Transition of a mesoscopic bosonic gas into a Bose-Einstein condensate

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The condensate number distribution during the transition of a dilute, weakly interacting gas of \( N = 200 \) bosonic atoms into a Bose-Einstein condensate is modeled within number conserving master equation theory of Bose-Einstein condensation. Initial strong quantum fluctuations occurring during the exponential cycle of condensate growth reduce in a subsequent saturation stage, before the Bose gas finally relaxes towards the Gibbs-Boltzmann equilibrium.

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I. INTRODUCTION

Bose-Einstein condensates have turned into exquisite tools to study fundamental quantum phenomena on the micrometer scale, and a vast range of different physical scenarios have been realized experimentally with ultracold matter in the last decade, confirming the fundamental importance and the broad applicational scope of Bose-Einstein condensation \[1\]. A microscopic, quantum dynamical description of the gas’ \( N \)-body state during the buildup of the condensed phase after a sudden switch of the gas temperature below the critical temperature expected for Bose-Einstein condensation, however, is still one of the most striking theoretical topics of ultracold matter physics up to date.

How can we model the quantum many-body dynamics during the transition of a dilute, weakly interacting gas of bosonic atoms into a Bose-Einstein condensate and link the resulting equilibrium statistics of the condensed phase to the roots of Bose statistics, i.e. to the statistics of quasi-ideal Bose gases, which was introduced almost one century ago by Bose and Einstein \[2\]? And under which conditions is the equilibrium statistics of a dilute and weakly interacting Bose-Einstein condensate of fixed particle number uniquely determined by the statistics of an ideal Gibbs-Boltzmann thermal gas – lacking any hysteresis on the condensate formation process \[3\]?

Since an exact numerical solution to the full \( N \)-body problem is out of the range of today’s supercomputing facilities already for rather small atomic samples with a few hundreds of atoms, these questions reduce to finding appropriate and numerically accessible effective equations for the quantum many-body dynamics of the Bose-Einstein phase transition. So far, extensive pioneering works \[4-6\] (and references cited therein) have led to accurate dynamic equations describing the evolution of the average condensate population for atomic gases with a few thousands to a few millions of atoms: the onset of Bose-Einstein condensation is marked by a spontaneously inserting exponential growth of the average ground state population, followed by a slow, subsequent saturation stage in which the condensate fraction converges towards an equilibrium value after suddenly cooling \[7\] the gas below its critical temperature.

In this Article, the relaxation dynamics of the entire state of a mesoscopic Bose gas during the transition of exactly \( N = 200 \) weakly interacting bosonic atoms into a Bose-Einstein condensate is reported for the first time within number-conserving master equation theory of Bose-Einstein condensation \[13, 15\]. In particular, focus is put on following the dynamics of the condensate number distribution during the Bose-Einstein condensation process. Detailed theoretical knowledge on the statistics and dynamics of mesoscopic (\( N \sim 200 – 1000 \) atoms), weakly interacting quantum gases is not only of importance for state-of-the-art experiments \[8\], but moreover contrasts fundamental postulates of classical, statistical mechanics to interacting, quantum degenerate many particle systems of finite size. The latter aspect arises from the neglect of number and energy fluctuations in standard thermodynamics, which is a reasonable assumption for classical, non-interacting gases in the thermodynamic limit (with particle numbers as large as Avogadro’s number, \( N \sim 10^{23} \)), whereas a vanishing impact of such quantum effects is in the quantum degenerate limit is a priori no longer irrefragable.

II. MASTER EQUATION THEORY

In order to model Bose-Einstein condensation for small atomic gases, it is sufficient to numerically monitor the condensate and non-condensate number distribution during condensation, as will be shown in the following. For this purpose, we derive a master equation for said number distributions assuming a 3-dimensional harmonic trapping potential, with \( p_N(\vec{N}_0, t) = p_N(N - \vec{N}_0, t) \) the condensate number distribution and \( \vec{N}_0 \) the number of condensed atoms, given a gas of \( N \) particles therein. The particle number \( N \) may be on the order of a few hundreds to a few millions of atoms, but is kept fixed during the final cycle of the condensation process. The derivation of the master equation is lengthy and relies on several approximations \[13, 15\], which can be summarized in the following way. We consider condensation onto one
simultaneously capturing the distribution of non-condensate particles, as the particle number in the gas is conserved. Each state \( \hat{\rho}_\perp(N - N_\perp, T) \) in eq. (1) denotes a thermal state projected onto the subspace of \( (N - N_\perp) \) non-condensate particles, given that \( N_\perp \) particles populate the condensate mode:

\[
\hat{\rho}_\perp(N - N_\perp, T) = \frac{\hat{Q}_{N-N_\perp} e^{-\beta \hat{H}_\perp} \hat{Q}_{N-N_\perp}}{Z_\perp(N - N_\perp, T)} ,
\]

with \( Z_\perp(N - N_\perp, T) = \sum_{\{N_k\}} \exp[-\sum_{k \neq 0} \beta \epsilon_k N_k] \), the partition function of \( (N - N_\perp) \) indistinguishable particles, in which the sum of the tuples \( \{N_{k_1}, N_{k_2}, \ldots\} \) is taken such that the total atom number is conserved, \( \sum_k N_k = (N - N_\perp) \). The operator \( \hat{H}_\perp = \sum_{k \neq 0} \epsilon_k \hat{a}_k^\dagger \hat{a}_k \) denotes the Hamiltonian of the non-condensate thermal vapor, \( \beta = (k_B T)^{-1} \) the inverse temperature of the gas, and \( \hat{Q}_{N-N_\perp} \) is a projector onto the Fock space of non-condensate number states with \( (N - N_\perp) \) particles.

The fact that the \( N \)-body state in eq. (2) is not a product state of a condensate and non-condensate density matrix doesn’t cause fundamental problems to derive a master equation for the reduced condensate density matrix. More explicit, as shown in Refs. [13, 15], the state in eq. (2) allows for the derivation of the master equation for a three-dimensional harmonic trapping potential without further approximations. Since the \( N \)-body state is diagonal in Fock number representation, we focus on the evolution of the diagonal elements characterized by \( p_N(N_\perp, t) = \langle N_\perp | \hat{\rho}(t) | N_\perp \rangle = \langle N_\perp | \hat{\rho}^{(N)}(t) | N_\perp \rangle \) in eq. (1). The corresponding master equation for the condensate number distribution in a gas of exactly \( N \) atoms describes Bose-Einstein condensation as due to quantum jumps \( N_\perp \rightarrow N_\perp + 1 \) of the condensate particle number:

\[
\frac{\partial p_N(N_\perp, t)}{\partial t} = - \left[ \xi_N^+ (N_\perp, T) + \xi_N^- (N_\perp, T) \right] p_N(N_\perp, t) + \xi_N^+ (N_\perp - 1, t) p_N(N_\perp - 1, t) + \xi_N^- (N_\perp + 1, t) p_N(N_\perp + 1, t) ,
\]

with a condensate feeding rate \( \xi_N^+ (N_\perp, T) = 2(N_\perp + 1) \lambda_\perp^+ (N - N_\perp, T) \), and a condensate loss rate \( \xi_N^- (N_\perp, T) = 2N_\perp \lambda_\perp^- (N - N_\perp, T) \). The single-particle transition rates \( \lambda_\perp^\pm (N - N_\perp, T) \) are given in Eq. (4).

Remarkably, even though eq. (3) describes Bose-Einstein condensation realistically in terms of two-body atomic collisions [3, 6, 13], it formally obeys the master equation for an ideal gas coupled to a thermal reservoir [14]. In contrast to the non-interacting case, however, the master eq. (3) accounts for the real-time dynamics of Bose-Einstein condensation in a dilute, weakly interacting gas. The master equation (3) is valid up to order \( aD^{1/3} \ll 1 \). Thus, even though we neglect terms
The quantum mechanical energy balances from atomic interactions.

The non-condensate single-particle modes originating which quantifies losses of condensate particles towards the quantum optical case \[12\]. Thus, the body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogies, and where \(\Delta\) is the off-resonance of a given two-body process and \(\Gamma\) the energy uncertainty, in analogy to the quantum optical case \[12\]. Thus, the \(\delta\)-distribution in eq. (4) reflects and ensures energy conservation on a certain width \(\Gamma\) arising from the finite decay time of non-condensate correlations \[13\] \[15\]. The \(\langle N^p_k\rangle(N^p_{\perp}, T)\) denote single-particle occupations, which are calculated with respect to each non-condensate thermal mixture of \(N^p_{\perp} = (N - N_0)\) particles in eq. (3), obeying \(\sum_k \langle N^p_k\rangle(N^p_{\perp}, T) = (N - N_0)\). The evaluation of \(\Gamma\) is beyond the scope of the present article, and will be presented elsewhere \[13\].

**III. DYNAMICS OF BOSE-EINSTEIN CONDENSATION**

The dynamics of the condensate number distribution during Bose-Einstein condensation is displayed in figs. 2 and 3 as a function of time \(t\) and condensate particle number \(N_0\) after a sudden switch of the atomic cloud’s temperature \(T\) below the ideal gas critical temperature \(T_c\) expected for Bose-Einstein condensation \[1\]. For numerical propagation of eq. (3), we consider a small Bose gas of \(N = 200\) weakly interacting \(^{87}\)Rb atoms (with s-wave scattering length \(a = 5.4\) nm \[9, 10\]), prepared in a time-independent, three-dimensional harmonic trapping potential with trapping frequencies \(\omega = 2\pi \times 2 \times 42.0\) Hz, \(\omega_y = 2\pi \times 42.0\) Hz, \(\omega_z = 2\pi \times 120.0\) Hz. Despite the well-known S-shape behavior \[3\] of the aver-
age condensate occupation number, the condensate number distribution in particular gives rise of non-condensate number fluctuations during the condensation process \[\text{[8]},\] since the total number of particles in the gas is fixed. Characteristic for a phase transition, we observe an initial spread of the condensate number distribution (large number fluctuations in the thermal vapor). While the condensate grows, these incipiently large fluctuations reduce until the reaching of a steady state. This steady state is in particular characterized in that the net particle flow between condensate and non-condensate is zero.

Achieving Bose-Einstein condensation hence relies on the atomic interactions in order to bring the gas into equilibrium in the quantum degenerate regime, number fluctuations are prominent during condensate formation as highlighted by figs. \[\text{[2]}\] and \[\text{[3]}\] and energy uncertainty (accounted for by the width \(\Gamma\) of the delta function in eq. \[\text{(4)}\]) is present due to the finite decorrelation time being condensate feeding and loss rates). According to eqs. \[\text{(1)}\] and \[\text{(5)}\], the steady \(N\)-body state reached by the atomic collisions remarkably thus obeys the statistics of a thermal Boltzmann state of \(N\) bosonic, non-interacting particles \[\text{[1]}\]:

\[
\hat{\sigma}^{(N)}(t \rightarrow \infty) = \hat{Q}_N \frac{e^{-\beta \hat{H}}}{Z(N,T)} \hat{Q}_N + \mathcal{O}(a_0^{1/3}) ,
\]  

with \(\hat{H} = \sum_k \epsilon_k \hat{a}_k^\dagger \hat{a}_k\), the Hamiltonian of a non-interacting gas, \(Z(N,T)\) the partition function of \(N\) indistinguishable particles, and \(\hat{Q}_N\), the projector onto the Fock subspace of \(N\) particles.

V. CONCLUSION

In conclusion, we have monitored the condensate and non-condensate number distribution during the phase transition of a mesoscopic Bose gas into a Bose-Einstein condensate. We find that the steady state of the gas in the condensed phase is a Gibbs-Boltzmann thermal state, obeying the Bose-Einstein statistics of an ideal gas for sufficiently dilute and weakly interacting atomic gases. The reported scenarios were numerically reproducible for total particle numbers up to \(N = 10^5\) \[\text{[15]}\]. The impact of environmental decoherence sources onto the condensate formation process during condensate formation such as detailed study of deviations of the final steady state from the Gibbs-Boltzmann equilibrium will be of future interest and discussed elsewhere.

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