An exact stochastic field method for the interacting Bose gas at thermal equilibrium

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ABSTRACT

We present a new exact method to numerically compute the thermodynamical properties of an interacting Bose gas in the canonical ensemble. As in our previous paper (Phys. Rev. A 63 023606 (2001) ), we write the density operator $\rho$ as an average of Hartree dyadics $|N : \phi_1\rangle\langle N : \phi_2|$ and we find stochastic evolution equations for the wave functions $\phi_1, \phi_2$ such that the exact imaginary-time evolution of $\rho$ is recovered after average over noise. In this way, the thermal equilibrium density operator can be obtained for any temperature $T$. The method is then applied to study the thermodynamical properties of a homogeneous one-dimensional $N$-boson system: although Bose-Einstein condensation can not occur in the thermodynamical limit, a macroscopic occupation of the lowest mode of a finite system is observed at sufficiently low temperatures. If $k_B T \gg \mu$, the main effect of interactions is to suppress density fluctuations and to reduce their correlation length. Different effects such as a spatial antibunching of the atoms are predicted for the opposite $k_B T \leq \mu$ regime. Our exact stochastic calculations have been compared to existing approximate theories.

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1. INTRODUCTION

The recent advances in the production and manipulation of ultra-cold atomic samples have opened the way to the investigation of the thermodynamical and dynamical properties of interacting Bose gases in different geometries and dimensionalities [1] [3]; in three dimensional traps, Bose-Einstein condensation was realized a few years ago [4] and now there is a great deal of experimental interest in lower-dimensional systems, for which a remarkably different physics is predicted [5] [10]. In presence of a condensate, i.e. when the coherence of the Bose field extends throughout the whole sample, a mean-field theory can be applied, which completely neglects the non-condensed atoms and describes the system in terms of the classical field corresponding to the condensate wave function [11]. In three dimensions, such an approach is clearly valid only when a small non-condensed fraction is present, which implies a low temperature and weak interaction regime; for low-dimensional systems a further constraint has to be imposed on the

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spatial size of the system, which has to be smaller than the finite coherence length of the field. Within mean-field theory, weak thermal excitations on top of a well populated condensate can be taken into account by means of the Bogoliubov approach which describes the low-lying part of the many-body spectrum as a collection of uncoupled harmonic oscillators. Clearly, this approximated theory is valid only at relatively low temperatures, when the density of thermal excitations is small enough for their mutual interaction to be neglected.

Exact results for the thermodynamical properties of interacting Bose gases at any temperature can in principle be obtained using Quantum Monte Carlo techniques, but such an approach is subjected to strict limitations in its applicability domain: first of all, it requires that the matrix elements of the Hamiltonian are real in the position representation; this condition excludes rotating systems such as the ones used to study vortices. The privileged role attributed to the position representation makes some observables hard to be sampled, e.g. the momentum distribution function or the occupation number statistics of a given mode. Finally, the thermodynamical calculations performed with the quantum Monte Carlo method can not be prolonged to real time so to determine the dynamical properties of the system.

In the present paper we present a new exact and numerically tractable approach to the calculation of thermodynamical properties of an interacting Bose gas in the canonical ensemble. This computational scheme is not restricted to Hamiltonians with real matrix elements in real space and gives access to all observables of the system. Also, this computational scheme can be easily integrated with our reformulation of the dynamical evolution and therefore used to describe the response of finite-temperature samples to perturbations away from equilibrium. The method is based on the stochastic evolution of Hartree dyadics \( \sigma = |N : \phi_1 \rangle \langle N : \phi_2| \) where \( \phi_{1,2} \) are non-normalized wave functions. In our previous paper we showed that it is possible to choose the stochastic evolution of \( \phi_{1,2} \) in such a way that the average evolution of \( \sigma \) over the stochastic noise exactly reproduces the full many-body time-evolution. Here, we show that similar arguments can be used to find a stochastic evolution which exactly reproduces the imaginary-time evolution of the Bose gas and therefore can be used to determine the thermodynamical properties of the interacting \( N \)-boson system in the canonical ensemble. Differently from previous theories such as Positive-\( P \) representation, our scheme is not subjected to instability problems.

After the general discussion on the method, we shall report its first application to a homogeneous one-dimensional interacting Bose gas: such a model is expected to accurately describe the physics of Bose condensates tightly confined in the transverse dimensions so to create an effective one-dimensional geometry.

The outline of the paper is the following: in Sec. we present the general theory underlying the method and we discuss the stochastic equations for the Hartree wave functions \( \phi_{1,2} \) to be used for the study of dynamics and thermodynamics of the interacting Bose gas.

In Sec. we give details on the algorithm used in numerical simulations in order to enhance the efficiency of Monte Carlo calculations; in particular, a large reduction in the statistical noise can be obtained by means of an importance sampling with an appropriate \( a \) priori distribution function.

In Sec. we shall apply the method to the thermodynamical properties of a homogeneous one-dimensional interacting Bose gas in the canonical ensemble and we shall compare the
results of our stochastic calculations with existing approximate theories. Conclusions are finally given in Sec.V.

II. THE STOCHASTIC WAVE FUNCTION APPROACH

The Hamiltonian of a trapped interacting Bose gas in $D$ dimensions can be written in a second-quantized form as

$$\mathcal{H} = \int d^Dx \hat{\Psi}^\dagger(x)h_0\hat{\Psi}(x) + \frac{1}{2}\int \int d^Dx d^Dx' \hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x')V_{\text{int}}(x-x')\hat{\Psi}(x')\hat{\Psi}(x)$$  (1)

where $h_0 = -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(x)$ is the single particle Hamiltonian in the external confining potential $V_{\text{ext}}(x)$. Interactions are modeled by the two-body potential $V_{\text{int}}(x-x')$ which is assumed to be repulsive. The field operators $\Psi(x)$ satisfy Bose commutation relations $[\hat{\Psi}(x), \hat{\Psi}^\dagger(x')] = \delta(x-x')$.

Although the exact dynamics of the many-body system could in principle be obtained from the quantum mechanical equation of motion for the $N$-body density operator

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

any explicit calculation results impossible for the experimentally relevant multi-mode systems because of the huge dimensionality of the corresponding $N$-body Hilbert space.

In this section we shall discuss a reformulation of the bosonic many-body problem in terms of stochastic wave functions. As we have shown in [17], the $N$-body density operator of the system can always be written as a statistical average of Hartree operators $|N : \phi_1\rangle\langle N : \phi_2|$ in which all $N$ atoms share the same, not necessarily normalized wave function (Sec.II A). In the same paper, we have shown that the exact time-evolution of the full many-body system can be reproduced by an appropriately chosen stochastic evolution of the pair of single-particle wave functions $\phi_{1,2}$ (Sec.II B). The central theoretical result of the present paper is presented in Sec.II C: a similar stochastic evolution of the single particle wave functions $\phi_{1,2}$ is able to reproduce the imaginary-time evolution:

$$\frac{\partial \rho(\tau)}{\partial \tau} = -\frac{1}{2}\{\mathcal{H}, \rho(\tau)\} = -\frac{1}{2}(\mathcal{H}\rho(\tau) + \rho(\tau)\mathcal{H})$$  (3)

of the many body system with initial condition $\rho(\tau = 0) = \text{Id}$; this gives access to the thermodynamical properties of the interacting Bose gas in the canonical ensemble at any desired temperature $T$ as the solution of (3) after an evolution “time” $\tau = 1/k_BT$ is $\rho(\tau = 1/k_BT) = e^{-\mathcal{H}/k_BT}$.

A. The Fock state Hartree dyadic ansatz

As in our precedent paper [17], we consider the $N$-body Fock state Hartree ansatz

$$\sigma = |N : \phi_1\rangle\langle N : \phi_2|$$  (4)
in which the two Hartree wave functions $\phi_{1,2}$ in the bra and the ket are in general different and not normalized.

Given the remarkable identity [17] ($\int D\phi$ denotes the functional integration over the set of wave functions of unit norm $\|\phi\| = 1$)

$$\text{Id} = \int D\phi \mid N : \phi \rangle \langle N : \phi |,$$  \hspace{1cm} (5)

any $N$-body density operator $\rho$ can be expanded over the family of dyadics (4)

$$\rho = \int \int D\phi_1 D\phi_2 \mathcal{P}(\phi_1, \phi_2) \mid N : \phi_1 \rangle \langle N : \phi_2 |$$  \hspace{1cm} (6)

with a positive probability distribution $\mathcal{P}(\phi_1, \phi_2)$. Note that this expansion is by no means unique and several distinct $\mathcal{P}(\phi_1, \phi_2)$ can be found which correspond to the same physical density operator $\rho$.

From the expansion (6), the mean values of the observables can be written as mean values of combinations of $\phi_1$ and $\phi_2$ over the probability distribution $\mathcal{P}(\phi_1, \phi_2)$. As simple examples, the one-body density matrix $\rho^{(1)}(x, x')$ can be written as

$$\rho^{(1)}(x, x') = \left\langle \hat{\Psi}^\dagger(x') \hat{\Psi}(x) \right\rangle = N \phi_1(x) \phi_2^\ast(x') \langle \phi_2 | \phi_1 \rangle^{N-1}$$  \hspace{1cm} (7)

and the second-order correlation function $C^{(2)}(x, x')$ as

$$C^{(2)}(x, x') = \left\langle \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x') \hat{\Psi}(x') \hat{\Psi}(x) \right\rangle = N(N-1) \phi_1(x) \phi_1(x') \phi_2^\ast(x') \phi_2^\ast(x) \langle \phi_2 | \phi_1 \rangle^{N-2}.$$  \hspace{1cm} (8)

**B. Real-time evolution: dynamics**

The central result of the paper [17] was the proof of the possibility of reproducing the exact time evolution (2) of $\rho$ by means of a Ito stochastic evolution for $\phi_{1,2}$

$$\phi_\alpha(t + dt) = \phi_\alpha(t) + F_\alpha dt + dB_\alpha \quad (\alpha = 1, 2);$$  \hspace{1cm} (9)

in all the paper, the noise term $dB_\alpha$ is treated in the standard Ito formalism [19]: it has a zero mean $dB_\alpha$ and $dB_\alpha^2 \propto dt$; the deterministic contribution is given by the force term $F_\alpha dt$.

In the infinitesimal time interval $[t, t + dt]$, the two wave functions $\phi_1(x)$ and $\phi_2(x)$ are assumed to evolve according to Ito stochastic differential equations (6). After $dt$, the dyadic $\sigma(t) = \mid N : \phi_1 \rangle \langle N : \phi_2 |$ has therefore evolved into

$$\sigma(t + dt) = \mid N : \phi_1 + d\phi_1 \rangle \langle N : \phi_2 + d\phi_2 |$$  \hspace{1cm} (10)

where $d\phi_{1,2}$ are defined according to (4). Imposing that this evolution reproduces in the average the exact many-body evolution

$$\bar{\sigma(t + dt)} = \sigma(t) + \frac{dt}{i\hbar} (\mathcal{H} \sigma(t) - \sigma(t) \mathcal{H})$$  \hspace{1cm} (11)
gives a set of constraints on the explicit form of the stochastic differential equations (9).

As we have shown in [17], many stochastic evolutions can be found which all satisfy the exactness constraints: their stability and statistical properties are however significantly different. In the following we shall limit our attention to the so-called simple scheme minimizing the growth of the statistical variance of $\sigma$: thanks to its stability, this scheme has in fact been found to be the most efficient for practical simulations.

Explicitly, the stochastic evolution of the wave functions $\phi_{1,2}$ reads

$$
 d\phi_\alpha = \frac{1}{i\hbar} \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) + \frac{(N - 1)}{\|\phi_\alpha\|^2} \int d\mathbf{x}' V_{\text{int}}(x - \mathbf{x}') |\phi_\alpha(\mathbf{x}')|^2 + \frac{(N - 1)}{2} \frac{\langle \phi_\alpha \phi_\alpha | V_{\text{int}} | \phi_\alpha \phi_\alpha \rangle}{\|\phi_\alpha\|^4} \right] \phi_\alpha \, dt + dB_\alpha; \quad (12)
$$

as expected, the deterministic term closely resembles the Gross-Pitaevskii evolution of mean-field theory; the noises $dB_1$ and $dB_2$ are statistically independent and are determined by the correlation properties

$$
 dB_\alpha(x) \, dB_\alpha(x') = \frac{dt}{i\hbar} Q_\alpha^x Q_\alpha^{x'} [V_{\text{int}}(x - x') \phi_\alpha(x) \phi_\alpha(x')], \quad (\alpha = 1, 2) \quad (13)
$$

where $Q_\alpha^x$ is the projector onto the subspace orthogonal to $\phi_\alpha(x)$. Thanks to the fact that the deterministic term is norm-preserving, a mathematically well-defined solution exist for all times [17] so that the simulation does not suffer from the divergence problems encountered by previous stochastic approaches such as Gardiner’s Positive-$P$ distribution [18,20–22]. The statistical error, although exponentially growing with time proportionally to $\exp[2N V_{\text{int}}(0) t/\hbar]$, is always finite [1]: this guarantees that reliable physical results can be obtained by means of a Monte Carlo simulation of the stochastic differential equations; the norm-preserving character of the deterministic force ensures that no intrinsically spiking trajectories [15] can occur in the numerical calculations. This fundamental fact has been verified in Monte Carlo simulations of simple systems.

Since any $N$-body density operator $\rho(t)$ can be expanded in Hartree dyadics [1], the time evolution of the many body system can be reproduced by the stochastic approach starting from any initial condition. In [17] we used as initial state a fully coherent mean-field state $\rho = |N : \phi \rangle \langle N : \phi|$, in order to be able to get information on the full dynamics keeping track of all quantum effects, a more physical initial state has to be chosen. In the following part of the paper we shall show how a related stochastic wave function approach can be found which is able to sample the thermal equilibrium density operator $\rho_{\text{eq}}(\beta)$ for a many-body system of $N$ interacting bosons at a given $\beta = 1/k_B T$ in the canonical ensemble. A simulation of the dynamics of the many body system at finite temperature $\beta$ can be then performed on the base of (9) using $\rho_{\text{eq}}(\beta)$ as the initial state.

\[1\] This result holds in the case of repulsive interaction potentials with a positive Fourier transform [17], for which $V_{\text{int}}(0) \geq |V_{\text{int}}(x)|$. This means, in particular, that the statistical error only vanishes in the absence of interactions.
C. Imaginary-time evolution: thermodynamics

It is a well-known fact of quantum statistical mechanics\cite{13} that the unnormalized thermal equilibrium density operator $\rho_{eq}$ at a given temperature $T$ in the canonical ensemble can be written as

$$\rho_{eq}(\beta) = e^{-\beta H}$$

with $\beta = 1/k_B T$. Starting from the infinite temperature equilibrium state

$$\rho_{eq}(\beta = 0) = \text{Id},$$

the density operator at any given $\beta$ can be obtained by means of the imaginary-time evolution

$$\frac{d\rho_{eq}(\tau)}{d\tau} = -\frac{1}{2} \{ \mathcal{H}, \rho_{eq}(\tau) \} = -\frac{1}{2} (\mathcal{H} \rho_{eq}(\tau) + \rho_{eq}(\tau) \mathcal{H})$$

during a “time” $\beta$. The mean values of the observables are then easily obtained from the equilibrium density operator

$$\langle \hat{O} \rangle = \frac{1}{\text{Tr}[\rho_{eq}]} \text{Tr}[\rho_{eq} \hat{O}].$$

Given the similarity of the real- and imaginary-time evolution equations (2) and (16), the same arguments which led to (12,13) can be generalized to the imaginary-time evolution: the stochastic equations for the wave functions $\phi_{1,2}$ within the simple scheme now read

$$d\phi_\alpha = -\frac{d\tau}{2} \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(x) + \frac{(N-1)}{\|\phi_\alpha\|^2} \int dx' V_{\text{int}}(x - x') |\phi_\alpha(x')|^2 + \right. \left. -\frac{(N-1)}{2} \frac{\langle \phi_\alpha \phi_\alpha | V_{\text{int}} | \phi_\alpha \phi_\alpha \rangle}{\|\phi_\alpha\|^4} \right] \phi_\alpha + dB_\alpha; \quad (18)$$

and the correlation functions of the statistically independent noise terms $dB_{1,2}$ are fixed by

$$dB_\alpha(x) dB_\alpha(x') = -\frac{d\tau}{2} Q_\alpha Q_\alpha' \left[ V_{\text{int}}(x - x') \phi_\alpha(x) \phi_\alpha(x') \right]; \quad (19)$$

it is apparent how these equations are obtained from the real-time ones by means of the simple substitution $dt \rightarrow -i\hbar \frac{d\tau}{2}$.

As the starting point of the imaginary-time evolution, one has to choose a representation of the identity operator describing the $T = \infty$ equilibrium state; even if not the most efficient one, the simplest choice is clearly the one dictated by (3)

$$\rho_{eq}(\tau = 0) = \int_1^D \mathcal{D}\phi \langle N : \phi \rangle \langle N : \phi \rangle; \quad (20)$$

in the following Sec.III, we shall discuss how the efficiency of an actual Monte Carlo simulation can be sensibly improved by choosing a non-trivial \textit{a priori} probability distribution.
Differently from what happened for the real-time evolution, the deterministic term now resembles an imaginary-time Gross-Pitaevskii equation and does not preserve any more the norm $\|\phi_{1,2}\|$ of the wave functions. In particular, the deterministic contribution to the norm variation is equal to

$$d\|\phi_\alpha\|^2 = -\epsilon_{GP}[\phi_\alpha] \|\phi_\alpha\|^2 d\tau$$

(21)

where the mean-field energy $\epsilon_{GP}[\phi]$ is defined in terms of the normalized wave function $\phi_\alpha = \phi_\alpha/\|\phi_\alpha\|$ as

$$\epsilon_{GP}[\phi_\alpha] = \langle \bar{\phi}_\alpha | h_0 | \bar{\phi}_\alpha \rangle + \frac{(N-1)}{2} \langle \bar{\phi}_\alpha \bar{\phi}_\alpha | V_{\text{int}} | \bar{\phi}_\alpha \bar{\phi}_\alpha \rangle.$$  

(22)

Since interactions are assumed to be repulsive and the atoms are assumed to be trapped (the spectrum of $h_0$ is bounded from below) the mean-field energy $\epsilon_{GP}$ is also bounded from below; this guarantees that the stochastic equations have regular and non-exploding solutions defined at all $\tau$'s and the stochastic dynamics can be safely simulated by means of Monte Carlo techniques.

III. THE SIMULATIONS

The mathematical manipulations of the previous section have led to a reformulation of the interacting $N$-body problem in terms of a pair of simple stochastic differential equations for the wave functions $\phi_{1,2}$. This is a good starting point for a Monte Carlo simulation of the full quantum dynamics of the many body system: in [17] we presented first examples of real-time simulations, in the present paper we shall present imaginary-time ones based on the theory of Sec.II C. The present section is devoted to a general analysis of the simulation algorithm, while the next Sec.IV will describe the application of the method to the thermodynamical properties of a one-dimensional interacting Bose gas.

The simplest Monte Carlo implementation of the simulation scheme consists in randomly choosing an initial wave function $\phi$ on the unit sphere with an uniform distribution as done in (20); the two wave functions $\phi_{1,2}$ are then evolved from their initial value $\phi_{1,2} = \phi$ according to the stochastic evolution (18) including the noise term (19).

Unfortunately, this simple procedure is not efficient to calculate the expectation value of the observables at a given $\beta$. Since the largest fraction of the randomly chosen wave functions initially have a large mean-field energy (22), their deterministic evolution according to (21) gives a fast reduction of the norm. The explicit expression of the physically interesting observables, (7) or (8), contains the norm of the wave function raised to a large power of the order $N$; in particular, the trace of the denominator of (17) involves a sum of stochastic realizations of

$$\langle \phi_2 | \phi_1 \rangle^N \propto \|\phi_1\|^N \|\phi_2\|^N.$$  

(23)

The contribution of most realizations to this sum is therefore negligible so that a large fraction of the computational time is effectively wasted and the convergence of the stochastic average is impractically slow.
A technique which is currently used in Monte Carlo integration to overcome this kind of problems is the so-called *importance sampling*, a general and comprehensive discussion of which can be found in [23, §7.8]. In our specific case, such a technique is equivalent to using the following equivalent representation of the identity operator instead of the simple (20)

$$\rho_{eq}(\tau = 0) = \int_1 P[\phi] D\phi \frac{|N : \phi\rangle\langle N : \phi|}{P[\phi]};$$

(24)

the initial wave function is now chosen according to the (arbitrarily chosen) *a priori* probability distribution $P[\phi]$, while the weight of the realization is correspondingly divided by a factor $P[\phi]$, which amounts to a global rescaling of $\phi$. By choosing a $P[\phi]$ concentrated on the realizations with largest weight at “time” $\beta$, an effectively flatter integrand is obtained for the expectation values of the observables which means a more efficient Monte Carlo sampling. Although different observables lead to different optimization schemes, a reasonable choice if we are mainly interested in few-body observables such as spatial and momentum densities and low-order correlation functions can be an optimization scheme taking the trace of $\rho$ as an optimization criterion: we wish that each dyadic $|N : \phi_1\rangle\langle N : \phi_2|$ in the simulation has approximately the same trace (23).

For a non-interacting gas, no stochastic noise is present in the evolution equation (18), so the two wave functions are always equal $\phi_1 = \phi_2$. Let us first consider a dyadic $\sigma$ with initial value $|N : \phi(0)\rangle\langle N : \phi(0)|/P[\phi(0)]$, where $\phi(0)$ is distributed over the unit sphere with the probability density $P[\phi(0)]$. After an imaginary-time evolution during $\tau$, the trace of $\sigma$ is given by $\|\phi(\tau)\|^2/N/P[\phi(0)]$ where $\phi(\tau)$ is the result of the imaginary-time evolution starting from $\phi(0)$. The imaginary-time evolution in the absence of interactions is simply written in the basis of eigenmodes of the trapping potential, that is the eigenvectors of $h_0$. We label these eigenmodes with $k$ and we note their eigenenergy $E_k$:

$$\phi_k(\tau) = \phi_k(0)e^{-\tau E_k/2};$$

(25)

$\phi_k(\tau)$ denotes the component of the wave function $\phi(\tau)$ on the eigenmode $k$. In this simple case, a unit trace for the dyadic $\sigma$ at “time” $\tau = \beta$ can be obtained for the following choice of $P[\phi(0)]$:

$$P[\phi(0)] = \|\phi(\beta)\|^2 = \left(\sum_k |\phi_k(0)|^2 e^{-\beta E_k}\right)^N.$$

(26)

Even if not the optimal one, this choice is able to provide good efficiency also in the interacting case as we shall see on numerical examples.

In the next subsections we shall discuss two different methods to numerically generate random initial wave functions according to the probability distribution $P[\phi]$ of (26). The first method (sec.III A) has to be used when no condensate is expected to be present. The second one (sec.III B) is to be preferred at low temperatures when there is a macroscopic occupation of a single mode; in this range of parameters, in fact, this second method is able to provide a quicker and more accurate sampling of $P[\phi]$, but it is extremely slow in the absence of a condensate.
A. Brownian motion sampling

A simple way to generate a random variable with a given probability distribution function \( P[\phi] \) consists in constructing a Brownian motion with a deterministic drift term \( F^{(\text{det})}[\phi] \) and a Langevin noise term \( d\phi^{(st)} \):

\[
d\phi = F^{(\text{det})}[\phi] \, dt + d\phi^{(st)}
\]  

(27)

whose equilibrium distribution function is exactly \( P[\phi] \); if the random variable is evolved for a sufficiently long time \( t_{\text{max}} \), its value will be independent from the initial value and distributed according to \( P[\phi] \). In practical simulations, \( t_{\text{max}} \) is chosen in a heuristic way so to make results not to change if it is further increased. Note that \( t \) is here a fictitious evolution time that we take dimensionless.

Provided the force term is integrable

\[
F^{(\text{det})}[\phi] = -2\nabla_{\phi^*} U[\phi]
\]  

(28)

and the diffusion is constant and isotropic

\[
\begin{align*}
 d\phi^{(st)}_{k} d\phi^{(st)}_{k'} &= 2\delta_{k,k'} \, dt, \\
 d\phi^{(st)}_{k} d\phi^{(st)}_{k'} &= 0
\end{align*}
\]  

(29)\hspace{1cm} (30)

the equilibrium density of the Brownian motion (27) can be shown to be equal to

\[
P_{\text{eq}}[\phi] = e^{-2U[\phi]}.
\]  

(31)

In our specific case, the Brownian motion has to be confined on the \( \|\phi\| = 1 \) sphere: this is actually done by keeping only the projection of both the deterministic force and the stochastic noise along the sphere surface (i.e. orthogonal to \( \phi \)) and then renormalizing the wave function to unity after each time step; the renormalization procedure is equivalent to adding a deterministic force along \( \phi \) which keeps the wave function on the sphere.

Explicitly, the deterministic and stochastic increments can be written in terms of the the projector \( \tilde{Q}^{\perp}_\phi = 1 - \frac{1}{\|\phi\|^2} |\phi\rangle\langle \phi| \) as

\[
\begin{align*}
 d\phi^{(st)}_{\text{st}} &= \tilde{Q}^{\perp}_\phi \, d\phi^{(st)} \\
 F^{(\text{det})}_{\text{det}}[\phi] &= \tilde{Q}^{\perp}_\phi \, F^{(\text{det})}[\phi]
\end{align*}
\]  

(32)\hspace{1cm} (33)

with the force \( F^{(\text{det})} \) being given by the derivative with respect to \( \phi^*_{k}(0) \) of the logarithm of (26).

\[
F^{(\text{det})}_{k} = \frac{N\phi_{k} e^{-\beta E_{k}}}{\sum_{k'} |\phi_{k'}|^{2} e^{-\beta E_{k'}}}.
\]  

(34)

In order to avoid systematic errors, an actual calculation requires a temporal step \( dt \) such that both the deterministic \( F^{(\text{det})}_{\text{det}} \, dt \) and the stochastic \( d\phi^{(st)}_{\text{st}} \) variations of \( \phi \) are small as compared to \( \|\phi\| = 1 \), which respectively means \( N \, dt \ll 1 \) and \( N \, dt \ll 1 \), \( N \) being the number of modes actually used in the simulation.
B. Bogoliubov rejection sampling

While the sampling method discussed in the previous section can be used for any choice of physical parameters, in the presence of a large population in a single mode, a different method based on a Bogoliubov sampling can be more efficient; it is also free from arbitrary parameters like $t_{\text{max}}$ or $dt$ of the previous Brownian motion sampling which are sources of systematic errors.

Taking into account the wave function normalization $\|\phi\| = 1$, we can eliminate from the probability distribution (26) the field variable $\phi_0$ using $|\phi_0|^2 = 1 - \sum_{k \neq 0} |\phi_k|^2$ (its phase is uniformly distributed) and derive a probability density for the $\phi_k$’s, $k \neq 0$, in terms of the $\phi_{k \neq 0}$ only:

$$dN = \frac{d\phi_0}{\pi} \left( \sum_k |\phi_k|^2 e^{-\beta E_k} \right)^N \delta \left[ \sum_k |\phi_k|^2 - 1 \right] \prod_{k \neq 0} d\phi_k =$$

$$= \left( 1 - \sum_{k \neq 0} \frac{|\phi_k|^2}{\lambda_k} \right)^N \Theta \left[ 1 - \sum_{k \neq 0} |\phi_k|^2 \right] \prod_{k \neq 0} d\phi_k \quad (35)$$

where the $d\phi_k$’s stand for the double integral over the real and the imaginary parts of $\phi_k$; the energy $E_0$ of the ground $k = 0$ mode is set to $E_0 = 0$. The coefficients $\lambda_{k \neq 0}$ are defined as

$$\lambda_k = \left( 1 - e^{-\beta E_k} \right)^{-1} \quad (36)$$

and satisfy $\lambda_k \geq 1$. Up to a global multiplicative factor, the distribution function (35) can be rewritten in terms of the reduced field $\psi_k = \phi_k / \sqrt{\lambda_k}$ as

$$dN = \left( 1 - \sum_{k \neq 0} |\psi_k|^2 \right)^N \Theta \left[ 1 - \sum_{k \neq 0} \lambda_k |\psi_k|^2 \right] \prod_{k \neq 0} d\psi_k \quad (37)$$

and in this form it is easily sampled: $\psi_{k \neq 0}$ are generated with a spherically symmetric
probability distribution proportional to

\[(1 - \sum_{k \neq 0} |\psi_k|^2)^N\]  

(40)

and then all the realizations which do not satisfy the \(\Theta\) function in (37) are rejected \[23\], i.e. the ones for which

\[\sum_{k \neq 0} \lambda_k |\psi_k|^2 > 1.\]  

(41)

At the end of this procedure, \(\phi\)'s are obtained which are distributed according to the desired distribution law (26).

The efficiency of this method clearly depends on the fraction of realizations which have to be rejected at some stage; the step which strongly depends on the physical parameters is the rejection governed by condition (41): the condition (41) can be reformulated in terms of the number \(N_k = N|\phi_k|^2\) of particles in the \(k\) excited mode as

\[\sum_{k \neq 0} N_k > N;\]  

(42)

the larger the occupation of the ground \(k = 0\) mode, the smaller the number of realizations rejected at this stage and thus the quicker the sampling. In presence of a macroscopic occupation, the most probable occupation number of the \(k = 0\) mode is non-zero (cfr. Sec. IV B 3) so that the rejection occurs very rarely and the Bogoliubov sampling method is very rapid.

**IV. APPLICATION: THERMODYNAMICAL PROPERTIES OF A 1D HOMOGENEOUS BOSE GAS**

In the previous sections we have described the principles of the stochastic approach to the imaginary-time evolution of an interacting Bose gas as well as the crucial points of its

\[2\] Thanks to the inequality

\[e^{-N \sum_{k \neq 0} |\psi_k|^2} \geq (1 - \sum_{k \neq 0} |\psi_k|^2)^N: \]  

(38)

the distribution function (40) can be sampled by means of the rejection method \[23, \S7.3\] with the Gaussian as the comparison function: this latter is sampled by standard methods \[23, \S7.2\]; for each realization, we then choose a random number \(z\) uniformly distributed in \([0, 1]\): if

\[z > \frac{(1 - \sum_{k \neq 0} |\psi_k|^2)^N}{e^{-N \sum_{k \neq 0} |\psi_k|^2}}\]  

(39)

the realization is rejected, otherwise it is retained. The remaining realizations are automatically distributed according to (40).
actual implementation in a Monte Carlo simulation. The present section is devoted to the application of the method developed in the previous sections to a physically relevant system such as $N$ interacting bosons in a one dimensional box of finite size $L$ with periodic boundary conditions.

The one-dimensional regime is not far from reach in present experiments on transversally confined Bose condensates [1]. In particular, the phase fluctuation of the field when the coherence length is smaller that the spatial extension of the gas have been recently observed in a harmonic potential [2].

A. Ideal Bose gas in a large box: quantum degeneracy

It is a well-known fact of thermodynamics that Bose-Einstein condensation does not occur in a one-dimensional and non-interacting homogeneous system in the thermodynamic limit $L \to \infty$ at a constant density $n = N/L$ [13]. Even in the absence of Bose condensation, effects coming from the Bose statistics are however apparent in the quantum degenerate regime [24]

$$T < T_{\text{deg}} = \frac{2\pi \hbar^2 n^2}{m k_B},$$

i.e. when the thermal de Broglie wavelength

$$\lambda_{\text{th}} = \sqrt{\frac{2\pi \hbar^2}{m k_B T}}$$

is larger than the mean inter particle spacing $d = n^{-1}$; in this case, Bose statistics strongly enhances population of the lowest modes so that the characteristic field coherence length

$$\ell_c = \frac{\hbar^2 n}{m k_B T} = \frac{n \lambda_{\text{th}}^2}{2\pi}$$

turns out to be much longer than in the case of a non-degenerate system for which the coherence length is equal to $\lambda_{\text{th}}/\sqrt{2\pi}$.

In fig.1 the results of our stochastic simulations for a non-interacting gas at temperatures both above and below the degeneracy temperature are compared with the analytical predictions of the grand-canonical ensemble. Provided the size of the box $L$ is chosen sufficiently larger than the coherence length $\ell_c$ (which is the case of fig.1), excellent agreement is found; in this limit the canonical and the grand-canonical ensembles are in fact equivalent. In the next section specific effects due to a fixed particle number and the finite size of the system will be addressed.

Differently from the 3D case in which a true condensate is present in the thermodynamical limit, the 1D first-order correlation function (fig.2a)

$$g^{(1)}(x) = \frac{1}{n} \langle \hat{\Psi}^\dagger(x) \hat{\Psi}(0) \rangle$$

(46)
has a vanishing long distance limit \( g^{(1)}(x \to \infty) = 0 \) and a similar behavior is found in the second-order correlation function (fig.2b):

\[
g^{(2)}(x) = \frac{1}{n^2} \langle \hat{\Psi}^\dagger(0) \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \hat{\Psi}(0) \rangle; \quad (47)
\]

in the short distance limit, \( g^{(2)} \) tends to the value 2 typical of thermal non-interacting Bose systems; for large \( x \), \( g^{(2)}(x) \) exponentially decays to the value 1 with a decay constant equal to \( \ell_c/2 \): the characteristic correlation length scales for the phase (46) and density (47) fluctuations are therefore of the same order.

All the calculations presented in this section have been performed by means of the Brownian motion sampling discussed in Sec.III A; in the present \( L \gg \ell_c \) regime, the efficiency of a Bogoliubov sampling would be definitely poorer.

**B. Ideal Bose gas in a small box: Bose-Einstein condensation**

In the present section we shall discuss the case of a true Bose-Einstein condensate in a finite 1D box: in particular, we shall study the effect of a macroscopic occupation of a single mode on different observables; differently from other techniques [16], our method is in fact able to give access to all the observables of the system.

1. **Macroscopic occupation of a single mode**

In the previous section, we have shown that the phase coherence in a 1D sample extends only over a finite length \( \ell_c \) and the absence of a true condensate in the thermodynamical limit corresponds to a vanishing limit \( g^{(1)}(x \to \infty) \). On the other hand, if the sample we are considering has a length \( L \) comparable to or smaller than the coherence length \( \ell_c \), phase coherence extends over the whole sample.

According to the Wiener-Khintchine theorem [21], the momentum distribution function \( N(k) \) of a homogeneous system is proportional to the Fourier transform of the field correlation function \( g^{(1)}(x) \); a phase coherence extending over the whole sample therefore implies a macroscopic occupation of a single mode \(^2\).

This finite-size induced Bose condensation occurs around the temperature

\[
k_B T_{BEC} = \frac{6N\hbar^2}{mL^2} \quad (48)
\]

\(^3\)Apart from a numerical factor of the order of unity, the analogous condition for an interacting harmonically trapped cloud \( \ell_c \simeq R_{TF} \) (\( R_{TF} \) is the Thomas-Fermi radius of the cloud) leads to the same condensation temperature \( T_{ph} = \frac{(\hbar \omega)^2}{\mu} N \) as predicted in [8] from a different point of view.
at which the maximum number \( N_{\text{max}} \) of atoms that can be stored in the excited modes

\[
N_{\text{max}} = \sum_{k \neq 0} \frac{1}{\mathrm{e}^{\beta \hbar^2 k^2/2m} - 1} \simeq \frac{m k_B T L^2}{6 \hbar^2}
\]  \hspace{1cm} (49)

equals the number \( N \) of atoms present in the sample; the longer \( L \), the smaller the “transition” temperature \( T_{\text{BEC}} \). In terms of the phase coherence length \( \ell_c \), the BEC condition \( N > N_{\text{max}} \) can be rewritten as \( L < 6 \ell_c \).

In fig.3 we have plotted the momentum distribution for a growing number of atoms \( N \) across the transition value \( N_{\text{BEC}} \): for \( N \ll N_{\text{BEC}} \) the atoms that are further added to the system spread over the whole distribution. On the other hand, for \( N \gg N_{\text{BEC}} \), the population of the excited modes saturates to the value \( N_{\text{max}} \) and the added atoms accumulate in the fundamental mode; this behavior is strictly analogous to what happens in three-dimensional systems.

For the three upper curves for which \( N \geq 2 N_{\text{BEC}} \), the Bogoliubov sampling technique of Sec.III B has revealed to be much more efficient than the Brownian motion one; for the lower ones, the Brownian motion technique of Sec.III A was instead more performing. As a further check, we have successfully verified that the predictions of the two methods really agree with each other; on the scale of fig.3 the corresponding curves are nearly indistinguishable.

2. Suppression of density fluctuations

In addition to the features of the momentum distribution function and the related field correlation function \( g^{(1)}(x) \) discussed in the previous section, the presence of a Bose-Einstein condensate can be detected also by looking at the density fluctuations quantified by the value \( g^{(2)}(0) \) of the second-order correlation function (47). For a non Bose-condensed gas, it is well-known that \( g^{(2)}(0) \) is close to 2 as for a chaotic beam of light; at zero temperature \( T = 0 \), all the \( N \gg 1 \) atoms of the system are in the fundamental mode, so that \( g^{(2)}(0) = 1 - \frac{1}{N} \simeq 1 \). As we immediately see in fig.4, the crossover between the two regimes occurs in the neighborhood of the Bose-Einstein condensation temperature \( T_{\text{BEC}} \).

A simple argument allows to estimate the value of \( g^{(2)}(0) \) at low temperatures, when the non-condensed fraction is small; the second order correlation function can in fact be written as

\[
\langle \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \hat{\Psi}(x) \rangle = \frac{1}{L^2} \left( 2 \sum_{k \neq k'} \langle \hat{a}^\dagger_k \hat{a}^\dagger_{k'} \hat{a}_{k'} \hat{a}_k \rangle + \sum_k \langle \hat{a}^\dagger_k \hat{a}^\dagger_k \hat{a}_k \hat{a}_k \rangle \right) =
\]

\[
= \frac{1}{L^2} \left( 2 \sum_{k \neq k'} \langle n_k n_{k'} \rangle + \sum_k \langle n_k^2 \rangle - \sum_k \langle n_k \rangle \right). \hspace{1cm} (50)
\]

\footnote{The sum can be analytically computed since the system is assumed to be degenerate: in this case, most of the population is concentrated in the lowest modes for which \( \beta \hbar^2 k^2/2m \ll 1 \), so that the exponential can be linearized \( e^{\beta \hbar^2 k^2/2m} - 1 \simeq \beta \hbar^2 k^2/2m \).}
Whenever the non-condensed fraction $N_{nc}/N = \sum_k \langle n_k \rangle / N$ is small enough, the probability for having a completely empty condensate results negligible; under this assumption, the non-symmetry-breaking Bogoliubov approach of [15] is exact for the non-interacting gas and the spectrum of excitations is composed of a set of harmonic oscillators, one for each $k \neq 0$ mode of the trap. At a given temperature $T$, each mode is thermally populated in an independent way with a mean occupation number

$$\langle n_k \rangle = \frac{1}{e^{\beta \hbar k^2/2m} - 1}$$

and a variance

$$\langle n_k^2 \rangle = 2 \langle n_k \rangle^2 + \langle n_k \rangle.$$  

By substituting (51) and (52) into (50), we get the simple result

$$g^{(2)}(0) = \left(1 - \frac{1}{N}\right) \left[1 + 2 \frac{N_{nc}}{N} \right] - \frac{N_{nc}^2}{N^2} - 3 \sum_{k \neq 0} \frac{\langle n_k \rangle^2}{N^2}$$

which is plotted as a solid line in fig.4. The agreement with the prediction of the stochastic calculation is excellent especially at low temperatures, when the non-condensed fraction $N_{nc}/N$ is substantially smaller than 1; the discrepancy becomes important only when the non-condensed fraction is as high as 1/2 and the probability of having an empty condensate mode is no longer negligible.

It is worth stressing that the present suppression of density fluctuations is a consequence of the statistics only and therefore completely different from the one originating from interactions that we shall discuss in Sec.IV C 1.

3. Ground mode population statistics

The probability of having $n$ atoms in the condensate is given by the expectation value of the projector $\hat{Q}(0; n)$ on the subspace in which the ground $k = 0$ mode contains exactly $n$ atoms:

$$Q_0(n) = \text{Tr}[\hat{Q}(0; n) \rho] \text{ Tr}[\rho]^{-1}$$

In terms of our Hartree ansatz (4), this quantity can be written as

$$\text{Tr}[\hat{Q}(0; n) \rho] = \frac{N!}{n! (N - n)!} \langle \phi_2^o^* \phi_1^o \rangle^n \langle \phi_2^+ \phi_1^+ \rangle^{N - n},$$

where $\phi_{1,2}^o$ are the components of the wave functions $\phi_{1,2}$ along the ground $k = 0$ mode and $\phi_{1,2}^+$ are the components along the orthogonal subspace spanned by the remaining $k \neq 0$ modes. In the non-interacting case in which $\phi_1 = \phi_2 = \phi$, this expression can be further simplified to

$$\text{Tr}[\hat{Q}(0; n) \rho] = \frac{N!}{n! (N - n)!} \langle \phi^o \rangle^{2n} \langle \|\phi\|^2 - |\phi^o|^2 \rangle^{N - n}.$$
At temperatures $T$ much higher than the condensation temperature $T_{BEC}$, the mean population of all the modes is only a small fraction of the total number of particles so that each of them sees all the others as a sort of particle reservoir and its occupation is accurately described within the grand-canonical ensemble by the thermal distribution function

$$Q_k(n) = \frac{\bar{n}^n}{(1 + \bar{n})^{n+1}}$$

of average occupation number $\bar{n}$. In this regime, the occupation probability $Q_0(n)$ of the ground mode $k = 0$ is a monotonically decreasing function and the most probable occupation number is $n = 0$ (fig.5, solid line).

As soon as $T$ approaches the condensation temperature $T_{BEC}$, the occupation statistics of the fundamental mode is drastically modified by the presence of a condensate (dotted and dot-dashed lines) and, in particular its slope at $n = 0$ changes its sign around $T = T_{BEC}$ [23]. For $T < T_{BEC}$ the occupation function $Q_0(n)$ has a peaked shape around its mean value (dashed line).

A similar transition is well known to occur for the photon distribution in a laser: below threshold the distribution has a thermal shape (57), while above threshold it tends to the Poisson distribution typical of a coherent state [21].

C. Interacting gas

In the case of the non-interacting system described in the previous section it has been possible to find the simple a priori distribution function $P[\phi]$ (26) which optimizes the efficiency of the Monte Carlo calculation at a given $\beta$. For an interacting system, such a optimum choice is no longer simple to implement; heuristically, the simulations of the interacting system described in the present section have been carried out using the same a priori $P[\phi]$ as used for non-interacting gases.

For simplicity of the analysis, we shall limit ourselves to the case of a zero-range interaction potential

$$V_{int}(x - x') = g \delta(x - x'); \quad (58)$$

the coupling constant $g$ is related to the 1D scattering length $a_{1D}$ by

$$g = \frac{\hbar^2}{ma_{1D}}. \quad (59)$$

On the discrete lattice we are actually using in the simulation, the delta interaction potential (58) translates into

$$V_{int}(x - x') = \frac{g}{\Delta x} \delta_{x,x'}, \quad (60)$$

$\Delta x$ being the lattice spacing.
1. Classical field regime

If the gas is well in the degenerate regime $T \ll T_{\text{deg}}$ but not condensed, the main effect of atom-atom interactions is the suppression of density fluctuations and the appearance of a new length scale $\xi = \sqrt{\hbar^2/2mng}$ over which the density fluctuations are correlated [24], the so-called healing length.

If interactions are extremely weak $\chi = \hbar^2 g \beta^2 n^3/m \ll 1$, i.e. $\xi \gg \ell_c$, then the gas can be considered as an ideal gas, the density fluctuations are close to the non-interacting value $g^{(2)}(0) = 2$ and the characteristic length scales for phase correlation and density fluctuations turn out being of the same order $\ell_c$ (fig. 6a). The fact that $g^{(2)}(0)$ in the figure is not exactly 2 even in a non-interacting case is due to the fact that the system we are considering is a finite one; we have in fact checked that for increasing box size $L$, $g^{(2)}(0)$ approaches its thermodynamical limit of 2 (fig. 6b).

For stronger interactions $\chi > 1$, density fluctuations are strongly suppressed by the interactions and their correlation is limited to the shorter length scale $\xi < \ell_c$; phase correlations are instead far less affected by the presence of the interactions than density correlations and, in particular, the field coherence length is increased by less than a factor 2.

From a quantitative point of view, the agreement of the result of our stochastic simulations with the approximated predictions of classical field theory [24] looks reasonable. We are in fact in a regime in which the classical field approximation can not be expected to be extremely accurate, since the classicity parameter $\eta = gn/k_BT \leq 0.1$ and the terms which were neglected are of order $\eta$.

If we neglect the stochastic noise in our calculations, we are led to an improved formulation of classical field theory: with respect to the usual one [24], we are now including one more “force” term in the imaginary-time evolution of the wave function in addition to the classical Boltzmann weight $e^{-\beta E[\phi]}$. The presence of this additional term makes the approach exact at least in the case of a non-interacting gas and, in particular, always immune from the so-called black-body catastrophe; the new deterministic term is in fact able to reproduce the correct Bose law even for the high energy modes, while the Boltzmann weight alone would predict a mean energy of $k_BT$ per mode. In practice, we have found that the result of the simulations is not appreciably modified if we neglect the stochastic term provided we are well within the classicity region $\eta \ll 1$; in other terms, this means that the predictions of the improved classical field theory are accurate in the $\eta \ll 1$ regime.

A similar improved classical field theory can also be formulated within the coherent state approach if we neglect the non-positive diffusion term in the Fokker-Planck equation [24]; also in this case, the approach gives exact predictions for the non-interacting gas.

A characteristic feature of classical field theories based on the Glauber-$P$ distribution such as the one in [24] is that the observables can be expressed as mean values of the corresponding classical field variables over a real and non-negative distribution function. Thanks to the Schwartz inequality, this implies that the second-order correlation $g^{(2)}(0)$ is always larger or equal to 1 and the field can never be antibunched.

In the next section we shall push our simulations over the boundary $\eta = 1$ of the classicity region and we shall look for signatures of non-classical behavior such as antibunching ($g^{(2)}(0)$). In previous stochastic field approaches such as the Glauber-$P$, such a parameter
2. Beyond the classical field regime: spatial antibunching of atoms

In the Sec. IV B we have seen that below the Bose-Einstein temperature $T_{\text{BEC}}$ a non-interacting gas is condensed in the zero-momentum mode. In the present section we discuss the effect of interactions on a condensed sample for $\eta \geq 1$, i.e. outside the classicality region. Since the mean occupation number of the fundamental mode is large, Bogoliubov rejection sampling will be used for the stochastic simulations.

In Fig. 7a we have plotted the value of $g^{(2)}(0)$ as a function of temperature for different values of the interaction constant $g$; as $T$ tends to zero, $g^{(2)}(0)$ tends to a finite value which is equal to $1 - 1/N$ for the non-interacting gas and equal to a smaller value in the presence of repulsive interactions; the stronger the interactions, the lower $g^{(2)}(0)$. In the other (b) panel, we show the behavior of $g^{(2)}(x)$ well below the condensation temperature: due to the repulsive interactions, a dip is present around $x = 0$. This effect is due to the stochastic term: the result of a calculation performed neglecting the noise term is shown as a long-dashed line; as expected $g^{(2)}(0)$ tends to $1 - 1/N$ for $T \to 0$. The disagreement with the exact calculation was expected since the classical approximation can not be accurate in the present definitely quantum regime $\eta \simeq 5$.

We now wish to compare our results for $g^{(2)}(0)$ to approximate analytical predictions. As a starting point we use the following result: given a Hamiltonian $\mathcal{H}$ which depends on a parameter $g$ (in our case, the interaction coupling constant), it follows from elementary quantum statistical mechanics that the partial derivative of the free energy $F = -k_B T \log Z$ (where $Z$ is the partition function $Z = \text{Tr}[e^{-\beta \mathcal{H}(g)}]$) with respect to the interaction parameter $g$ is equal to

$$ \frac{\partial F}{\partial g} = \langle \frac{\partial \mathcal{H}}{\partial g} \rangle; \quad (61) $$

in the case of a local interaction potential \cite{18}, this brings to the remarkable expression

$$ g^{(2)}(0) = \frac{2}{gnN} \frac{\partial F}{\partial g} \quad (62) $$

which can be used to obtain an analytical prediction to be compared with the results of stochastic simulations.

Furthermore, we are in a regime where the temperature is well below the transition temperature $T_{\text{BEC}}$ and the interactions are sufficiently weak $n\xi \gg 1$, most of the particles are therefore in the condensate and the system is accurately described by a Bogoliubov approximation in which the Hamiltonian of the many-body system is approximated as a system of uncoupled harmonic oscillators corresponding to the different elementary excitations of the system \cite{12, 14}.

In this case, the free energy $F$ of the system of uncoupled harmonic oscillators is immediately
calculated as
\[ F(g) = E_0(g) + k_B T \sum_{k \neq 0} \log(1 - e^{-\beta \epsilon_k}) \] (63)
and its derivative with respect to \( g \) has the following simple form
\[ \frac{\partial F}{\partial g} = \frac{dE_0}{dg} + \sum_{k \neq 0} \frac{d\epsilon_k}{dg} \frac{1}{e^{\beta \epsilon_k} - 1}. \] (64)

The index \( k \neq 0 \) runs over the different modes whose energies are given by the well-known Bogoliubov expression
\[ \epsilon_k = \sqrt{\frac{\hbar^2 k^2}{2m} \left( \frac{\hbar^2 k^2}{2m} + 2gn \right)} \] (65)
and the ground state energy \( E_0(g) \) is equal to \[ E_0(g) = \frac{N(N-1)g}{2L} - \sum_k \epsilon_k |v_k|^2 \] (66) with \( v_k = |\sinh \theta_k|^2 \) and
\[ \tanh 2\theta_k = \frac{gn}{\epsilon_k + gn}. \] (67)

Inserting the explicit expressions (65,66,67) into (64), numerically performing the sum over the different modes of a finite homogeneous box and finally inserting the result into (62) we are led to the finite temperature Bogoliubov predictions for \( g^{(2)}(0) \) which are plotted in fig.7a as dashed lines.

These results can be compared to stochastic simulations: for \( T \to 0 \), Bogoliubov theory is most accurate for weak interactions, when the quantum depletion of the condensate is small. At finite temperatures (but much lower that the condensation temperature), thermal excitations are present on top of the condensate: since the free-energy (63) only keeps track of the lowest order terms in the excitation density, the agreement of the approximated Bogoliubov predictions with stochastic simulations is best at low temperatures when the density of non-condensed atoms is small.

In the non-interacting case, the stochastic simulations can be compared also with the theory of Sec.IV.B2, as expected, that approach is more accurate that the Bogoliubov calculations of the present section (fig.7a); in the Bogoliubov approach, in fact, the \( g = 0 \) result is obtained as the limit for \( g \to 0 \) of a theory which is linearized in the excitation density and thus able to reproduce only the terms in (53) which are linear in the \( n_k \)'s; the quadratic terms are instead not included at all.

V. CONCLUSIONS

In this paper, we have developed a new method for the exact calculation of the thermodynamical quantities of an interacting \( N \)-boson system in the canonical ensemble. This
method is the imaginary-time version of the one discussed in our previous paper [17] for the real time evolution of the system.

In order to have an efficient sampling of the observables, an importance sampling method has been used with an \textit{a priori} distribution based on the non-interacting gas. We have applied the simulation scheme to a homogeneous one-dimensional interacting Bose gas and, whenever available, we have successfully compared the predictions of stochastic simulations with the ones of existing theories, such as the grand-canonical ensemble, the classical field approach [24] and Bogoliubov theory [12–15].

In particular, we have discussed the effect of Bose condensation in finite-size systems on the different observables, such as the momentum distribution, the density fluctuations and the occupation statistics of the ground mode.

In the case of a non-condensed system, the main effect of interactions is to suppress density fluctuations without affecting in a dramatic way the phase coherence properties of the sample. In the classical field regime $k_B T \gg \mu$, the effect of the noise term is negligible so that the system is already accurately described by the deterministic force term alone. For the opposite case of a condensed sample at very low temperatures $k_B T \leq \mu$, interesting features have been predicted such as an spatial antibunching of the atoms.

In the future, we plan to combine the imaginary-time evolution discussed in the present paper with the real-time evolution discussed in [17] in order to dispose of a tool for the numerical calculation of dynamical properties of finite temperature Bose gases. Improvements of the statistical properties of the stochastic simulations will hopefully be investigated both in terms of better \textit{a priori} distribution functions and in terms of the extension of the ansatz to include more sophisticated states such as Bogoliubov vacua. Finally, we plan to generalize the stochastic approaches in order to consider also multi-mode nonlinear optical systems in which driving and damping play an essential role [21].

The first part of the work on the real-time evolution has been done in collaboration with Jean Dalibard, to whom we are indebted for many stimulating discussions. Laboratoire Kastler Brossel is a Unité de Recherche de l’École Normale Supérieure et de l’Université Paris 6, associée au CNRS.
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FIG. 1. Homogeneous non-interacting gas in a large $L \gg \ell_c$ box with periodic boundary conditions. Mean occupation number of the different plane wave modes of the box in the non-degenerate ($T = 8 T_{\text{deg}}$) regime (a) and in the degenerate ($T = 0.02 T_{\text{deg}}$) regime (b); the disks are the result of stochastic calculation with $N_r = 2048$ realizations, the solid line is the prediction of grand-canonical ensemble in the thermodynamical limit. $N = 6$ atoms (a) in a box of length $L = 6\ell$; $N = 96$ atoms (b) in a box of length $L = 96\ell$ ($\ell$ is an arbitrary length unit).

FIG. 2. Homogeneous non-interacting gas in a large $L \gg \ell_c$ box. First (a) and second (b) order correlation functions below degeneracy for $T = 0.02 T_{\text{deg}}$ (dot-dashed) and $T = 0.08 T_{\text{deg}}$ (solid). $N = 96$ atoms in a box of length $L = 96\ell$ ($\ell$ is an arbitrary length unit). Stochastic simulation with $N_r = 400$ realizations. The deviation of $g^{(2)}(0)$ from the grand-canonical prediction $g^{(2)}(0) = 2$ is a finite size effect (see Sec. IV B 2.)
FIG. 3. Degenerate non-interacting gas in a finite box: mean occupation number of the different momentum modes for growing number of particles across the Bose-Einstein condensation threshold $N/N_{BEC} = 0.25$ (circles), $N/N_{BEC} = 0.5$ (squares), $N/N_{BEC} = 1$ (diamonds), 2 (triangles), 3 (crosses) and 4 (stars). Stochastic calculation with $N_r = 2048$ realizations. $L = 48l$, $\beta = 16 \frac{m^2}{\hbar^2}$ ($l$ is an arbitrary length unit).

FIG. 4. Degenerate non-interacting gas in a finite box: second-order correlation function across the Bose-Einstein condensation threshold at $T \simeq T_{BEC}$. Solid line: analytical prediction (53). Disks: stochastic calculation with $N_r = 256$ realizations. $N = 192$ atoms in a $L = 48l$ box ($l$ is an arbitrary length unit).
FIG. 5. Non-interacting Bose gas: probability distribution of the ground mode occupation number for different temperatures across the Bose-Einstein transition: $T/T_{BEC} = 30$ (solid), 3 (dotted), 1 (dot-dashed), 0.5 (dashed). Stochastic calculation with $N_r = 1024$ realizations. $N = 32$ atoms in a $L = 24l$ box ($l$ is an arbitrary length unit).

FIG. 6. Left panel: first $g^{(1)}(x)$ and second-order $g^{(2)}(x)$ correlation functions for different values of the interaction strength $g/(\hbar^2/ml) = 0$ (solid), 0.005 (dotted), 0.01 (long-dashed) and 0.02 (dot-dashed) ($\chi = \hbar^2 g \beta^2 n^3/m = 0,1,2,4$), all within the classical field regime ($gn/k_B T \leq 0.1 \ll 1$). Right panel: comparison of the approximate classical field predictions in the thermodynamical limit with stochastic simulations for finite boxes of growing size $L/\ell_c = 9$ (circles), 18 (squares). Stochastic simulation with $N_r = 2048$ realizations, $\beta = 0.8 ml^2/\hbar^2$. $N = 324$, $L = 48l$ (circles); $N = 648$, $L = 96l$ (squares) ($l$ is an arbitrary length unit).
FIG. 7. Left panel: second order correlation $g^{(2)}(0)$ as a function of temperature for different values of the interaction strength; from below $\frac{m\ell}{\hbar^2}g = 0.1, 0.05, 0$. Disks: stochastic calculation with $N_r = 2048$ realizations. Dashed line: Bogoliubov prediction. Dotted line: analytical prediction for the non-interacting gas (nearly superimposed to the disks). Dot-dashed line: stochastic calculation neglecting the noise term for $\frac{m\ell}{\hbar^2}g = 0.05$; notice the low temperature limit equal to $1 - 1/N$. Right panel: second order correlation function $g^{(2)}(x)$ for $\frac{m\ell}{\hbar^2}g = 0.1$ (solid) at $T_{BEC}/T = 21$ obtained by means of a stochastic calculation with $N_r = 2048$ realizations. $N = 42$ atoms in a $L = 6\ell$ box ($\ell$ is an arbitrary length unit).