Norm preserving stochastic field equation for an ideal Bose gas in a trap: numerical implementation and applications

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Received 16 September 2010
Published 1 December 2010
Online at stacks.iop.org/JPhysB/43/245302

Abstract

Stochastic field equations represent a powerful tool to describe the thermal state of a trapped Bose gas. Often, such approaches are confronted with the old problem of an ultraviolet catastrophe, which demands a cutoff at high energies. In Heller and Strunz (2009 J. Phys. B: At. Mol. Opt. Phys. 42 081001) we introduce a quantum stochastic field equation, avoiding the cutoff problem through a fully quantum approach based on the Glauber–Sudarshan P-function. For a close link to actual experimental setups, the theory is formulated for a fixed particle number and thus based on the canonical ensemble. In this work the derivation and the non-trivial numerical implementation of the equation is explained in detail. We present applications for finite Bose gases trapped in a variety of potentials and show results for ground state occupation numbers and their equilibrium fluctuations. Moreover, we investigate spatial coherence properties by studying correlation functions of various orders.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The enormous progress in experimental and theoretical studies of ultracold quantum gases leads to a much deeper understanding of quantum many-body physics [2–4]. In particular, Bose–Einstein condensation in traps enables us to investigate profoundly quantum statistical phenomena in finite systems. In more recent experiments, spatial and temporal coherences [5–9] of ultracold Bose gases are investigated in terms of correlation functions. Moreover, dynamics from non-equilibrium to equilibrium states [10] and the spatial dependence of equilibrium density fluctuations [11] are considered. For a theoretical description of these phenomena, it is desirable to consider nonzero temperature, finite size and—as no particle bath is present—a canonical description of the many-body quantum system. For most experiments, interaction between the atoms are of crucial importance. In systems with a Feshbach resonance, the interaction strength may even be tuned over a wide range—allowing the study of ideal gases, too. In this paper we deal almost exclusively with an ideal gas and comment on the interacting case briefly at the end.

It is clear that many properties of ultracold gases are sensitive to temperature not least due to the different size of the condensed fraction of the gas. Moreover, for these finite systems with a fixed number of particles, it is preferable to base a theoretical description on the canonical ensemble rather than the usual grand canonical ensemble. For an ideal gas, the best known example for the significance of choosing the canonical ensemble is the fluctuation of the ground state occupation number $\langle N_0^2 \rangle - \langle N_0 \rangle^2$ [12]. Clearly, it approaches zero as temperature tends to zero in a canonical ensemble. Yet it is of the size of the average particle number $N$ in a grand canonical description. A detailed study of the fluctuations of the ground state particle number in the microcanonical and the canonical ensembles is given in [13–18]. Spatial correlations are among other quantities of relevance for which a grand canonical formulation differs significantly from a canonical description [19].

Recently, we presented a norm preserving stochastic field equation that describes the canonical state of an ideal Bose gas [1]. The resulting equation fully reflects quantum statistics and was given in [1] in a representation independent form. Therefore, it can be propagated in position space, meaning that it is not necessary to know eigenfunctions and -energies of the trapped atoms. While in [1] we simply state the equation and display a few applications, here we want to elaborate...
on its derivation, its numerical implementation and further applications in much more detail.

As we will show, spatial correlations and fluctuations can easily be calculated in position space. Due to the quantum framework, the equation—despite representing a c-number field—does not suffer from any cutoff problems which usually occur for classical field equations. Thus, numerical simulations can be performed with sufficient precision and reasonable effort.

Let us relate our approach to previous stochastic equations for the grand canonical ensemble. Note that most of these investigations are concerned with an interacting gas, while here, as a first step, we restrict ourselves to the case of the ideal gas. Since our theory can be formulated in position space, we clearly expect to be able to include interactions in a mean field sense in the next step.

Detailed discussions of different approaches to (interacting) ultracold gases in terms of stochastic field equations are given in [20, 21]. Exact methods based on the positive P-representation of the full density operator are used by Drummond and co-workers [22]. This theory brings about numerical challenges and is applied mainly to one-dimensional systems. More recently, also a 3D free gas at temperatures well below the transition temperature has been discussed [23]. Other approaches [20, 24–27] can be seen as classical field methods, in which the lowly occupied energy levels must be treated in a different formalism or, due to ultraviolet problems. Davis and co-workers apply a projection on a subspace of highly occupied energy levels, using a cutoff [24], while Gardiner and co-workers separate the field operator in a highly and lowly occupied part [20, 25]. We see our approach more in the spirit of Stoof and co-worker, who start from a path integral approach and arrive at a functional Fokker–Planck equation for the Wigner functional of the thermal field [26]. After additional simplifications, in their work the corresponding Langevin equation takes the form of a classical stochastic field equation as given by Hohenberg and Halperin [28].

Apart from these grand canonical approaches, theories for a fixed particle number have also been presented more recently [29–32]. Xu and co-workers describe Bose gases with first order perturbation theory and in a Bogoliubov approximation [29]. An exact phase-space description for a finite number of particles is worked out by Korsch and co-workers. Exact evolution equations for the Husimi-Q- and the Glauber–Sudarshan-P-distribution function based on a Bose–Hubbard Hamiltonian are derived [30, 31]. Stochastic methods in phase space for the canonical ensemble of qubit and spin models have been presented by Drummond and co-workers [32]. While all these theories based on a canonical ensemble focus on different systems, e.g. lattices or spin models, we here aim to describe the full canonical thermal state of a Bose gas in any given trap.

Our novel equation presented in [1] has been found on the basis of the Glauber–Sudarshan P-representation—being exact for an ideal gas. In this paper we aim to explain in more detail the derivation of the equation, its properties, its numerical implementation, and we show its power by discussing further applications. The paper is structured as follows: in the second section we show the theoretical background and the derivation of the stochastic field equation. The third section is devoted to the discussion of some crucial properties of the equation. In the fourth section we demonstrate how we propagate the equation in energy and in position space numerically. Results of these numerical applications are shown in the fifth section, before we draw conclusions in the final section.

2. Stochastic field equation for the canonical ensemble

In order to derive a quantum stochastic field equation for the canonical ensemble of an ideal Bose gas, our first aim is to express quantum expectation values for a fixed particle number in terms of c-number integrals. The desired stochastic field equation should enable us to calculate these expectation values. We use the corresponding Fokker–Planck equation to demonstrate the equivalence of stochastic and canonical quantum ensemble mean.

We begin with the canonical density operator for N particles:

\[
\hat{\rho}_N = \frac{1}{Z_N} e^{-\hat{H}_N} \rho_N. \tag{1}
\]

As usual, the Hamiltonian \(\hat{H} = \sum_k \epsilon_k \hat{a}_k^\dagger \hat{a}_k\) can be expressed in terms of occupation numbers of single-particle states (\(\epsilon_k\) denotes the energy of single-particle state \(k\)). Furthermore, the canonical partition function is denoted by \(Z_N\), with the usual \(\beta = \frac{1}{kT}\) incorporating Boltzmann’s constant \(k\) and temperature \(T\). Crucially, a projector \(\hat{P}_N = \sum_{|n_k\rangle} \langle |n_k\rangle |n_k\rangle\) on the N-particle subspace appears, with the usual number states \(|n_k\rangle = \frac{1}{\sqrt{n_k!}} \prod_k (\hat{a}_k^\dagger)^{n_k} |0\rangle\). The operator \(\hat{P}_N\) projects the exponential \(e^{-\hat{H}}\) on a subspace of \(N\) particles. In order to arrive at a c-number representation of quantum expectation values, one can express \(e^{-\hat{H}}\) from (1) as a mixture of coherent states using the (Glauber–Sudarshan) P-function representation [33]:

\[
e^{-\hat{H}} = \frac{1}{Z} \int d\mu[z] \exp \left( -\sum_k |z_k\rangle \langle z_k| e^{\hat{a}_k^\dagger \hat{a}_k} - 1 \right) \langle \{ z \}, \{ \rangle \{ \} \rangle =: \int d\mu[z] P(\{ z \}, \{ z \}) \langle \{ \rangle \{ \} \rangle. \tag{2}
\]

Here, we abbreviate the normalization factor with \(\tilde{n} = \prod_k (e^{\hat{a}_k^\dagger \hat{a}_k} - 1)^{-1}\), and products of coherent states with \(| \{ z \} \rangle = |z_0\rangle |z_1\rangle \cdots |z_N\rangle \cdots\). The appropriate measure is \(d\mu[z] = \frac{1}{\pi^N} \prod_k \frac{dz_k}{2}\).

Of particular interest are correlation functions of quantum field operators. Using the P-representation (2), we can determine canonical quantum expectation values with the help of \(| \langle \{ z \} | \hat{P}_N | \{ z \} \rangle \rangle = \frac{1}{N!} (\sum_k |z_k|^2)^N e^{-\sum_k |z_k|^2} \langle \{ z \}, \{ \rangle \{ \} \rangle \langle \{ \rangle \{ \} \rangle \rangle \) (see [34]) and obtain a weight function \(W_N(\{ z \}) = \frac{1}{N!} \langle \{ z \}, \{ \rangle \{ \} \rangle \langle \{ \rangle \{ \} \rangle \rangle \) of \(| \langle \{ z \} | \hat{P}_N | \{ z \} \rangle \rangle \). With the latter, quantum expectation values can be written as integrals over c-numbers, 

\[
\langle \hat{a}_i^\dagger \hat{a}_j \rangle_N = \text{tr}(\hat{a}_i^\dagger \hat{a}_j \hat{P}_N) = \frac{1}{C} \int d\mu[z] z_i^* z_j W_{N-1}(\{ z \}). \tag{3}
\]

with \(C = \int d\mu[z] W_N(\{ z \})\).
In this work we focus on spatial correlation functions. Therefore, we are interested in ensemble averages for the bosonic field operator \( \hat{\psi}(x) \sum_{\xi} \xi \hat{a}^\dagger \) with \( \xi \) the single-particle eigenstate corresponding to energy \( E_\xi \).

First, the weight function is rewritten as \( W_N(\{\psi\}) = \frac{1}{N!} \left( \int d\chi |\psi(\chi)|^2 \right)^N e^{-\int d\chi |\psi(\chi)|^2} P(\psi^*, \psi) \) using \( \psi(x) = \sum_{\xi} \xi \hat{a}^\dagger \psi(x) \) which is the eigenvalue of the field operator when applied to the coherent state \( |\{z\}\rangle \), i.e. \( \psi(x)|\{z\}\rangle = \psi(x)|\{z\}\rangle \). Further, we obtain

\[
\langle \hat{\psi}^\dagger(x)\hat{\psi}(x') \rangle_N = \frac{1}{C} \int d\mu[\psi] \psi^\dagger(x)\psi(x') W_{N-1}(\{\psi\}),
\]

(4)

with the normalization constant \( C = \int d\mu[\psi] W_N(\{\psi\}) \). It should be mentioned here that for quantum expectation values of second (or higher) order one has to use weight functions of different \( N \). For \( \langle \hat{\psi}^\dagger(x)\hat{\psi}(x') \hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x') \rangle \), for instance, the first order \( W_{N-1}(\{\psi\}) \) has to be replaced by \( W_{N-2}(\{\psi\}) \) —for higher orders the result changes accordingly (4th order: chose \( W_{N-3}(\{\psi\}) \)).

In order to calculate these expectation values we were able to construct a new, norm-preserving stochastic field equation [1]. The equivalence of quantum statistical and stochastic ensemble is based on the fact that the weight functions \( W_n (n = N, N - 1, \ldots) \) turn out to be stationary solutions of the corresponding Fokker–Planck equation.

In representation independent form \( \langle \psi(x, t) = \langle x |\psi(t)\rangle \rangle \) and using Stratonovich calculus [35] it reads (\( \hbar = 1 \) throughout)

\[
(S) \frac{d}{dt} |\psi\rangle = -(A + i)H - \Lambda \frac{\langle \hat{\psi}^\dagger H \hat{\psi} \rangle}{\langle \hat{\psi}^\dagger \hat{\psi} \rangle} |\psi\rangle dt + \sqrt{2\Lambda} \left( \sqrt{\langle \hat{\psi}^\dagger \hat{\psi} \rangle} \langle \hat{\psi} \rangle \frac{d\hat{\xi}}{dt} - \frac{\langle \hat{\psi} \rangle \sqrt{\langle \hat{\psi}^\dagger \hat{\psi} \rangle} \langle \hat{\psi}^\dagger \hat{\psi} \rangle \langle \hat{\psi} \rangle}{\langle \hat{\psi}^\dagger \hat{\psi} \rangle} K |\psi\rangle \right).
\]

(5)

Here, the single-particle Hamiltonian \( H = \frac{p^2}{2m} + V(x) = \sum_{\xi} \xi \hat{a}^\dagger \xi \hat{a} \hat{a}^\dagger \) appears, and a damping parameter \( \Lambda \). Crucially, temperature enters through an operator

\[
K = \frac{H}{e^{\beta H} - 1}.
\]

(6)

The noise increment \( d\xi \) is uncorrelated in space and time \( \langle x |d\xi(t)\rangle\langle d\xi(t')|x'\rangle = \delta(x - x')\delta(t - t') \). Equation (5) is a norm preserving, nonlinear stochastic equation that enables us to obtain canonical expectation values on average.

It is important to stress that the dependence of the stochastic fields \( |\psi(t)\rangle \) on the particle number \( N \) is indirectly given through their norm \( N = \langle \hat{\psi}^\dagger \hat{\psi} \rangle \) which is preserved during propagation and thus determined by the initial condition. One might expect \( N \approx N \) to be a reasonable choice; however, matters are more delicate and a distribution of norms \( N \) is required in order to obtain exact quantum expectation values. We devote the whole next section 3 to the relation between norm \( N \) and particle number \( N \).

Sometimes it is useful to express (5) as an Ito-stochastic equation, reading

\[
(1) \frac{d}{dt} |\psi\rangle = -(A + i)H - \Lambda \frac{\langle \hat{\psi}^\dagger H \hat{\psi} \rangle}{\langle \hat{\psi}^\dagger \hat{\psi} \rangle} |\psi\rangle dt + \sqrt{2\Lambda} \left( \sqrt{\langle \hat{\psi}^\dagger \hat{\psi} \rangle} \langle \hat{\psi} \rangle \frac{d\hat{\xi}}{dt} - \frac{\langle \hat{\psi} \rangle \sqrt{\langle \hat{\psi}^\dagger \hat{\psi} \rangle} \langle \hat{\psi}^\dagger \hat{\psi} \rangle \langle \hat{\psi} \rangle}{\langle \hat{\psi}^\dagger \hat{\psi} \rangle} K |\psi\rangle \right).
\]

(7)

The novel stochastic field equation can easily be solved numerically and used in different representations. An implementation in the position representation is particularly useful as it can be applied to arbitrary external potentials \( V(x) \). Based on the assumption of sufficient ergodicity, in applications the ensemble averages are replaced by a long time limit \( \langle \hat{\psi}^\dagger(x)\hat{\psi}(x') \rangle_N = \lim_{t \to \infty} \int f \int d\mu \langle \psi^\dagger(x, s)\psi(x', s) \rangle \) over a single realization \( \psi(x, s) \) of the stochastic field equation.

The term \( (A + i) \) consists of a phenomenological damping \( \Lambda \), while \( 'i' \) describes ‘real’ dynamics. So, in a phenomenological manner, our equation can also be used to mimic the transition from a non-equilibrium to an equilibrium state.

It is important to point out the crucial role of the operator \( K \). Its meaning becomes most apparent when we omit the nonlinear terms in our equation (5) and think of \( H \) to represent \( H - \mu \) which also affects the operator \( K \). One obtains an equation which gives us the thermal state of the grand canonical ensemble [36]

\[
\frac{d}{dt} |\psi\rangle = -(A + i)H |\psi\rangle dt + \sqrt{2\Lambda K} |d\xi\rangle,
\]

(8)

with \( \mu \) the chemical potential used to fix the average particle number \( N \). It should be mentioned here that the canonical equation (5) is not merely a normalized version of the grand canonical equation. The linear equation (8) is closely related to the classical field equation for the thermal state of the grand canonical ensemble for any Hamiltonian energy functional \( \mathcal{H}(\psi, \psi^\dagger) \) [28]:

\[
\frac{d}{dt} \langle x |\psi(t)\rangle = -(A + i) \frac{\delta H}{\delta \psi^\dagger} |x\rangle dt + \sqrt{2\Lambda kT} |d\xi\rangle,
\]

(9)

which has well-known ultraviolet problems. If one sets \( \frac{\delta H}{\delta \psi} = H \psi \), there is only one difference between classical (9) and quantum equation (8): the classical temperature \( kT \) is substituted by the operator \( K \). As discussed in [24], for instance, the classical equation satisfies the equipartition theorem and therefore the infinite degrees of freedom of a field \( \psi(x, t) \) lead to an ultraviolet catastrophe. This can also be seen in equation (9) looking at a formulation in position space: the white noise term which is uncorrelated in position induces arbitrarily high momentum kicks. However, if we consider the operator \( K = \frac{\hbar}{\sqrt{2\mu} \gamma(x)} \) acting on the white noise \( |d\xi\rangle \) in position space representation, the former white noise becomes spatially correlated, and we no longer get unphysical momentum. In other words, proper quantum statistics requires the replacement of spatially uncorrelated noise \( \sqrt{kT} |d\xi\rangle \) in (9) by spatially correlated effective noise \( |d\xi'\rangle = \sqrt{kT} |d\xi\rangle \), as in (8). The correlation function of the effective noise \( \langle x |d\xi(t)\rangle|d\xi(t')|x'\rangle = \langle x |K|x'\rangle dt \) is now a smooth function.
Figure 1. Correlation function $\langle x|K|x'\rangle$ of the noise $|dx\rangle = \sqrt{K}|dx\rangle$ of our stochastic field equation (5) for a harmonic potential. We show the correlation function for temperature $kT = 1.2\hbar\omega$ (left) and for a higher temperature $kT = 4.5\hbar\omega$ (right).

in position space and shown in figure 1 for two different temperatures.

In the low energy limit $H \ll kT$, indeed, the operator tends to the classical temperature $K \approx kT$. Yet in the case of high energies $H \gg kT$, the operator tends to zero $K \to 0$. We see that in the quantum equations (5, 8) the required cutoff for preventing ultraviolet problems is built in.

3. Stochastic average and quantum expectation value

In this section we want to investigate the relationship between quantum expectation values of arbitrary order $\langle a_i \cdots a_j a_i \cdots a_j \rangle$ (3) and those obtained with the stochastic field equation (SFE) $\langle \langle z_i^* z_j \cdots z_k \rangle \rangle_{\text{SFE}}$. For the following, we introduce the norm $N \equiv \sum_k |z_k|^2 = \langle \psi |\psi \rangle$ of the wavefunction. The stochastic equation keeps the norm fixed, while the integral of the quantum expectation values (3) extends over a range of values of the quantity $\sum_k |z_k|^2$. The norm stays constant and for any stochastic method $\langle \langle 1 \rangle \rangle_{\text{SFE}} = 1$. Hence, we can write the first order expectation values we obtain from the stochastic equation as

$$\langle \langle z_i^* z_j \rangle \rangle_{\text{SFE}}(N, \epsilon_0) = \frac{\int \mu(\{z\}) \delta(N - \sum_k |z_k|^2) W_{N-1}(\{z\})}{\int \mu(\{z\}) \delta(N - \sum_k |z_k|^2) W_{N-1}(\{z\})}.$$

We find that this expression depends on the ground state energy $\epsilon_0$. It can be seen easily by a substitution $z \to z e^{\beta \epsilon_0}/2$ that the simple identity $\langle \langle z_i^* z_j \rangle \rangle_{\text{SFE}}(N e^{-\beta \epsilon_0}, \epsilon_0) = \langle \langle z_i^* z_j \rangle \rangle_{\text{SFE}}(N, 0)$ holds. The relation between the average values given by the stochastic field equation and quantum expectation values is now obvious

$$\langle \hat{a}_i^\dagger \hat{a}_j \rangle_N = \frac{\int dN \hat{P}(N) \langle \langle z_i^* z_j \rangle \rangle_{\text{SFE}}(N, \epsilon_0)}{\int dN \hat{P}(N) \delta(N - \sum_k |z_k|^2) W_{N-1}(\{z\})},$$

with $\hat{a}_i = \prod_{\ell} e^{\beta \epsilon_i} - e^{\beta \epsilon_i})^{-1}$. Well below the critical temperature it is sufficient to consider only the first term of the sum $\sum_k c_k e^{-\beta \epsilon_k N}$ because the remaining terms are smaller by a factor $e^{-\beta \epsilon_k} - e^{-\beta \epsilon_k} N$. Numerical investigations of the factors $c_k$ showed that this approximation is justified in the temperature region considered here. Then our distribution $\hat{P}(N)$ is normalized to

$$\int_0^\infty dN \hat{P}(N) = \sum_k c_k e^{-\beta \epsilon_k N} \approx e^{\beta \epsilon_0}.$$

Within this approximation we have a Poisson-like distribution

$$\hat{P}(N) \sim N^{N-1} \exp(-e^{\beta \epsilon_0} N),$$

This distribution is centred around

$$\langle N \rangle = \frac{\int_0^\infty dN \hat{P}(N) N}{\int_0^\infty dN \hat{P}(N)} = N e^{-\beta \epsilon_0},$$

and the standard deviation equals $\Delta N = \sqrt{N e^{-\beta \epsilon_0}}$. For large $N$, the ratio of variance and mean goes to zero $\Delta N \to 0$. Hence, in general it is sufficient to propagate equation (5) with a single norm i.e. we replace $\hat{P}(N) \sim N^{N-1} \exp(-e^{\beta \epsilon_0} N)$.

As a consequence, from (11) we obtain the simple relation $\langle \langle \hat{a}_i^\dagger \hat{a}_j \rangle \rangle_N = e^{\beta \epsilon_0} \langle \langle z_i^* z_j \rangle \rangle_{\text{SFE}}(N e^{-\beta \epsilon_0}, \epsilon_0)$ between the canonical quantum correlation function and the ensemble average of the stochastic field equation. As further elaborated upon in section 5, it is for very high precision only, that it is necessary to take into account the full norm distribution. Let us also remark that for higher order expectation values these considerations apply similarly.

It should be noted here that if the norm of our numerical simulation of the stochastic field equation $N$ should correspond to the particle number $N$, we have to choose $\epsilon_0 = 0$. However, it is also possible to choose a norm different from the particle number according to (16). This freedom is useful for an easier numerical implementation, as shown in section 4. It should also be mentioned that for temperatures above and near the critical temperature, the approximations leading to expression (14) are no longer valid and the exact norm distribution needs to be known. Still, using (14), for many quantities we observe satisfying results even in this temperature region.

4. Numerical implementation

In this section it is shown how one can solve the novel stochastic field equation numerically. The implementations can be performed in different representations, whichever is convenient for a given trap potential. If the single-particle eigenenergies are known (recall that we neglect interatomic interactions here) a propagation in energy space is the easiest way to solve our equation. In a box potential this is analogous to a propagation in momentum space. For a trap potential $V(x)$ with an unknown energy spectrum, one can solve the equation in position space directly, using a split operator method based on fast Fourier transformation. This implementation is more challenging but the program can easily be adjusted to any trap just by changing the single line of code where the potential is defined.
If the eigenvalues for the given trap potential are known, a numerical implementation in energy space does not contain any challenging aspects. As already explained above, it is more convenient to pass to position space, if we want to solve problems with arbitrary external potential, for which the eigenenergies are not known. We turn to a discretized case that allows only easy solutions using standard fast Fourier transformation methods [37].

The challenging aspect is the evaluation of matrix elements of the operator (6) appearing in (7), i.e., the determination of

\[ \langle x_i | K | x_j \rangle = \left\{ x_i \left| \frac{p_i^2}{2m} + V(x) \right| e^{\frac{\beta p_i^2}{2m}} + V(x) - 1 \right\} x_j \]

For an efficient implementation, a Wigner–Weyl approximation is helpful. The Wigner–Weyl correspondence [33] of the operator \( K \) in 2D phase space is defined as

\[ K(x, p) = \int d^D s e^{ip\cdot s} \left( x + \frac{s}{2} \right) K \left( x - \frac{s}{2} \right), \]

(17)

with the help of which we can obtain the matrix elements as

\[ \langle x_i | K | x_j \rangle = \frac{1}{(2\pi)^D} \int d^D p e^{ip\cdot (x_i - x_j)} K \left( \frac{x_i + x_j}{2} \right). \]

(18)

In order to simplify, we consider only zeroth order in \( \hbar \), and find the classical expression

\[ K(x, p) \approx \frac{\left( V(x) + \frac{p^2}{2m} \right)}{e^{\beta V(x)} + \frac{p^2}{2m} - 1}. \]

(19)

This approximation will be justified by comparing the approximated numerical result with exact numerical calculations.

Expanding the denominator in a geometric series we get

\[ \langle x_i | K | x_j \rangle \approx \frac{1}{(2\pi)^D} \int d^D p e^{ip\cdot (x_i - x_j)} \left( V \left( \frac{x_i + x_j}{2} \right) + \frac{p^2}{2} \right) \times \sum_{n=1}^{\infty} e^{-\beta p V \left( \frac{x_i + x_j}{2} \right)} e^{-\frac{p^2}{2}} \]

(20)

The momentum integration can now be carried out without any difficulty which leads to the following expression:

\[ \langle x_i | K | x_j \rangle \approx \frac{1}{(2\pi)^D} \sum_{n=1}^{\infty} e^{-\beta p V \left( \frac{x_i + x_j}{2} \right)} \times \left( V \left( \frac{x_i + x_j}{2} \right) + \frac{D}{2\beta n} - \frac{(x_i - x_j)^2}{2(\beta n)^2} \right) e^{-\frac{p^2}{2\beta n}}. \]

(21)

It is important to note that the convergence of the geometric series in (20) very much depends on the minimum of the potential energy. Indeed, rapid convergence can be assured by adding some (physically irrelevant) constant to \( V(x) \). However, as this shift also affects the ground state energy \( \epsilon_0 \), it also has a significant influence on the norm distribution of the wavefunction as can be witnessed in (16). Therefore, in practice one tries to identify some optimal shift that assures both, rapid convergence and a reasonable norm of the wavefunction.

An efficient generation of \( \langle x_i | K | x_j \rangle \) is given in equation (21). Now, in order to propagate equation (7), it is necessary to think about the numerical implementation of the correlated noise \( d\zeta \) = \( \sqrt{K} d\xi \), too. Obviously, the (discretized) noise \( d\zeta = \langle x_i | d\xi \rangle \) must be generated in a way that

\[ d\zeta_i d\zeta_j^* = \langle x_i | K | x_j \rangle \]d\tau \]

holds. In order to find an efficient way to obtain the noise, we start with equation (20). Based on the substitution \( p \to \sqrt{n\beta} p \) we get

\[ \langle x_i | K | x_j \rangle \approx \frac{1}{(2\pi)^D} \sum_{n=1}^{\infty} e^{-\beta p V \left( \frac{x_i + x_j}{2} \right)} \times \left( V \left( \frac{x_i + x_j}{2} \right) + \frac{D}{2\beta n} - \frac{(x_i - x_j)^2}{2(\beta n)^2} \right) e^{-\frac{p^2}{2\beta n}} + \frac{1}{n\beta} \int d^D p \frac{p^2}{2} e^{\frac{p^2}{2\beta n}} e^{-\frac{p^2}{2\beta n}}. \]

(22)

For simplicity, the following derivation of an efficient noise generating method will be restricted to the one-dimensional case \( D = 1 \). For higher dimensions, the strategy follows the very same lines.

The first integral \( \int d^D p e^{\frac{p^2}{2\beta n}} e^{-\frac{p^2}{2\beta n}} \) can be obtained from a Monte Carlo integration of \( \langle x_i | e^{\sqrt{n\beta} \xi_1} \rangle \) over a normally distributed real random variable \( \eta_1 \). For the second momentum integral in (22), note that the integral \( \int d^D p \frac{p^2}{2} e^{\frac{p^2}{2\beta n}} e^{-\frac{p^2}{2\beta n}} \)
Ground state, the Wigner function reflects the ground state Wigner function $T < T_c(N)$. Gaussian random numbers we display a single realization with our stochastic field equation (5), and on the right-hand side a long-time average over 25 000 time steps. Wigner function of a Bose gas of 100 particles trapped in a harmonic potential (left) and in the quartic potential Figure 3.

\[ V(x, y, z) = x^2 + y^2 + z^2 \] (right) above (top), at (middle), and below (bottom) the critical temperature. On the left-hand side of both pictures we display a single realization with our stochastic field equation (5), and on the right the exact correlation function $\langle V(x_i)V(x_j) \rangle$.

\[ V(x, y, z) = x^2 + y^2 + z^2 \]

\[ \langle x_i \mid \sqrt{K} \mid x_j \rangle \approx \sum_{n=1}^{\infty} e^{-\beta n/2} V^{(\frac{\mu}{2})} \left( V \left( x_i + x_j \right) \right) \]

\[ \times e^{\eta_1(\eta_1-x)} + \frac{1}{2n\beta} \cos \left( \sqrt{\eta_1^2 + \eta_3^2 + \eta_4^2 x_2} \right) \]

\[ \times \cos \left( \sqrt{\eta_2^2 + \eta_3^2 + \eta_4^2 x_3} \right) \]

\[ + \frac{1}{2n\beta} \sin \left( \sqrt{\eta_2^2 + \eta_3^2 + \eta_4^2 x_3} \right) \]

\[ \times \sin \left( \sqrt{\eta_2^2 + \eta_3^2 + \eta_4^2 x_3} \right) \right)_{\eta} \]

(24)

The good agreement of the correlation function of the noise in the Wigner–Weyl approximation from (25) and the exact correlation function can be seen in figure 2, where we show on the left an average over numerical realizations from (25) and on the right the exact correlation function $\langle x_i \mid \sqrt{K} \mid x_j \rangle$ for an isotropic harmonic oscillator at $kT = 3\hbar\omega$.

To summarize this section, we are able to obtain the non-trivial noise and matrix elements of $K$ with reasonable effort. The other terms of the equation can be propagated using fast Fourier transformation. Thus, we are able to propagate the whole stochastic field equation in $D$ spatial dimensions. Results of such numerical simulations are presented in the following section.

5. Results of numerical simulations

Our equation is applied here to a 3D Bose gas of fixed particle number trapped in various 3D potentials and different quantities are calculated. The results are obtained in energy or position representation. The applicability of our equation is
first shown by determining the Wigner function $W(x,p) = \frac{1}{2\pi} \int dy \, e^{i px} \langle \hat{\psi}(x + \frac{1}{2} y) \hat{\psi}(x - \frac{1}{2} y) \rangle$ of a Bose gas. The propagation itself is performed in 3D position space, while the right columns show the Wigner function integrated over the remaining four phase-space coordinates. As already explained in section 4 we use a Wigner–Weyl approximation for the spatial correlation functions are quantities which are often measured in experiments. In [1] we investigated second order correlation functions and their remarkable differences between a canonical and a grand canonical description. We also showed the good agreement of our values with corrected grand canonical results from [19]. Here we want to go beyond these well-known results and show correlation functions for the potential $V(x,y,z) = x^4 + y^4 + z^4$. In figure 5 we present calculations of first $G_2(x,0) = \langle \hat{\psi}(x) \hat{\psi}(0) \rangle$ and second order $G_2(x,0) = \langle \hat{\psi}(x) \hat{\psi}(0) \hat{\psi}(0) \hat{\psi}(x) \rangle$ correlation functions as they depend on the $x$-coordinate for a Bose gas of 200 particles for temperatures below $T_c$ (plus signs, crosses).

The differences of the grand canonical and the canonical ensemble become very obvious when considering the fluctuations of the ground state occupation as a function of temperature. As already mentioned in the introduction, in a grand canonical description the variance for temperature near zero would be of the order of the particle number $N$. In figure 6 we display the ground state number fluctuations for a Bose gas of 200 particles in an isotropic harmonic potential in the canonical ensemble that clearly tend to zero as temperature lowers. We compare our calculations with the analytical canonical result of [18] which is based on the known eigenenergies for the harmonic potential.

So far, for the determination of the graphs in figures 3–5, it was sufficient to simulate with a single norm as elaborated upon in section 3. Now, we find that the number fluctuations are very sensitive with respect to slight errors of first $\langle N_0 \rangle$ or second order $\langle N_0^2 \rangle$ expectation values. Therefore, for this application, in order to reach the precision shown in figure 6, it is necessary to simulate with a distribution of norms. We use the simplified Poisson-type distribution from (15), which explains why near the critical temperature deviations from the exact result occur.
Figure 5. First and second order spatial correlations $G_1(x, 0)$ (top) and $G_2(x, 0)$ (bottom) obtained with our stochastic field equation for a Bose gas trapped in the potential $V(x, y, z) = x^4 + y^4 + z^4$ for different temperatures ($0.5T_c$: crosses, $0.8T_c$: stars).

Figure 6. Simulation (plus signs) of the variance of the ground state occupation for a 3D ideal Bose gas in an isotropic harmonic potential compared to results from [18] (full line).

One can summarize our simulations by pointing out that with our stochastic field equation (5) in combination with the Wigner–Weyl approximation for the noise generation, one obtains good numerical results for many different temperature-dependent quantities in arbitrary potentials, also embracing the fixed particle number in these systems.

6. Conclusion and outlook

In this paper we have discussed a novel stochastic field equation for a Bose gas with a finite and fixed particle number: our theory is based on the canonical ensemble referring to the conditions found in actual experiments with atomic gases in traps. The equation is exact for ideal gases. A generalization including atomic interactions appears possible on the basis of the inclusion of a mean-field interaction term in the potential.

Our approach to a numerical solution of the equation is explained in great detail. We focus on the implementation in position space, in which it is not necessary to know the single-particle eigenenergies of the system. By changing the specification of the external potential in the numerical code, we can easily determine equilibrium properties of the gas for
many trap geometries. We can calculate correlation functions of arbitrary order and in principle obtain information about the full thermal canonical state. We show that it is possible to achieve results with satisfying precision for many different quantities of the ideal gas like first and second order correlation functions, ground state occupations and the variance of the ground state occupation.

Acknowledgments

We are grateful for inspiring discussions with Markus Oberthaler and Thimo Grotz. Sigmund Heller acknowledges support from the International Max Planck Research School for Dynamical Processes in Atoms, Molecules and Solids, Dresden. Computing resources have been provided by the Zentrum für Informationsdienste und Hochleistungsrechnen (ZIH), TU Dresden.

Appendix. Calculation of the norm distribution \( \hat{P}(\mathcal{N}) \)

In this appendix we derive expression (13) for the distribution of the norm:

\[
P(\mathcal{N}) = \frac{\int d\mu[z]\delta(\mathcal{N} - \sum_i |z_i|^2)W_{N-1}(\{z_i\})}{\int d\mu[z]W_N(\{z\})},
\]

(A.1)

with

\[
W_{N-1}[z] = \frac{1}{(N-1)!} \left( \sum_i |z_i|^2 \right)^{N-1} e^{-\sum_i \beta \epsilon_i |z_i|^2},
\]

(A.2)

which we use in section 3. Suppose the number of considered eigenstates equals \( M \), which is arbitrary. We perform the transformation of variables: \( |z_i|^2 \rightarrow x_i \) and find

\[
\hat{P}(\mathcal{N}) = \frac{2}{C} \int_0^\infty d^{(M-1)x} x \int_0^\infty dx_0 \delta \left( x_0 - (N - \sum_i x_i) \right)
\]

\[
\times \frac{1}{(N-1)!} \left( \sum_i x_i \right)^{(N-1)} e^{-\sum_i \beta \epsilon_i x_i}
\]

\[
= \frac{2}{C(N-1)!} \mathcal{N}^{(N-1)} e^{-\epsilon \mathcal{N}}
\]

\[
\times \int_0^{x_0} \cdots \int_0^{x_0} \int_0^{x_0} \cdots \int_0^{x_0} dx_{M-1} e^{-\sum_{i=1}^{M-1} (\beta \epsilon_i - \epsilon \mathcal{N}) x_i},
\]

(A.3)

with \( C = \int d\mu[z]W_N(\{z\}) \). First, we calculate the integral

\[
F_M = \int_0^\infty \cdots \int_0^\infty dx_{M-1} e^{-\sum_{i=1}^{M-1} \beta \epsilon_i x_i - \epsilon \mathcal{N}}
\]

(A.4)

Now we substitute \( \bar{x}_1 = x_1, \bar{x}_2 = x_2 + x_1, \bar{x}_3 = x_3 + \bar{x}_2, \) etc and rewrite the integral as

\[
F_M = \int_0^\infty \cdots \int_0^\infty d\bar{x}_1 e^{-\sum_{i=1}^{M-1} \beta \epsilon_i x_i - \epsilon \mathcal{N}}
\]

\[
\times \int_0^\infty d\mathcal{N} e^{-(\epsilon \mathcal{N} - \epsilon \mathcal{N}) \bar{x}_M},
\]

(A.5)

By considering a derivative with respect to \( \mathcal{N} \) of equation (A.5) we succeeded to find a solution with the ansatz

\[
F_M(\mathcal{N}) = \frac{1}{M!} \sum_{k=0}^{M} \frac{1}{\epsilon \mathcal{N} - \epsilon \mathcal{N}_k} e^{-(\epsilon \mathcal{N} - \epsilon \mathcal{N}_k) \mathcal{N}}
\]

(A.6)

with \( g_k = \prod_{l=k}^{M-1} \frac{1}{\epsilon \mathcal{N}_l - \epsilon \mathcal{N}_k} \) and \( g_k = \frac{1}{\epsilon \mathcal{N}_l - \epsilon \mathcal{N}_k} \). In this way we can obtain all coefficients \( g_k \) iteratively. With a bit of analysis we find

\[
F_M = \sum_{k=0}^{M} \frac{1}{\epsilon \mathcal{N}_l - \epsilon \mathcal{N}_k} e^{-(\epsilon \mathcal{N} - \epsilon \mathcal{N}_k) \mathcal{N}}.
\]

(A.7)

Finally, we plug expression (A.7) into equation (A.3) and use \( C = \int d\mu[z]W_N(\{z\}) = \int d\mathcal{N} \int d\mu[z] \delta(\mathcal{N} - \sum_k |z_k|^2)W_N(\{z\}) \) to write the norm distribution in the form

\[
\hat{P}(\mathcal{N}) = \frac{1}{(N-1)!} \sum_k c_k e^{-\epsilon \mathcal{N}_k \mathcal{N}}.
\]

(A.8)

with \( c_k = \frac{1}{\sum_{l=0}^{\infty} \frac{1}{\epsilon \mathcal{N}_l - \epsilon \mathcal{N}_{k-1}}}, \) as it is written in equation (13) of section 3.

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