerically applied the simulation schemes to a two-mode model and to a one-dimensional Bose gas. In both cases we found that the constant trace schemes lead to some diverging realizations, while the simple schemes lead to a statistical spread on the *N*-body density operator increasing exponentially with time with an exponent $\gamma \propto NV(0)/\hbar$. The simple schemes are therefore not well suited to determine small deviations from the mean-field approximation in the large *N* limit but can be more efficiently applied to systems with a small number of particles, such as small atomic clouds tightly trapped at the nodes or antinodes of an optical lattice.

In the one-dimensional numerical example of this paper we have presented results for a simple one-body observable, the size of the atomic cloud. We have actually extended the calculations to more elaborate observables such as the first order and the second order correlation functions of the field. We have not presented the results here as the initial state of the gas was taken to be a (not very physical) Hartree-Fock state. We are presently working on the possibility to generate a more realistic initial state such as a thermal equilibrium for the gas, by extending our stochastic approach to evolution in imaginary time.

This work has several possible perspectives of extension. One can first use as building block a more sophisticated ansatz than the Hartree-Fock state $|N:\phi\rangle$, such as Bogoliubov vacua (that is squeezed states of the atomic field) or a multimode Hartree-Fock ansatz (that is an arbitrary coherent superposition of number states in several adjustable modes of the field). One can also look for *approximate* rather than *exact* stochastic solutions to the *N*-body problem but that would be better than mean-field approaches in some given situations. We hope to address some of these perspectives in the near future.

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