Canonical ensemble of an interacting Bose gas: Stochastic matter fields and their coherence

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Abstract – We present a novel quantum stochastic evolution equation for a matter field describing the canonical state of a weakly interacting ultracold Bose gas. In the ideal gas limit our approach is exact. This numerically very stable equation suppresses high-energy fluctuations exponentially, which enables us to describe condensed and thermal atoms within the same formalism. We present applications to ground-state occupation and fluctuations, density profile of ground-state and thermal cloud, and ground-state number statistics. Our main aim are spatial coherence properties which we investigate through the determination of interference contrast and spatial density correlations. Parameters are taken from actual experiments.

Equilibrium fluctuations in ultracold gases reveal detailed information about states and phases of interacting many-body quantum systems [1]. Recent experiments permit to control ultracold quantum gases in a hitherto unknown precision and to investigate temperature-dependent quantities like the thermal density and ground-state occupancy [2], spatial correlation functions [3–6] density fluctuations [7] or interference contrast [8].

In this work we determine the canonical state of an interacting ultracold Bose gas. A novel quantum stochastic evolution equation for a c-number field $\psi(x)$ is presented such that canonical quantum statistical expectation values can be replaced by an ensemble mean over these stochastic matter fields. The equation allows to determine coherence properties and other relevant observables; it is based on a mean-field-type approximation and strictly valid for the non-interacting case, for which the relevance of the canonical ensemble has been emphasized by studying coherence properties [9,10].

Most theoretical descriptions of interacting ultracold Bose gases at finite temperature are based on grand canonical statistics [1,11]. For actual experiments involving a fixed and finite number of particles, however, a canonical description is natural. In studying the role of the chosen ensemble, attention so far has been paid to ground-state number fluctuations [12,13]. While for the ideal gas canonical and grand canonical ensemble give vastly different predictions [14], this ceases to be true for interacting gases in the thermodynamical limit [15]. Our work is based on canonical statistics right from the start and allows us to not only investigate occupation fluctuations but also spatial coherence properties.

Many stochastic field methods exist for the description of Bose gases at finite temperature. All of these are based on grand canonical statistics, and nicely overviewed and compared in [11,16]. In the truncated Wigner approach, the evolution of the field Wigner functional is determined approximately from a sampling over random initial fields whose dynamics is given by the Gross-Pitaevskii equation [17,18]. Based on a quantum kinetic theory and a separation of condensed and non-condensed part, Gardiner and co-workers derive a stochastic Gross-Pitaevskii equation [19]. With a similar result, a functional integral approach to the evolution of the field Wigner distribution is worked out in an approach by Stoof and co-workers [20]. Care has to be taken with respect to the white noise driving these equations. Exact methods based on the positive $P$-representation are used by Drummond and co-workers [21]. It is possible to use this approach for 3D systems; still, the long-time numerical solution has to be exercised with caution. We see the strength of our approach in its unified applicability to a vast number of different phenomena: from ground-state fluctuations to properties of the thermal cloud, to coherence properties and contrast in Bose gas interferometry. For the latter we obtain nice agreement.
with experiments of the Schmiedmayer group that may be well described by the Luttinger liquid theory [8] or by a stochastic phase model [22].

Two properties of our novel equation should be emphasized: first, unlike in our previous attempt [23], the equation is not norm preserving. Still, the norm fluctuations are small compared to those of related stochastic equations used for grand canonical simulations. Secondly, as in [23], ultraviolet cutoff problems do not appear due to the use of the Glauber-Sudarshan $P$-function. Our treatment leads to spatially correlated and thus spatially smooth noise. This avoids high absolute values of spatial derivatives. Unphysically large momenta do not arise. These properties allow us to also be able to treat full 3D gases within our approach [24].

We propose to use the stochastic (Ito) equation

$$d\psi = -\frac{1}{\hbar} \left( (\Lambda + i)H - \frac{\Lambda}{\langle \psi \rangle} \int H e^{-H/kT} \right) |\psi\rangle dt$$

$$+ \sqrt{\frac{2\Lambda}{\hbar}} \int H e^{-H/kT} |d\xi\rangle$$

(1)

for a $c$-number matter field $\psi(\vec{x}, t) = \langle \vec{x} | \psi(t) \rangle$ to determine all equilibrium properties of a weakly interacting Bose gas of $N$ particles at arbitrary temperature $T$ ($k$ is Boltzmann's constant). Throughout, we will refer to (1) as the stochastic matter field equation (SMFE) for finite temperature. Crucially, the operator $H$ is the effective (mean-field) one-particle energy operator

$$H = \frac{\vec{p}^2}{2m} + V(\vec{x}) + g(N-1) \frac{|\psi(\vec{x}, t)|^2}{\langle \psi(t) | \psi(t) \rangle},$$

(2)

such that eq. (1) may also be seen as a stochastic Gross-Pitaevskii equation. As usual, $V(\vec{x})$ denotes the trap potential, the interaction parameter $g$ is proportional to the s-wave scattering length $a_s$ and $m$ is the mass of a Boson. The parameter $\Lambda$ appearing in (1) is a phenomenological damping rate that sets the time scale for transition to equilibrium. Its appearance as square root with the fluctuations reflects a fluctuation-dissipation relation. The fluctuating part is driven by complex Ito increments $|d\xi\rangle$ with $|d\xi\rangle \langle d\xi | = 1 dt$, $|d\xi\rangle \langle d\xi | = 0$. Note, however, that the operator $\sqrt{H} e^{-H/kT}$ acts on the noise, effectively leading to spatially correlated noise [23].

Before we show the versatility and accuracy of the SMFE in applications, let us sketch how we arrive at (1). Our aim is to determine mean values $\langle \ldots \rangle_N = \text{tr} | \ldots \rangle \rho_N$ with the canonical density operator

$$\hat{\rho}_N = \frac{1}{Z_N} e^{-\hat{H}/kT} \hat{\Pi}_N$$

(3)

in second quantization with Hamiltonian $\hat{H}$, canonical partition function $Z_N$, and projector $\hat{\Pi}_N = \sum_{\{n_k\}} |\{n_k\}\rangle \langle \{n_k\}|$ onto the $N$-particle subspace. For the latter we use the relation given in [25]

$$\langle \{z\} | \hat{\Pi}_N | \{z\} \rangle = \left( \sum_k |z_k|^2 \right)^N \exp\left( - \sum_k |z_k|^2 / N! \right)$$

with products of coherent states $\{z\} = |z_0| |z_1| \cdots |z_k| \cdots$. Normally ordered matter field correlation functions are expressed in terms of functional phase space integrals [23], for instance

$$\langle \psi(\vec{x}) \psi(\vec{x'}) \rangle_N = \frac{1}{C_N} \int \mathcal{D}[\psi] \psi^\dagger(\vec{x}) \psi(\vec{x'}) W_{N-1}(\psi),$$

(4)

with the weight functions

$$W_N(\psi) = \frac{1}{N!} \langle \psi | \psi \rangle^N e^{-\langle \psi | H | \psi \rangle} P(\psi),$$

where $P(\psi)$ denotes the Glauber-Sudarshan $P$-function [26] of state $\exp(-\hat{H}/kT)$ and $C_N = \int \mathcal{D}[\psi] W_N(\psi)$. Note that second- (or higher-) order correlations require the use of $W_{N-2}$ (or lower index) in expression (4), while $C_N$ remains.

For the ideal gas case ($g = 0$), we prove that the SMFE (1) corresponds to a Fokker-Planck equation [27] whose stationary solution is just the weight functional $W_N(\psi)$. Thus, equilibrium expectation values of the canonical ensemble are obtained from propagating eq. (1) and averaging. In practice, we use a long-time-average over a single trajectory $\psi(x, t)$.

The SMFE (1) is exact for an ideal gas; interactions can be included with great success: we propose to use the single equation (1) with (2), containing the current stochastic mean-field energy, to describe all properties of weakly interacting Bose gases in a unified way. Indeed, we emphasize that (1) interpolates smoothly between the high-temperature limit $T \gg T_c$, where interactions are negligible and thus our description is exact anyway. At the opposite end, when $T \ll T_c$, the SMFE (1) with (2) is just mean-field Gross-Pitaevskii theory and is again expected to give good results. Clearly, the fluctuations we describe are of thermal origin; quantum fluctuations are taken into account to some extent through the use of the $P$-representation. Note also that it is of crucial importance to use the current, stochastic $\psi(x, t)$ in (2), such that on average $\langle \hat{H}(\psi) \rangle_{N-1} = \bar{p}^2/2m + V(\vec{x}) + \bar{g}(\vec{x}) \langle \psi(x) \psi(x) \rangle_{N-1}$. The quality of choice (2) was tested by solving eq. (1) for a two-mode system and comparing with numerically exact quantum results over a wide temperature range.

We convince ourselves of the validity of (1) by first considering an ideal Bose gas of 200 particles in a 3D harmonic trap. In fig. 1 results for ground-state occupation, its variance and further centered moments are compared with exact results for the canonical ensemble obtained from a recursion relation [28].

As a first application to the interacting case in fig. 2, the density profile (green solid line) of a quasi-1D Bose gas of 20240 atoms in a trap with a coupling constant $g_{1D} = 0.01 \hbar \omega_l$ at a temperature of $kT = 430 \hbar \omega_l$ is shown (we use the oscillator length $l = \sqrt{\hbar/m \omega_l}$). The blue dashed line is the contribution with off-diagonal long-range order (ODLRO) whose wave function
ψ_0(z) is obtained from a diagonalization of the full ρ(z, z') = ⟨ψ(ψ(z)ψ(z'))⟩_N applying the Penrose-Onsager criterion [29]. Moreover, a histogram of the stochastic occupation n_0 = ⟨ψ_0|ρ|ψ_0⟩ leads to the ground-state number statistics P(n_0) (inset in fig. 2). The average number of particles in state ψ_0 turns out to be 12573. Our findings are nicely compatible with the “stochastic Gross-Pitaevskii” results of [16], without, however overestimating lowly occupied regions. In fact, as can be seen in fig. 3, our results for the lowly occupied thermal wings of the density of the gas are in very good agreement with the local Bose-Einstein (rather than Boltzmann) distribution ρ_{BE}(z) = 1/(2πℏω_{l})^{3/2}g_{1/2}(μ-V(z)/kT) with g_{1/2}(x) = ∑_{n=1}^{∞}n^{3}e^{-nx} and the chemical potential μ (see [16]).

The SMFE (1) is ideally suited to study the coherence properties of interacting matter waves through the determination of spatial correlation functions. As an application we show results of our SMFE applied to recent experiments in the Schmiedmayer group [8]: two independent condensates are prepared in quasi-1D; after expansion they interfere; the observed interference pattern is integrated over a length L which determines the contrast |A(L)|^2, where A(L) = ∫_{-L/2}^{L/2} dz ψ_1(z)ψ_2(z).

Both, mean value ⟨|A(L)|^2⟩ (fig. 4) and the full distribution W(α) of the normalized moments defined through ∫_{0}^{∞} W(α)α^m dα = ⟨α^m⟩ = ⟨|A|^m⟩/|A|^2 are determined (fig. 5). In [8] it is shown that experimental results are well described by Luttinger-liquid theory (LLT) to which we will compare our SMFE results.

In fig. 4 we show the average contrast ⟨|A(L)|^2⟩ as a function of length L for different temperatures and find very good agreement with LLT (and thus with experiment). Deviations for large L arise from density variations along the gas. LLT results are based on a uniform density. The gas contains some 4400 ^87Rb atoms with a central density of n_{1D} ≈ 50 μm^{-1}. The interaction strength for this 1D case is g_{1D} = 2ℏω_⊥a_s, with ω_⊥ = 2π × 3.9 kHz. In fig. 5 we show the distribution function of the interference contrast W(α) as a histogram with α(L) = |A(L)|^2/⟨|A(L)|^2⟩ obtained from our simulations. We use a central density n_{1D} = 50 μm^{-1} in line with the experimental setup (see [8]). LLT predicts a change of...
The length-dependent normalized interference contrast for different lengths $L$ and different temperatures of 33 nK, 47 nK and 68 nK ($n_{1D} \approx 50 \mu m^{-1}$, $\omega_{\perp} = 2\pi \times 3.0 \text{kHz}$). The data from the SMFE (black plus signs, green crosses, brown stars) is compared to Luttinger-liquid theory (LLT) (red solid line, blue dashed line, yellow dashed-dotted line) which agrees well with the experimental measurements [8]. Small deviations arise from the variation of the density in the harmonic trap, while the Luttinger-liquid theory applies to a uniform density.

Our results are in good agreement with the Luttinger liquid theory which has proven to describe the experiments adequately.

Let us summarize our achievement: We present a novel quantum stochastic matter field equation (SMFE) for a gas of $N$ particles trapped in an arbitrary potential at any temperature $T$ (canonical ensemble). The equation is strictly valid for a non-interacting gas; we include interactions in a stochastic mean-field sense and obtain promising results over the entire relevant temperature regime. The SMFE is capable of tackling problems in 1D to 3D with arbitrary trapping potentials. Results for ground-state occupation distribution and density profiles are shown. Of particular interest is the determination of spatial correlation functions of arbitrary order. We apply our approach to calculate interference contrast distributions and density ripples as recently measured. Our results are in good agreement with the Luttinger liquid theory which has proven to describe the experiments adequately.

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