Number-conserving master equation theory for a dilute Bose-Einstein condensate

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We describe the transition of $N$ weakly interacting atoms into a Bose-Einstein condensate within a number-conserving quantum master equation theory. Based on the separation of time scales for condensate formation and non-condensate thermalization, we derive a master equation for the condensate subsystem in the presence of the non-condensate environment under the inclusion of all two-body interaction processes. We numerically monitor the condensate particle number distribution during condensate formation, and derive a condition under which the unique equilibrium steady state of a dilute, weakly interacting Bose-Einstein condensate is given by a Gibbs-Boltzmann thermal state of $N$ non-interacting atoms.

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I. INTRODUCTION

After almost one century of theoretical works to understand the existence, analysis and creation of a new state of matter at ultracold temperatures, the first experimental observation of a Bose-Einstein condensate was presented in Refs. [1, 2]. Nowadays, Bose-Einstein condensates are well established as a distinguished form of quantum matter enabling in situ studies of most disparate physical phenomena, such as Josephson oscillations [3], or Anderson localization [4, 5], on a micrometer scale.

In the limit of zero temperature and weak interactions, where all atoms of the gas can be assumed to share the same single particle quantum state, the dynamics of the condensate is described accurately by the nonlinear Gross-Pitaevskii equation [6]. Finite temperature effects at thermal equilibrium are accounted for within higher order perturbation theories [7, 8]. In contrast, only few theoretical works have been developed to model the non-equilibrium process of condensate formation itself. Pioneering works, such as of Refs. [9–12], pointed primarily on the different dynamical stages of condensate formation in terms of kinetic growth equations, and numerous efforts have led to highly accurate predictions for the time scale of condensate formation.

Less is known about the condensate particle number distribution’s dynamics in a dilute, weakly interacting Bose gas consisting of a fixed number of $N$ particles. Another question under current study [13] is whether the equilibrium steady state of a dilute Bose-Einstein condensate – which is finally reached only due to interatomic collisions, even in the case of very weak interactions – is unique, and characterized by thermodynamics and statistics of an ideal gas? And, how do quantum effects, such as number and energy fluctuations of the condensate and the non-condensate, which should become important especially for mesoscopic Bose-Einstein condensates, evolve during Bose-Einstein condensation and eventually drive the Bose gas into the final Gibbs-Boltzmann equilibrium state?

Here, we present a quantum master equation theory for a dilute Bose-Einstein condensate consisting of a fixed number of $N$ particles.

In contrast to previously derived effective equations for the condensate dynamics under the influence of the non-condensate environment, based for example on quantum kinetic theory [11] or on an analogy with the laser master equation [14], our condensate master equation fully takes into account conservation of the total number of particles, i.e. of condensate plus non-condensate particles. In particular, the depletion of the non-condensate during the process of condensate formation results in condensate feeding and loss rates which are different from the case where the Bose gas is coupled to an external particle reservoir with a fixed chemical potential.

Apart from particle number conservation, our approach relies on the separation of time scales between the condensate and non-condensate dynamics. The time scale $\tau_0$ for condensate growth [15–21] is typically of the order of $1–4$ s, and thus much slower than the timescale $\tau_{\text{col}} \sim 10–50$ ms of two-body collisions within the non-condensate [12, 17, 18]. We assume that these collisions lead to an effective thermalization of the non-condensate within each subspace of fixed non-condensate particle number, and to a rapid decay of non-condensate correlation functions with a rate $\Gamma \approx \tau_{\text{col}}^{-1}$. Under these conditions, particle exchange between condensate and non-condensate leads to a Markovian master equation for the condensate’s particle number distribution. Finally, we will show that its equilibrium steady state is given by a Gibbs-Boltzmann thermal state of non-interacting particles under the condition that the Bose gas is sufficiently dilute, and that the decay of non-condensate correlations does not occur too fast, i.e. $\hbar \beta \Gamma \ll 1$, where $\beta = 1/k_B T$ ($k_B$ being the Boltzmann constant and $T$ the temperature of the gas).

The paper is organized as follows: The derivation of the quantum master equation is given in section [11] First,
we define the condensate and non-condensate Hamiltonians, and decompose all two body interaction terms in a physically motivated way. Using the assumptions mentioned above, we then derive the quantum master equation of Lindblad type for the reduced condensate density matrix. For dilute atomic gases in three-dimensional harmonic trapping potentials, the Lindblad master equation reduces to a simple rate equation for the condensate number distribution, describing transitions $N_0 \rightarrow N_0 \pm 1$ of the condensate particle number $N_0$.

In Sec. III the rate equation is used to study the dynamics of condensate formation, and its equilibrium steady state. We numerically monitor the condensate dynamics of condensate formation, and its equilibrium composition of the gas into a condensate “system” and a non-condensate “environment” part, see Sec. II A. In Sec. II B we then examine the two particle interactions between these subsystems as described by the Hamiltonian, Eq. (5). They fall into three different classes which we denote as single particle, pair and scattering events. Under the inclusion of all these two body interaction processes, the quantum master equation of Bose-Einstein condensation in a Bose gas with conserved particle number $N$ is finally derived in Secs. II C and II D.

II. QUANTUM MASTER EQUATION THEORY

The separation of time scales between non-condensate thermalization and condensate growth motivates a decomposition of the gas into a condensate “system” and a non-condensate “environment” part, see Sec. II A. In Sec. II B we then examine the two particle interactions between these subsystems as described by the Hamiltonian, Eq. (5). They fall into three different classes which we denote as single particle, pair and scattering events. Under the inclusion of all these two body interaction processes, the quantum master equation of Bose-Einstein condensation in a Bose gas with conserved particle number $N$ is finally derived in Secs. II C and II D.

A. Condensate and non-condensate subsystem

After defining the condensate mode, we examine the decomposition of the full two body Hamiltonian in Eq. (4) into a condensate and a non-condensate part, and the interactions between them.

1. Separation of the second-quantized field

Quantitatively, we determine the condensate wave function $\Psi_0(\vec{r})$ (assuming all $N$ particles occupying the same condensate mode) by the Gross-Pitaevskii equation

$$-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + gN|\Psi_0(\vec{r})|^2 - \mu_0 \right) \Psi_0(\vec{r}) = 0 \;,$$

which, as discussed in Ref. [22, 23], gives a good approximation to the exact condensate mode at sufficiently low final temperatures, and sufficiently dilute atomic gases.

In our following treatment, we will use $\Psi_0(\vec{r})$ as defined by Eq. (11) to describe the condensate wave function also in a situation where initially not all particles occupy the condensate, and hence the condensate particle number will change as a function of time. Neglecting the associated time dependences of $\Psi_0(\vec{r})$ is justified because it changes over the characteristic time scale for condensation, much longer than the time scale $\tau_{\text{col}}$. We can thus employ an adiabatic approximation and compute the rates in the master equation for a fixed $\Psi_0$ and at the end of the calculation only take into account their dependence on $\Psi_0$, hence on time. In the limit of very weak interactions, where the condensate state is approximated, at all times, by the ground state of the external trapping potential, $|\chi_0\rangle$, or, if the initial state of the gas is already close to its equilibrium value, the situation is even simpler as the $\Psi_0$ dependence can be entirely forgotten.

The total bosonic field $\hat{\Psi}$, expressed in an orthonormal basis $\{|\Psi_k\rangle, k \in N_0\}$, where $|\Psi_0\rangle$ is the Gross-Pitaevskii ket, separates into

$$\hat{\Psi} = |\Psi_0\rangle \hat{a}_0 + \sum_{k \neq 0} |\Psi_k\rangle \hat{a}_k \equiv \hat{\Psi}_0 + \hat{\Psi}_{\perp} \;,$$

with creation and annihilation operators $\hat{a}_k$ and $\hat{a}_k^\dagger$, respectively, satisfying usual bosonic commutation relations $[\hat{a}_k, \hat{a}_l^\dagger] = \delta_{kl}$, and $[\hat{a}_k, \hat{a}_l] = [\hat{a}_k^\dagger, \hat{a}_l^\dagger] = 0$.

2. Fock-Hilbert space

The corresponding Fock states, forming a complete basis of the many particle Hilbert space $\mathcal{F}$ on which these operators act on are denoted by $|N_0, \{N_k\}\rangle$. The interpretation of a many particle Fock state is hence to find $N_0$ particles in the condensate mode $|\Psi_0\rangle$, and $\{N_k\} = \{N_1, N_2, \ldots\}$ particles in the modes $\{|\Psi_1\rangle, |\Psi_2\rangle, \ldots\}$. The basis $\{|\Psi_k\rangle, k \in N\}$ is chosen such as to diagonalize the non-condensate Hamiltonian, see Eq. (5). Let us point out briefly the tensor structure of the total Fock-Hilbert space $\mathcal{F}$, corresponding to the subsystems condensate and non-condensate, respectively:

$$\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_{\perp} \;.$$

As the condensate Hilbert space $\mathcal{F}_0$ is defined by $\mathcal{F}_0 = \text{span} \{|N_0\} : N_0 \in \mathbb{N}\}$, so is the Hilbert space $\mathcal{F}_{\perp}$ of the
non-condensate by $\mathcal{F}_\perp = \text{span}\{|N_1, N_2, \ldots : N_k \in \mathbb{N}\}$. Partial traces will be taken according to Eq. [3] in the following.

3. Decomposition of the Hamiltonian

The following decomposition of the Hamiltonian only requires the validity of the Gross-Pitaevskii equation for the condensate mode, and the orthogonality of the two fields $\hat{\Psi}_0$ and $\hat{\Psi}_\perp$, in the sense that

$$\int d\vec{r} \hat{\Psi}_0^\dagger(\vec{r}) \hat{\Psi}_\perp(\vec{r}) = 0.$$  \hspace{1cm} (4)

The Hamiltonian $\hat{\mathcal{H}}$ in second quantization, including two body interactions $[5]$, is given by

$$\hat{\mathcal{H}} = \int d\vec{r} \hat{\Psi}_0^\dagger(\vec{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) \right] \hat{\Psi}_0(\vec{r}) + \frac{g}{2} \int d\vec{r} \hat{\Psi}_0^\dagger(\vec{r}) \hat{\Psi}_\perp^\dagger(\vec{r}) \hat{\Psi}_\perp(\vec{r}) \hat{\Psi}(\vec{r}),$$ \hspace{1cm} (5)

where $\hat{\Psi}(\vec{r}) = \hat{\Psi}_0(\vec{r}) + \hat{\Psi}_\perp(\vec{r})$ denotes the second-quantized bosonic field, and with $g = \alpha a \hbar^2 / m$ quantifying the interaction strength in terms of the s-wave scattering length $a$. The neglect of three-body collisions implied by Eq. (3) is justified in the dilute regime $a \rho^{1/3} \ll 1$, with $\rho$ the density of the atomic gas. The field decomposition in Eq. [2] splits the Hamiltonian $\mathcal{H}$ into three basic contributions,

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_\perp + \hat{\mathcal{V}}_{0\perp},$$ \hspace{1cm} (6)

where $\hat{\mathcal{H}}_0$ and $\hat{\mathcal{H}}_\perp$ describe a pure condensate and non-condensate, respectively.

The condensate Hamiltonian $\hat{\mathcal{H}}_0$ contains the single particle contribution linear in the field $\hat{\Psi}_0$, as well as the nonlinear, self-interacting two body term, and is given by

$$\hat{\mathcal{H}}_0 = \int d\vec{r} \hat{\Psi}_0^\dagger(\vec{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) \right] \hat{\Psi}_0(\vec{r}) + \frac{g}{2} \int d\vec{r} \hat{\Psi}_0^\dagger(\vec{r}) \hat{\Psi}_\perp^\dagger(\vec{r}) \hat{\Psi}_\perp(\vec{r}) \hat{\Psi}_0(\vec{r}).$$ \hspace{1cm} (7)

When the average number of particles in the condensate is much larger than unity, a mean field approximation can be used to compute the ground state of $\hat{\mathcal{H}}_0$, which allows to recover the ordinary Gross-Pitaevskii equation [1].

Concerning the Hamiltonian of the background gas, $\hat{\mathcal{H}}_\perp$, we first write down the contribution bilinear in the non-condensate fields $\hat{\Psi}_\perp$ and $\hat{\Psi}_\perp^\dagger$, respectively:

$$\hat{\mathcal{H}}_\perp = \int d\vec{r} \hat{\Psi}_\perp^\dagger(\vec{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) \right] \hat{\Psi}_\perp(\vec{r}) + \sum_{k \neq 0} \epsilon_k a_k^\dagger a_k,$$ \hspace{1cm} (8)

where $\epsilon_k$ are single particle energies of non-condensate particles. To model interactions between non-condensate particles, we assume that these lead to a rapid thermalization in the non-condensate thermal vapor, as will be further discussed in Sec. II D 1 below.

Finally, the last term in Eq. (6), $\hat{\mathcal{V}}_{0\perp}$, describes all two body interactions between condensate and non-condensate. This term will be examined in the following subsection.

B. Two-body interaction processes

Inserting the decomposition of the field $\hat{\Psi}(\vec{r})$, Eq. [2], into the Hamiltonian $\hat{\mathcal{H}}$, Eq. [5], we find, besides the condensate and non-condensate Hamiltonians, Eqs. [7] [8], various terms describing two particle interaction processes. Sorting these according to the number of condensate and non-condensate particles, which are created or annihilated during a two body collision event, we obtain

$$\hat{\mathcal{V}}_{\perp 0} = \hat{\mathcal{V}}_\perp + \hat{\mathcal{V}}_{\perp 0} + \hat{\mathcal{V}}_0.$$ \hspace{1cm} (9)

where

$$\hat{\mathcal{V}}_\perp = g \int d\vec{r} \hat{\Psi}_\perp^\dagger(\vec{r}) \hat{\Psi}_\perp(\vec{r}) \hat{\Psi}_\perp(\vec{r}) \hat{\Psi}_0(\vec{r}),$$ \hspace{1cm} (10)

accounts for single particle events, where the condensate particle number changes by $\Delta N_0 = \pm 1$, and correspondingly, the number of non-condensate particles by $\Delta N_\perp = \mp 1$.

Second,

$$\hat{\mathcal{V}}_{\perp 0} = \frac{g}{2} \int d\vec{r} \hat{\Psi}_0^\dagger(\vec{r}) \hat{\Psi}_\perp^\dagger(\vec{r}) \hat{\Psi}_\perp(\vec{r}) \hat{\Psi}_\perp(\vec{r}) + \frac{g}{2} \int d\vec{r} \hat{\Psi}_\perp^\dagger(\vec{r}) \hat{\Psi}_\perp^\dagger(\vec{r}) \hat{\Psi}_\perp(\vec{r}) \hat{\Psi}_\perp(\vec{r}),$$ \hspace{1cm} (11)

describes pair events, where two condensate particles are created or annihilated, i.e., $\Delta N_0 = \pm 2$ and $\Delta N_\perp = \mp 2$.

Finally, the term

$$\hat{\mathcal{V}}_0 = 2g \int d\vec{r} \hat{\Psi}_0^\dagger(\vec{r}) \hat{\Psi}_\perp^\dagger(\vec{r}) \hat{\Psi}_\perp(\vec{r}) \hat{\Psi}_\perp(\vec{r})$$ \hspace{1cm} (12)

describes scattering events, where the number of condensate and non-condensate particles is unchanged ($\Delta N_0 =$...
\[ \Delta N_\perp = 0. \] As we will see later, scattering events do not contribute to the master equation for the condensate density matrix, which will mainly be governed by single particle events, with negligible influence of pair events.

To illustrate the different interaction terms, we introduce a diagrammatic representation of the interaction matrix elements \([14, 23]\). These are depicted in Fig. 1. Annihilation and creation of condensate particles are denoted by 0 and \(0^*\), respectively, whereas \(k, l, m\) and \(k^*, l^*, m^*\) refer to annihilated, or created particles of the corresponding non-condensate modes. Note that Fig. 1 contains only condensate loss events, where the number of condensate particles decreases. The conjugate processes, corresponding to condensate feeding, are obtained by exchanging the corresponding labels with respect to the diagram center.

Furthermore, Fig. 1 also shows processes of first order in the non-condensate field (upper left diagram), which are, however, not contained in Eq. (4). The reason is that these processes cancel out with mixed, single particle contributions between condensate and non-condensate fields in the Hamiltonian in Eq. (5). This is a consequence of the orthogonality of the two fields, \(\hat{\Psi}_0(\vec{r})\) and \(\hat{\Psi}_\perp(\vec{r})\), see Eq. (3), and the fact that \(\Psi_0(\vec{r})\) is an approximate solution of the Gross-Pitaevskii equation, Eq. (1), for sufficiently low temperatures (i.e., a sufficiently peaked condensate number distribution close to \(N\)). Indeed, when we combine upper left diagrams in Fig. 1 and their hermitian conjugates, with mixed single particle contributions in Eq. (5), we get the vanishing term

\[
\int d\vec{r} \hat{\Psi}_\perp(\vec{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + \hat{\Psi}_0^\dagger(\vec{r}) \hat{\Psi}_0(\vec{r}) \right] \hat{\Psi}_0(\vec{r}) \\
\simeq \sum_{k \neq 0} \hat{a}_k^\dagger \int d\vec{r} \hat{\Psi}_k^\dagger(\vec{r}) \hat{\Psi}_0(\vec{r}) \mu_0 a_0 = 0.
\]

In total, the Hamiltonian \(\hat{H}\) in Eq. (5) thus decomposes into

\[
\hat{H} = \hat{H}_0 + \hat{H}_\perp + \hat{V}_\rightarrow + \hat{V}_\leftarrow + \hat{V}_\odot,
\]

where the different interaction terms \(\hat{V}_\rightarrow\) in Eq. (10), \(\hat{V}_\leftarrow\) in Eq. (11), and \(\hat{V}_\odot\) in Eq. (12), account for single particle (\(\rightarrow\)), pair (\(\leftarrow\)) and scattering (\(\odot\)) contributions.

C. Evolution equation for the total density matrix

In analogy to the standard quantum optical derivation \([15, 10]\), we start with the von-Neumann equation, considering a many particle state \(\hat{\Psi}(t)\) of the condensate and the non-condensate field, \(\hat{\Psi}_0(\vec{r})\) and \(\hat{\Psi}_\perp(\vec{r})\), as well as the density matrix \(\hat{\sigma}(N)(t)\), to the interaction picture (denoted by the label \(I\)), which is carried out with respect to the Hamiltonian parts \(\hat{H}_0\) and \(\hat{H}_\perp\) of the subsystems condensate and non-condensate. The different operators hence undergo the transformation

\[
X(t) \rightarrow X^{(I)}(t) = \hat{U}(t) X(t) \hat{U}^\dagger(t) ,
\]

with respect to the time evolution operator \(\hat{U}(t)\) given by

\[
\hat{U}(t) = \exp \left[ \frac{i}{\hbar} \left( \hat{H}_0 + \hat{H}_\perp \right) t \right].
\]
The time evolution of the full density operator $\hat{\sigma}^{(N,I)}(t)$ in the interaction picture is then determined by the interaction between condensate and non-condensate particles, according to:

$$\frac{\partial \hat{\sigma}^{(N,I)}(t)}{\partial t} = -\frac{i}{\hbar} \{ \hat{V}^{(I)}_{0\perp}(t), \hat{\sigma}^{(N,I)}(t) \} .$$

(19)

where $\hat{V}^{(I)}_{0\perp}(t)$ is obtained by inserting the time dependent annihilation (and creation) operators, e.g. $a_0(t) = a_0 e^{-i\omega_0 t/\hbar}$ and $a_k(t) = a_k e^{-i\omega k t/\hbar}$ in the corresponding time independent expressions derived in the previous section. Integration of Eq. (19) between $t$ and $t + \Delta t$ leads to

$$\hat{\sigma}^{(N,I)}(t + \Delta t) = \hat{\sigma}^{(N,I)}(t) - \frac{i}{\hbar} \int_t^{t + \Delta t} dt' \left[ \hat{V}^{(I)}_{0\perp}(t'), \hat{\sigma}^{(N,I)}(t') \right] .$$

(20)

For short times, $\Delta t$, a good approximate solution of Eq. (20) is obtained by its iteration up to second order in $\hat{V}^{(I)}_{0\perp}$ (which is required since the first-order terms vanish, as we will see later):

$$\Delta \hat{\sigma}^{(N,I)}(t) = \frac{i}{\hbar} \int_t^{t + \Delta t} dt' \left[ \hat{V}^{(I)}_{0\perp}(t'), \hat{\sigma}^{(N,I)}(t) \right]$$

(21)

$$- \int_t^{t + \Delta t} dt' \int_t^{t + \Delta t} dt'' \left[ \hat{V}^{(I)}_{0\perp}(t'), \hat{V}^{(I)}_{0\perp}(t''), \hat{\sigma}^{(N,I)}(t) \right] ,$$

where we have set $\Delta \hat{\sigma}^{(N,I)}(t) = \hat{\sigma}^{(N,I)}(t + \Delta t) - \hat{\sigma}^{(N,I)}(t)$. Note that Eq. (21) expresses the state at time $t + \Delta t$ (left-hand side) fully, as a function of the state $\hat{\sigma}^{(N,I)}(t)$ at time $t$ - in contrast to the exact Eq. (20), where states $\hat{\sigma}^{(N,I)}(t')$ at all intermediate times $t'$ appear on the right-hand side.

D. Time evolution of the reduced condensate density matrix

The time evolution of the condensate in the presence of the non-condensate gas is obtained by taking the partial trace over $F_{\perp}$ in Eq. (21). To get a Markovian master equation for the reduced condensate density matrix, $\hat{\rho}_0^{(N)}(t) = \text{Tr}_{\perp} \hat{\sigma}^{(N)}(t)$, we use a Born-Markov ansatz generalized for the $N$-particle state $\sigma^{(N)}(t)$ which allows to express $\sigma^{(N)}(t)$ completely in terms of the reduced condensate density matrix $\hat{\rho}_0^{(N)}(t)$ at time $t$, see Eq. (22).

$$\sigma^{(N)}(t) = \sum_{N_0=0}^N p_N(N_0,t)|N_0\rangle\langle N_0| \otimes \hat{\rho}_{\perp}(N - N_0, T) ,$$

(22)

for the environment, which is supposed to be unchanged by the interaction with the system. Then, the total state $\hat{\sigma}(t)$ would be given by the product $\hat{\sigma}(t) = \hat{\rho}(t) \otimes \hat{\rho}_E(T)$, hence completely determined by the reduced state $\hat{\rho}(t)$ of the (condensate) subsystem. However, in our case, this simple product ansatz cannot be applied, since condensate and non-condensate are correlated by particle number conservation: If one finds $N_0$ particles in the condensate, the particle number in the non-condensate is determined as $N_{\perp} = N - N_0$, and vice versa.

The physical origin of the non-condensate thermalization is the interaction between non-condensate particles, which leaves the number of non-condensate particles unchanged. We hence couple the non-condensate to a heat bath only allowing for exchange of energy, but not of particles, see Fig. 2. The thermalization then occurs only within subspaces of fixed particle number. In addition, we assume that coherences between subspaces of different particle number are destroyed due to the coupling with the heat bath. Under this assumption, the total $N$-particle state is obtained as:

$$\hat{\sigma}^{(N)}(t) = \sum_{N_0=0}^N p_N(N_0,t)|N_0\rangle\langle N_0| \otimes \hat{\rho}_{\perp}(N - N_0, T) ,$$

where $p_N(N_0,t)$ denotes the probability of finding $N_0$ particles in the condensate (or, equivalently, $N - N_0$ par-
particles in the non-condensate), and
\[
\hat{\rho}_\perp(N - N_0, T) = \frac{\hat{Q}_{N - N_0} e^{-\beta \hat{H}_\perp} \hat{Q}_{N - N_0}}{Z_\perp(N - N_0, T)}
\]  
(23)
describes a thermal state projected onto the subspace of \(N - N_0\) non-condensate particles, with corresponding projector \(\hat{Q}_{N - N_0}\), and normalization factor \(Z_\perp\).

Furthermore, it can be shown that scattering events, described by \(\hat{\rho}_\perp\), are dynamically independent from each other. Hence, single particle, pair and scattering events in the non-condensate particles in the non-condensate), and
\[
\hat{\rho}_\perp(N - N_0, T) = \text{Tr}_{\rho_\perp} \left\{ \hat{Q}_{N - N_0} e^{-\beta \hat{H}_\perp} \hat{Q}_{N - N_0} \right\} .
\]  
(24)
Note that, since \(\hat{\sigma}(N)(t)\) is diagonal in the Fock basis, it is invariant under the free evolution \(\hat{U}(t)\), Eq. (18), and hence \(\hat{\sigma}(N,I)(t) = \hat{\sigma}(N)(t)\). In the following, we hence drop the index ‘I’ referring to the interaction picture for the \(N\)-particle state \(\hat{\sigma}(N)(t)\), or its reduced condensate state \(\hat{\sigma}_0(N)(t)\), see below.

2. Evolution equation for the condensate density matrix

Taking the partial trace over the non-condensate, we obtain the reduced condensate density matrix:
\[
\hat{\rho}_0(N)(t) = \text{Tr}_{\rho_\perp} \left\{ \hat{\sigma}(N)(t) \right\} = \sum_{N_0=0}^{N} p_N(N_0, t)|N_0\rangle\langle N_0| .
\]  
(25)

Inserting Eq. (22) in the right-hand side of Eq. (21), and taking the partial trace over the non-condensate, leads to a closed evolution equation for the reduced condensate density matrix. Moreover, it can be shown that the terms of first order in the interaction \(\hat{V}_{0,1}(t)\) vanish after taking the partial trace over \(\mathcal{F}_{\perp}\). Indeed, from the diagonal form of the \(N\)-particle state \(\hat{\sigma}(N)(t)\), see Eq. (22), it follows that
\[
\text{Tr}_{\rho_\perp} \left\{ \hat{V}_{0,1}(t'), \hat{\sigma}(N)(t) \right\} = 0 .
\]  
(26)
From the remaining second order terms, we obtain:
\[
\Delta \hat{\rho}_0(N)(t) = - \sum_{N_0=0}^{N} \int \frac{d\tau}{t} \int t' \frac{dt''}{\hbar^2} \text{Tr}_{\rho_\perp} \left[ \hat{V}_{0,1}(t'), \left[ \hat{V}_{0,1}(t''), p_N(N_0, t)|N_0\rangle\langle N_0| \otimes \hat{\rho}_\perp(N - N_0, T) \right] \right] .
\]  
(27)
Writing the interaction term \(\hat{V}_{0,1}(t')\) as a sum over the three different processes (single particle, pair and scattering events), see Eq. (19), we can now verify that any mixed commutator in Eq. (27) vanishes - again as a consequence of the diagonality of \(\hat{\sigma}(N)(t)\).

Hence, single particle, pair and scattering events in the gas are dynamically independent from each other. Furthermore, it can be shown that scattering events, described by \(\hat{V}_{\perp}\), do not contribute, since they leave the number of condensate particles unchanged. We are left with:
\[
\frac{\Delta \hat{\rho}_0(N)(t)}{\Delta t} = \frac{\Delta \hat{\rho}_0(N)(t)}{\Delta t} \bigg|_{\sim} + \frac{\Delta \hat{\rho}_0(N)(t)}{\Delta t} \bigg|_{\sim} ,
\]  
(28)
where the two terms on the right-hand side of Eq. (28) are obtained by inserting the corresponding interaction terms \(\hat{V}_{\sim}\) and \(\hat{V}_{\sim,\sim}\), instead of the full interaction \(\hat{V}_{\perp,0}\) into Eq. (27).

3. Quantum master equation of Lindblad type

In order to perform the time integration in Eq. (27), we first notice that the right-hand side depends only on the time difference \(\tau = t' - t''\). Second, we assume that only times \(\tau \ll \Delta t\) contribute to the integral, due to the rapid decay of non-condensate correlation functions. To implement this rapid decay, we assume that the two point correlation functions of the non-condensate decay on the average time scale \(\tau_{\text{col}}\) of a two body collision event. Performing the time integral as
where the quantum jump operators \( \hat{S}_\pm(N_0) \) and \( \hat{P}_\pm(N_0) \) are defined by
\[
\begin{align*}
\hat{S}_+(N_0) &= |N_0 + 1\rangle \langle N_0|, \\
\hat{S}_-(N_0) &= |N_0 - 1\rangle \langle N_0|, \\
\hat{P}_+(N_0) &= |N_0 + 2\rangle \langle N_0|, \\
\hat{P}_-(N_0) &= |N_0 - 2\rangle \langle N_0|.
\end{align*}
\]

Obviously, \( \hat{S}_+(N_0) \) adds one particle to the condensate with a rate \( \xi^+_N(N_0, T) = 2(N_0 + 1)\lambda_+^+(N - N_0, T) \), whereas \( \hat{S}_-(N_0) \) destroys a condensate particle with the rate \( \xi^-_N(N_0, T) = 2N_0\lambda_-^-(N - N_0, T) \), given a number of \( (N - N_0) \) non-condensate particles, and a temperature \( T \) of the heat reservoir. In a similar way, \( \hat{P}_\pm(N_0) \) describe the simultaneous creation of two condensate particles with a rate \( \gamma^+_N(N_0, T) = (N_0 + 1)(N_0 + 2)\lambda_+^+(N - N_0, T) \), and the depletion of two condensate particles with a rate \( \gamma^-_N(N_0, T) = N_0(N_0 - 1)\lambda_-^-(N - N_0, T) \). The different transition rates \( \xi^+_N(N_0, T) \) and \( \gamma^+_N(N_0, T) \) are defined by the following integrals over non-condensate correlation functions:

\[
\begin{align*}
\lambda_-^-(N - N_0, T) &= \text{Re} \left\{ \frac{g^2}{\hbar^2} \int d\vec{r} \int d\vec{r}' \Psi^*_0(\vec{r})\Psi_0(\vec{r}') \int_0^\infty d\tau \ e^{-\Gamma^2\tau} e^{\pm \frac{imc}{\hbar} \sqrt{\lambda_-^-(N - N_0, T)}} \right\}, \\
\lambda_+^+(N - N_0, T) &= \text{Re} \left\{ \frac{g^2}{4\hbar^2} \int d\vec{r} \int d\vec{r}' \Psi^*_0(\vec{r})\Psi_0(\vec{r}') \Psi^*_0(\vec{r}')\Psi_0(\vec{r}) \int_0^\infty d\tau \ e^{-\Gamma^2\tau} e^{\pm \frac{2imc}{\hbar} \sqrt{\lambda_+^+(N - N_0, T)}} \right\}.
\end{align*}
\]

where \( \mathcal{G}^{(\pm)}(\vec{r}, \vec{r}', N - N_0, T, \tau) \) and \( \mathcal{G}^{(\pm)}_{\text{cor}}(\vec{r}, \vec{r}', N - N_0, T, \tau) \) are correlation functions of the non-condensate field for single particle (\(-\)) and pair (\(-\)) events, given that \((N - N_0)\) particle are in the non-condensate gas. In Eqs. \((32)\) and \((33)\), we have extended the time integral from \(\Delta t\) to \(\infty\), assuming a Gaussian decay of non-condensate correlations due to thermalization which occurs within a time interval on the order of the average time \( \Gamma = \tau_{\text{col}}^{-1} \) for two-body collisions.

The remaining coherent parts \( \mathcal{G}^{(\pm)} \) and \( \mathcal{G}^{(\pm)}_{\text{cor}} \) of non-condensate correlations are determined by the thermalized state in Eq. \((29)\):
\[ G_{\pm}^{(+)}(\vec{r}, \vec{r}', N - N_0, T, \tau) = \left\langle \hat{\Psi}_\bot^\dagger(\vec{r}, \tau)\hat{\Psi}_\bot^\dagger(\vec{r}', \tau)\hat{\Psi}_\bot(\vec{r}', 0)\hat{\Psi}_\bot(\vec{r}, 0) \right\rangle^{(N-N_0)}_{\mathcal{F}_\bot}, \]

\[ G_{\pm}^{(-)}(\vec{r}, \vec{r}', N - N_0, T, \tau) = \left\langle \hat{\Psi}_\bot(\vec{r}, \tau)\hat{\Psi}_\bot(\vec{r}', \tau)\hat{\Psi}_\bot^\dagger(\vec{r}', 0)\hat{\Psi}_\bot^\dagger(\vec{r}, 0) \right\rangle^{(N-N_0)}_{\mathcal{F}_\bot}, \]

for single particle events, and by

\[ G_{\pm}^{(+)}(\vec{r}, \vec{r}', N - N_0, T, \tau) = \left\langle \hat{\Psi}^\dagger_\bot(\vec{r}, \tau)\hat{\Psi}^\dagger_\bot(\vec{r}', \tau)\hat{\Psi}_\bot(\vec{r}', 0)\hat{\Psi}_\bot(\vec{r}, 0) \right\rangle^{(N-N_0)}_{\mathcal{F}_\bot}, \]

\[ G_{\pm}^{(-)}(\vec{r}, \vec{r}', N - N_0, T, \tau) = \left\langle \hat{\Psi}_\bot(\vec{r}, \tau)\hat{\Psi}_\bot(\vec{r}', \tau)\hat{\Psi}^\dagger_\bot(\vec{r}', 0)\hat{\Psi}^\dagger_\bot(\vec{r}, 0) \right\rangle^{(N-N_0)}_{\mathcal{F}_\bot}, \]

4. Quantum master equation of Bose-Einstein condensation

From the master equation of Lindblad type in Eq. (30), we can derive the evolution equation for the condensate particle number distribution, \( p_N(N_0, t) = \langle N_0 | \rho(t) | N_0 \rangle \). Considering only single particle processes (\( \to \)), since they dominate the condensate process in three-dimensional harmonic traps, see section II D 7, leads to the quantum master equation for quantum jump processes with \( \Delta N_0 = \pm 1 \):

\[ \frac{\partial p_N(N_0, t)}{\partial t} = - [\xi^+_N(N_0, T) + \xi^-_N(N_0, T)] p_N(N_0, t) + \xi^+_N(N_0 - 1, T) p_N(N_0 - 1, t) + \xi^-_N(N_0 + 1, T) p_N(N_0 + 1, t), \]

with \( \xi^+_N(N_0, T) = 2(N_0 + 1) \lambda^+_N(N - N_0, T) \) and \( \xi^-_N(N_0, T) = 2N_0 \lambda^-_N(N - N_0, T) \), where the transition rates \( \lambda^\pm_N(N - N_0, T) \) are given by Eq. (32).

Bose-Einstein condensation is now reduced to a simple rate equation, the master Eq. (33), which describes in particular the buildup of a macroscopic condensate occupation from the fluctuating thermal vapor. As sketched in Fig. 3, net particle flow towards a state \( |N_0\rangle \langle N_0| \) is described by the current \( \xi^+_N(N_0, T) p_N(N_0 - 1, t) + \xi^-_N(N_0 + 1, T) p_N(N_0 + 1, t) \), and particle flow from the state \( |N_0\rangle \langle N_0| \) by the current \( \xi^+_N(N_0, T) p_N(N_0, t) + \xi^-_N(N_0, T) p_N(N_0, t) \). As will be shown in section II D 7, the steady state of the system is therefore reached, if, and only if the net probability flux for every state \( |N_0\rangle \langle N_0| \) (\( \to \) detailed balance of probability flow) is zero, i.e. \( \xi^+_N(N_0, T) p_N(N_0, T) = \xi^-_N(N_0 + 1, T) p_N(N_0 + 1, T) \) for all \( N_0 = 0 \ldots N \).

5. Transition rates for Lindblad dynamics

We now evaluate the different decay rates, Eqs. (32) and (33). For this purpose, we decompose the higher order correlation functions of the non-condensate fields into second order correlation functions according to the Wick theorem [26] and perform the integrals over \( \vec{r}, \vec{r}' \) and \( \tau \), see appendix A. For the single particle creation and
loss events, the result is:

\[
\lambda_{\pm}(N_{\perp}, T) = \frac{16\pi^3 \hbar^2 a^2}{m^2} \sum_{k,l,m \neq 0} \left[ f_{\pm}^{-}(k, l, m, N_{\perp}, T) \times \delta^{(\Gamma)}(\omega_k + \omega_l - \omega_m - \omega_0) + g_{\pm}^{-}(k, l, m, N_{\perp}, T) \delta^{(\Gamma)}(\omega_l - \omega_0) \right]
\]

(37)

where \(\omega_k \equiv \epsilon_k / \hbar\), \(\omega_0 \equiv \mu_0 / \hbar\), and where

\[
f_{\pm}^{-}(k, l, m, N_{\perp}, T) = \langle N_k \rangle(N_{\perp}, T) \langle N_l \rangle(N_{\perp}, T) \times \langle N_m \rangle(N_{\perp}, T) + 1 \rangle |\zeta_{kl}^0|^2
\]

(38)

and

\[
g_{\pm}^{-}(k, l, m, N_{\perp}, T) = 2 \langle N_k \rangle(N_{\perp}, T) \langle N_l \rangle(N_{\perp}, T) \times \langle N_m \rangle(N_{\perp}, T) |\zeta_{kl}^0|^2
\]

(39)

are the weight functions for condensate particle feedings. Correspondingly,

\[
f^{-}(k, l, m, N_{\perp}, T) = [\langle N_k \rangle(N_{\perp}, T) + 1] \times \langle N_l \rangle(N_{\perp}, T) + 1 \rangle \langle N_m \rangle(N_{\perp}, T) |\zeta_{kl}^0|^2
\]

(40)

and

\[
g_{-}^{-}(k, l, m, N_{\perp}, T) = 2 \langle N_k \rangle(N_{\perp}, T) \times \langle N_l \rangle(N_{\perp}, T) + 1 \rangle \langle N_m \rangle(N_{\perp}, T) |\zeta_{kl}^0|^2
\]

(41)

are the weight functions for condensate particle losses. The functions \(f_{\pm}^{-}(k, l, m, N_{\perp}, T)\) and \(g_{\pm}^{-}(k, l, m, N_{\perp}, T)\) depend on temperature, the number of non-condensate particles, \(N_{\perp} = (N - N_0)\), and on the quantum mechanical probability amplitudes

\[
\zeta_{kl}^0 = \left(\zeta_{kl}^0\right)^* = \int d\vec{r} \Psi_0^* (\vec{r}) \Psi_m^* (\vec{r}) \Psi_k (\vec{r}) \Psi_l (\vec{r})
\]

(42)

for the different microscopic single particle feeding and loss processes with energy balances \(\Delta \epsilon_{\pm} = \Delta \epsilon_{\pm}/\hbar = (\omega_k + \omega_l - \omega_m - \omega_0)\) or \((\omega_l - \omega_0)\). The \(\delta\)-distribution in Eq. (37), \(\delta^{(\Gamma)}(\Delta \omega_{\pm}) = 1/2\Gamma \exp[-(\Delta \omega_{\pm})^2/4\Gamma^2]\), reflects conservation of energy during the single particle feeding and loss processes on a certain width \(\sqrt{2\Gamma}\) arising from the decay of the non-condensate field correlation functions in Eqs. (32) (33). Therefore, only single particle processes with energy balances \(\Delta \epsilon_{\pm}/\hbar < \Gamma\) will contribute to the rates in Eq. (37).

The average occupation number \(\langle N_k \rangle(N_{\perp}, T)\) of a non-condensate single particle state \(|\Psi_k\rangle\) of a thermal state projected onto the subspace of \(N_{\perp} = (N - N_0)\) non-condensate atoms, reads (see appendix [44])

\[
\langle N_k \rangle(N_{\perp}, T) = \frac{1}{\exp[\beta(\epsilon_k - \mu_\perp(N_{\perp}, T))] - 1}
\]

(43)

where \(\mu_\perp(N_{\perp}, T)\) is defined by the normalization condition: \(\sum_{k \neq 0} \langle N_k \rangle(N_{\perp}, T) = N_{\perp}\). According to this definition, \(\mu_\perp(N_{\perp}, T)\) equals the chemical potential of a thermal state of \(N_{\perp} = (N - N_0)\) non-condensate particles \([23]\). From \(\langle N_k \rangle + 1 = \langle N_k \rangle \exp[\beta(\epsilon_k - \mu_\perp)]\), and using the energy conservation as expressed by the \(\delta\)-function in Eq. (37), one can derive the following relation between the single particle loss and feeding rates:

\[
\lambda_{\pm}(N - N_0, 0, T) = e^{\beta \Delta \mu(N - N_0, T)} \lambda_{-}(N - N_0, 0, T),
\]

(44)

where \(\Delta \mu(N - N_0) = \mu_\perp(N - N_0, T) - \mu_0\). To obtain Eq. (14), the finite width \(\Gamma\) of the \(\delta\)-function is neglected, which is justified under the condition \(\hbar \Gamma \beta \ll 1\). The relation (44) will be useful in Sec. 11 to determine the equilibrium state of the Bose gas.

Note that Eq. (13) takes into account the depletion of the non-condensate during condensate formation, ensuring that \(\langle N_k \rangle \to 0\) as \(N_0 \to N\). According to Eqs. (35, 40), also the condensate feeding and loss rates tend to zero in this limit. In contrast, the rates obtained within quantum kinetic theory (1) increase with increasing condensate particle number \(N_0\).

Finally, the rates for pair events turn into:

\[
\lambda_{\pm}^{-}(N_{\perp}, T) = \frac{4\pi^3 \hbar^2 a^2}{m^2} \sum_{k,l \neq 0} f_{\pm}^{-}(k, l, N_{\perp}, T) \times \delta^{(\Gamma)}(\omega_k + \omega_l - 2\omega_0),
\]

(45)

with the weight function

\[
f_{\pm}^{-}(k, l, N_{\perp}, T) = \langle N_k \rangle(N_{\perp}, T) \langle N_l \rangle(N_{\perp}, T) |\zeta_{kl}^0|^2
\]

(46)

for pair feedings, and correspondingly

\[
f^{-}(k, l, N_{\perp}, T) = \langle N_k \rangle(N_{\perp}, T) + 1 \rangle \langle N_l \rangle(N_{\perp}, T) + 1 \rangle |\zeta_{kl}^0|^2
\]

(47)

for pair losses, with

\[
\zeta_{kl}^0 = \int d\vec{r} (\Psi_0^* (\vec{r})^* \Psi_k (\vec{r}) \Psi_l (\vec{r})
\]

(48)

Looking at the energy balance of a pair event, \(\Delta \epsilon_{\pm}/\hbar = \omega_k + \omega_l - 2\omega_0\), we see that pair events occur as energy non-conserving processes, i.e., \(\Delta \epsilon_{\pm}/\hbar \gg \Gamma \sim 10-20\) Hz, since the single particle energy \(\mu_\perp\) of condensate particles is smaller than the energies \(\epsilon_k, l \gg \hbar \Gamma\) of non-condensate particles in a three-dimensional harmonic trap. Therefore, pair events can be neglected in comparison with the single-particle events in the master equation (36). For the same reason, we can neglect the terms associated to the \(g_{\pm}^{-}\) functions in Eq. (37) as compared to those associated to the \(f_{\pm}^{-}\) functions.
III. RESULTS

In this section, we present numerical studies of the condensate particle number distribution obtained from Eq. (36) during Bose-Einstein condensation, and derive the unique equilibrium steady state of the Bose-Einstein condensate. Under the assumption \( \hbar \Gamma / E \ll 1 \), the equilibrium steady state is proven to be a Gibbs-Boltzmann (thermal) state of non-interacting particles in the dilute equilibrium steady state is proven to be a Gibbs-Boltzmann condensate. Under the assumption the unique equilibrium steady state of the Bose-Einstein condensation, and derive condensate particle number distribution obtained from their non-interacting limits. Hence, the basis states Pitaevskii equation turn into the single particle eigenstates are proportional to \( a \). cesses of second order in the interaction \( \hat{\chi} \) rates derived in the previous section originate from processes of second order in the interaction \( \hat{\chi} \), all the rates are proportional to \( a^2 \), as evident from the prefactors in Eqs. (37) (45). The remaining dependence of the rates on the interaction strength originates from the single particle wave functions \( |\Psi_k\rangle \), the eigenvalue of the Gross-Pitaevskii equation \( \mu_0 \), and the non-condensate single particle energies \( \epsilon_k \), which are themselves functions on the parameter \( a_0 \), see Eq. (1).

Interested in the case of dilute and weakly interacting gases, we thus expand these quantities (i.e. \( |\Psi_0\rangle \), \( \mu_0 \) and \( \epsilon_k \)) in terms of the scattering length \( a \), taking into account only the first non-vanishing contribution, given by their non-interacting limits. Hence, the basis states \( |\Psi_k\rangle \) turn into the single particle eigenstates \( |\chi_k\rangle \) of the trapping potential, with corresponding ground state energy \( \epsilon_0 \), whereas the \( \epsilon_k \)'s are the energies of the excited states. Thereby, we evaluate the transition rates to lowest non-vanishing order – proportional to \( a^2 \) – in the s-wave scattering length.

Quantitatively, this procedure is correct as long as the ground state of the Gross-Pitaevskii equation \( |\Psi_0\rangle \) is well approximated by the single-particle ground state. This, in turn, is the case if the interaction energy \( gN|\Psi_0|^2 \) is much smaller than the harmonic oscillator energy \( h\omega \), or, in other words, if \( aN/L \ll 1 \), where \( L = \hbar / m\omega \) denotes the extension of the harmonic oscillator ground state.

When \( aN/L \) increases, the ground state of the Gross-Pitaevskii equation is progressively distorted, as well as the various excited states, making the explicit calculation of the rates, Eqs. (37) (42), more difficult. However, no drastic change is likely to take place, making the following predictions qualitatively and maybe semi-quantitatively correct for a realistic situation like Bose-Einstein condensation of a Rb or Na gas.

B. Dynamics of Bose-Einstein condensation

Equation (36) is solved numerically to propagate the condensate particle number distribution \( p_N(N_0, t) \) in time. Figure 4 displays a typical example for the time evolution of \( p_N(N_0, t) \) for a gas of \( N = 2000 \) \(^{87}\)Rb atoms which undergoes the Bose-Einstein condensation phase transition in a three-dimensional harmonic trap with frequencies \( \omega_x = \omega_y = 2\pi \times 42.0 \) Hz, \( \omega_z = 2\pi \times 120.0 \) Hz. The final temperature of the gas is \( T = 20.31 \) nK, and the critical temperature of the harmonic oscillator ground state.

To calculate the transition rates leading to the condensate growth scenario in Fig. 4, we used the semi-classical limit \( a \ll 1 \) [21], where the discrete sums in the feeding and loss rates in Eq. (37) are replaced by an integral over the density of states \( g(\epsilon) = \epsilon^2 / 2(\hbar^2 \omega_\perp \omega_\parallel) \). This shifts the final condensate fraction by approx. 10% as compared to the exact numerical evaluation of the discrete sums (employed in Figs. 5 and 6 below), but does not change the qualitative behavior observed in Fig. 4.

C. Average condensate growth

From the time evolution of the distribution \( p_N(N_0, t) \) defined by Eq. (36) the growth of the average condensate population can be extracted using

\[
\langle N_0 \rangle (t) = \sum_{N_0=0}^{N} N_0 p_N(N_0, t),
\]

(49)
and deriving a corresponding condensate growth equation [11]. For this purpose, we assume a sufficiently narrow peaked distribution \( p_N(N_0, t) \) around the mean value \( \langle N_0 \rangle \) as indicated by Fig. 4 such that the rates are approximately constant in this narrow region, meaning that

\[
\lambda^+(N - N_0, T) \approx \lambda^-(N - \langle N_0 \rangle, T) ,
\]

for \( N_0 \) close enough to \( \langle N_0 \rangle \). Taking the average \( N_0 \partial p(N_0, t)/\partial t \) with \( \partial p(N_0, t)/\partial t \) given by Eq. (50) finally leads to the following growth equation for the average condensate occupation:

\[
\frac{\partial \langle N_0 \rangle}{\partial t} = \xi^+((N_0), T) - \xi^-((N_0) + 1, T) ,
\]

with \( \xi^+((N_0), T) = 2(\langle N_0 \rangle + 1)\lambda^+(N - \langle N_0 \rangle, T) \), and \( \xi^-((N_0) + 1, T) = 2(\langle N_0 \rangle + 1)\lambda^-(N - \langle N_0 \rangle, T) \). The equilibrium value of \( \langle N_0 \rangle \) is hence defined by the detailed particle balance condition \( \lambda^+_+(N - \langle N_0 \rangle, T) = \lambda^-_-(N - \langle N_0 \rangle, T) \). According to the above relation between the rates \( \lambda^+_+ \) and \( \lambda^-_- \), see Eq. (13), this implies equality of the chemical potentials on average:

\[
\mu_0 = \mu_0(N - \langle N_0 \rangle, T) .
\]

In the next section, we will show that not only the average condensate occupation, but also the whole steady state distribution \( p_N(N_0, T) \) agrees with the thermodynamical prediction.

### D. Steady state distribution

For this purpose, we solve Eq. (22) for the steady state distribution, defined by \( \partial p_N(N_0, t)/\partial t = 0 \), which leads to:

\[
p_N(N_0, T) = N \prod_{\sigma = 1}^{N_0 - 1} \frac{\xi^+_{\sigma}(\sigma - 1, T)}{\xi^-_{\sigma}(\sigma, T)} .
\]

Let us now compare this steady state to a thermal state of \( N \) non-interacting particles at temperature \( T \):

\[
\hat{\sigma}_{N, th} = \hat{Q}_N e^{-\beta \hat{H}} \frac{Z(N, T)}{Z(N, T)} \hat{Q}_N ,
\]

with the partition function \( Z(N, T) \) of \( N \) indistinguishable particles, and the projector \( \hat{Q}_N \) onto the Fock space of \( N \) particles. In the absence of interactions, \( \hat{H} \) in Eq. (54) is the Hamiltonian of the gas in Eq. (4), with \( g \equiv 0 \). To proof the equality of the state \( \hat{\sigma}_{N, th} \) and the steady state of the Bose gas in Eq. (22), with \( p_N(N_0, T) \) given by Eq. (53), it needs to be shown that the recursion relation for the condensate particle number distribution,

\[
\frac{p_{N, th}(N_0, T)}{p_{N, th}(N_0 + 1, T)} = e^{\beta \epsilon_0} \frac{Z(N - N_0, T)}{Z(N - N_0 - 1, T)} ,
\]

which results from tracing Eq. (54) over the non-condensate, applies as well for the steady state, Eq. (53),
of the master equation. In Eq. (53), $\mathcal{Z}_\perp(N - N_0, T)$ is the partition function of $(N - N_0)$ non-condensate particles, see Eq. (24), and $\epsilon_0$ the single particle ground state energy of a non-interacting gas. This can be seen if we approximate $\lambda_\perp(N - N_0, T) \approx \lambda_\perp(N - N_0 + 1, T)$, neglecting terms of the order of $N^{-1}$. In this case, we obtain from Eq. (53):

$$\frac{p_N(N_0, T)}{p_N(N_0 + 1, T)} \approx \frac{\lambda_\perp(N - N_0, T)}{\lambda_\perp(N - N_0, T)} = e^{\beta(\epsilon_0 - \mu_\perp(N, T))},$$

(56)

where we used Eq. (44), and $\epsilon_0 = \mu_0$ (in the regime of small interactions, $aN/L \ll 1$, see Sec. IIIA).

Now, the non-condensate chemical potential, as defined by the normalization condition in Eq. (43), can be shown [25] to be related to the non-condensate partition function, via $-\beta\mu_\perp(N - N_0, T) = \ln\mathcal{Z}_\perp(N - N_0, T) - \ln\mathcal{Z}_\perp(N - N_0 - 1, T)$. Therewith, we arrive at the recurrence relation in Eq. (55), which was to be shown. Hence, the steady state of the entire Bose gas in Eq. (22) is given by the thermal state in Eq. (54), in the case of weak interactions, and under the condition $\beta\hbar \ll 1$ for which Eq. (44) is proven to be valid.

The $1/N$ approximation required for the above proof is confirmed by comparing the exact numerical calculation of the steady state condensate particle number distribution to the prediction of the Boltzmann ansatz in Eqs. (54). Fig. 5 shows the stationary particle number distribution for the same parameters as in Fig. 4. In order to show that the agreement holds up to the critical temperature (and beyond), Fig. 6 displays the comparison of average condensate occupations, and the standard deviation of the stationary condensate particle number distributions (such as the one depicted in Fig. 5) as a function of the entire range of relative temperatures, $T/T_c$, for $N = 2000$ atoms for the same trap parameters as in Fig. 6. Again, we observe close agreement between master equation and the Boltzmann ansatz: The shift of the critical temperature is about 10% with respect to the critical temperature $T_c$ of Bose-Einstein statistics in the semiclassical limit [1] in both cases.

IV. CONCLUSION

We have presented the conceptual part and first numerical results of a number-conserving quantum master equation theory to describe the transition of a dilute gas of $N$ bosonic atoms into a Bose-Einstein condensate. The central result of our theory is the quantum master equation in Eq. (36) which describes the time evolution of the reduced condensate state in contact with the non-condensate environment for a fixed total atom number. In the dilute gas regime, we numerically monitored the full condensate particle number distribution $p_N(N_0, t)$ during condensate formation.

The theory predicts condensate formation times of the order of seconds, matching experimentally and theoretically observed times scales [1, 2]. The derived steady state for a dilute, weakly interacting Bose-Einstein condensate undergoing Markovian dynamics is unique, and proven to obey the same statistics as a Gibbs-Boltzmann thermal state of non-interacting particles, in the case of weak interactions $aN/L \ll 1$, and for the case $\hbar\beta \ll 1$ of not too rapidly decaying non-condensate correlation functions.

Future improvements of our model will consist in a microscopic derivation of the rate $\Gamma$ describing the decay of non-condensate field correlation functions (e.g. by diagrammatic expansion techniques for higher order correlation functions), which, in the present version, has been introduced in a rather phenomenological way. Furthermore, the condition $aN/L \ll 1$ of weak interactions may be relaxed. Since, in this case, the condensate wave function will depend on the number of condensate particles, this will in particular require to introduce time-dependent condensate and non-condensate wave functions. Finally, it remains to be studied whether deviations from the Gibbs-Boltzmann occur if the condition $\hbar\beta \ll 1$ is not fulfilled.

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Appendix A: Two point correlation functions

Here, we decompose the correlation functions of the non-condensate field for single particle $(\cdots)$ and pair $(\cdots)$ processes into products of two-point correlation functions with Wick’s theorem, which applies to thermal expectation values [26, 27].

We begin with the correlation function for single particle processes $G_{\perp}^{(1)}(\vec{r}, \vec{r}'; N - N_0, T, \tau)$ in Eq. (41):
Any two point correlation function of products of two non-condensate fields in Eqs. (A1) and (A2) can thus be written

\[ G^{(+)\cdots}(\vec{r}, \vec{r}', N - N_0, T, \tau) = \langle \hat{\Psi}^{\dagger}_\Lambda(\vec{r}, \tau) \hat{\Psi}^{\dagger}_\Lambda(\vec{r}, \tau) \hat{\Psi}_\Lambda(\vec{r}', \tau) \hat{\Psi}_\Lambda(\vec{r}', 0) \hat{\Psi}_\Lambda(\vec{r}', 0) \hat{\Psi}_\Lambda(\vec{r}', 0) \rangle_{\mathcal{F}_\Lambda} \]

and similarly:

\[ G^{(-)}(\vec{r}, \vec{r}', N - N_0, T, \tau) = \langle \hat{\Psi}^{\dagger}_\Lambda(\vec{r}, \tau) \hat{\Psi}^{\dagger}_\Lambda(\vec{r}, \tau) \hat{\Psi}_\Lambda(\vec{r}', \tau) \hat{\Psi}_\Lambda(\vec{r}', 0) \hat{\Psi}_\Lambda(\vec{r}', 0) \hat{\Psi}_\Lambda(\vec{r}', 0) \rangle_{\mathcal{F}_\Lambda} \]

The non-condensate field \( \hat{\Psi}_\Lambda(\vec{r}, \tau) \) in the interaction picture with respect to \( \hat{\mathcal{H}}_\perp \) in Eq. (8), written in the single particle basis set \( \{ | \Psi_k \rangle, k \in \mathbb{N} \} \), turns into

\[ \hat{\Psi}_\perp(\vec{r}, \tau) = \hat{U}_\perp(\tau) \hat{\Psi}(\vec{r}) \hat{U}_\perp(\tau) = \sum_{k \neq 0} \Psi_k(\vec{r}) \hat{a}_k \exp \left[ -\frac{i \epsilon_k \tau}{\hbar} \right] \]  

Any two point correlation function of products of two non-condensate fields in Eqs. (A1) and (A2) can thus be written in terms of the average occupation of different non-condensate single particle states \( | \Psi_k \rangle \in \mathcal{F}_\perp \), e.g.:

\[ \langle \hat{\Psi}^{\dagger}_\Lambda(\vec{r}, \tau) \hat{\Psi}_\Lambda(\vec{r}', 0) \rangle_{\mathcal{F}_\perp} = \sum_{k \neq 0} \Psi_k(\vec{r}) \Psi_k(\vec{r}') \langle N_k \rangle (N - N_0, T) \exp \left[ -\frac{i \epsilon_k \tau}{\hbar} \right] \]  

where we used that \( \langle \hat{a}_k^{\dagger} \hat{a}_l \rangle_{\mathcal{F}_\perp}^{(N-N_0)} = \langle \hat{a}_k^{\dagger} \hat{a}_l \rangle_{\mathcal{F}_\perp}^{(N-N_0)} \delta_{kl} = \langle N_k \rangle (N - N_0, T) \delta_{kl} \). The function

\[ \langle N_k \rangle (N - N_0, T) = \text{Tr}_{\mathcal{F}_\perp} \left\{ \hat{a}_k^{\dagger} \hat{a}_k \hat{Q}_{N-N_0} \frac{e^{-\beta \hat{\mathcal{H}}_\perp}}{Z_{\perp}(N - N_0)} \hat{Q}_{N-N_0} \right\} \]

describes the average many particle occupation of a non-condensate single particle state \( | \Psi_k \rangle \), given that \( (N - N_0) \) particles are in the non-condensate, and given a temperature \( T \) of the external heat reservoir. For the explicit derivation of analytical expressions for the occupation numbers \( \langle N_k \rangle (N - N_0, T) \), see appendix [B] Anti-normally ordered products of two point correlation functions of two non-condensate fields in the interaction picture arising in Eqs. (A1) and (A2) can be obtained correspondingly, turning into

\[ \langle \hat{\Psi}_\perp(\vec{r}, \tau) \hat{\Psi}^{\dagger}_\perp(\vec{r}', 0) \rangle_{\mathcal{F}_\perp}^{(N-N_0)} = \sum_{k \neq 0} \Psi_k(\vec{r}) \Psi_k(\vec{r}') \langle N_k \rangle (N - N_0, T) + 1 \exp \left[ \frac{i \epsilon_k \tau}{\hbar} \right] \],

where we have used that

\[ \langle \hat{a}_k \hat{a}_k^{\dagger} \rangle_{\mathcal{F}_\perp}^{(N-N_0)} = \langle N_k \rangle (N - N_0, T) + 1 \delta_{kl} \]
feeding rates in Eq. (37).

Integration of processes:

\[
G^{(+)}(\vec{r}, \vec{r}^\prime, N - N_0, T, \tau) = 2 \sum_{k,l,m \neq 0} \Psi_k^*(\vec{r}) \Psi_k(\vec{r}^\prime) \Psi_l^*(\vec{r}) \Psi_l(\vec{r}^\prime) \Psi_m^*(\vec{r}) \Psi_m(\vec{r}^\prime) \langle (N_k)(N - N_0, T) + 1 \rangle \times \exp \left[ \frac{-i (\epsilon_k - \epsilon_l - \epsilon_m) \tau}{\hbar} \right] + 
\]

\[
+ 4 \sum_{k,l,m \neq 0} |\Psi_k(\vec{r})|^2 |\Psi_l^*(\vec{r})| |\Psi_l(\vec{r}^\prime)|^2 |\Psi_m(\vec{r}^\prime)|^2 \langle N_k \rangle (N - N_0, T) \times \exp \left[ \frac{i \epsilon_l \tau}{\hbar} \right].
\]

Next, we decompose the correlation functions for pair events, \( G^{(\pm)}(\vec{r}, \vec{r}^\prime, N - N_0, T, \tau) \). Using Eq. (A8) [A9], the normally ordered correlation function for pair events is given by:

\[
G^{(\pm)}(\vec{r}, \vec{r}^\prime, N - N_0, T, \tau) = 2 \sum_{k,l,m \neq 0} \Psi_k^*(\vec{r}) \Psi_k(\vec{r}^\prime) \Psi_l^*(\vec{r}) \Psi_l(\vec{r}^\prime) \Psi_m^*(\vec{r}) \Psi_m(\vec{r}^\prime) \langle (N_k)(N - N_0, T) \rangle \exp \left[ \frac{-i (\epsilon_k - \epsilon_l - \epsilon_m) \tau}{\hbar} \right] + 
\]

\[
+ 4 \sum_{k,l,m \neq 0} |\Psi_k(\vec{r})|^2 |\Psi_l^*(\vec{r})| |\Psi_l(\vec{r}^\prime)|^2 |\Psi_m(\vec{r}^\prime)|^2 \langle N_k \rangle (N - N_0, T) \times \exp \left[ \frac{i \epsilon_l \tau}{\hbar} \right].
\]

The anti-normally ordered pair correlation function \( G^{(-)}(\vec{r}, \vec{r}^\prime, N - N_0, T, \tau) \) can be decomposed similarly:

\[
G^{(-)}(\vec{r}, \vec{r}^\prime, N - N_0, T, \tau) = \langle \Psi_l^+(\vec{r}, \tau) \Psi_l^+(\vec{r}^\prime, \tau) \Psi_k^+(\vec{r}^\prime, 0) \Psi_k^+(\vec{r}, 0) \rangle^{(N - N_0)}_{F_{\perp}} = 
\]

\[
2 \langle \Psi_l^+(\vec{r}, \tau) \Psi_l^+(\vec{r}^\prime, 0) \rangle^{(N - N_0)}_{F_{\perp}} \langle \Psi_k^+(\vec{r}^\prime, \tau) \Psi_k^+(\vec{r}, 0) \rangle^{(N - N_0)}_{F_{\perp}} = 
\]

\[
2 \sum_{k,l \neq 0} \Psi_k^*(\vec{r}) \Psi_k(\vec{r}^\prime) \Psi_l^*(\vec{r}) \Psi_l(\vec{r}^\prime) \langle N_k \rangle (N - N_0, T) + 1 |\langle N_l \rangle (N - N_0, T) + 1 \rangle \exp \left[ \frac{-i (\epsilon_k + \epsilon_l) \tau}{\hbar} \right].
\]

which again, after multiplication with \( \Psi_0^*(\vec{r}) \) \( \Psi_0^*(\vec{r}^\prime) \|^2 \exp[\pm 2i \mu_0 \tau] \) and integration over \( \tau \), turns into the pair feeding and loss rates in Eq. (A5).

Appendix B: Single particle non-condensate occupations

The state of the non-condensate in Eq. (22) allows to determine the average number of particles, \( \langle N_k \rangle = \langle N_k \rangle (N - N_0, T) \) in Eq. (A6), for each particular non-
condensate single particle mode $|\Psi_k\rangle$, given that $N_0$ particles populate the condensate mode, and consequently $(N - N_0)$ particles populate the non-condensate single particle modes. According to Eq. (A5), we hence consider the expectation value of the number operator $\hat{N}_k$ in a non-condensate state of $(N - N_0)$ particles, which leads to

$$
\langle N_k \rangle(N - N_0, T) = Z^{-1}_\perp(N - N_0) \sum_{N_k=0}^{(N-N_0)} N_k \exp \left[ -\beta \beta_k N_k \right] , \quad (B1)
$$

where $Z_\perp(N - N_0)$ is the partition function of $(N - N_0)$ indistinguishable particles in the non-condensate in Eq. (24). In terms of the partial partition sum, $Z_\perp^{(k)}(N - N_0)$ [24], which excludes the sum over one particular non-condensate single particle mode $|\Psi_k\rangle$, Eq. (B1) can be written as

$$
\langle N_k \rangle(N - N_0, T) = Z^{-1}_\perp(N - N_0 - N_k) \sum_{N_k=0}^{(N-N_0)} N_k \exp \left[ -\beta \epsilon_k N_k \right] Z^{(k)}_\perp(N - N_0 - N_k) \ , \quad (B2)
$$

For small enough $N_k$ (it suffices to start at $N_k = 1$ and to determine $Z^{(k)}_\perp(N - N_0 - N_k)$ iteratively), we can expand

$$
\ln \left[ Z^{(k)}_\perp(N - N_0 - 1) \right] \simeq \ln \left[ Z^{(k)}_\perp(N - N_0) \right] + \alpha^{(k)}_\perp(N - N_0, T) , \quad (B3)
$$

which introduces the parameter

$$
\alpha^{(k)}_\perp(N - N_0, T) = \frac{\partial \ln \left[ Z^{(k)}_\perp(N - N_0) \right]}{\partial (N - N_0)} . \quad (B4)
$$

From Eq. (B3), we hence find the recursion relation

$$
\frac{Z^{(k)}_\perp(N - N_0 - 1)}{Z^{(k)}_\perp(N - N_0)} = \exp \left[ -\alpha^{(k)}_\perp(N - N_0, T) \right] , \quad (B5)
$$

between the partial partition sums $Z^{(k)}_\perp(N - N_0)$ of $(N - N_0)$ and $Z^{(k)}_\perp(N - N_0 - 1)$ of $(N - N_0 - 1)$ non-condensate particles. Multiple iteration of Eq. (B5) hence leads to

$$
\frac{Z^{(k)}_\perp(N - N_0 - N_k)}{Z^{(k)}_\perp(N - N_0)} = \exp \left[ -N_k \alpha^{(k)}_\perp(N - N_0, T) \right] , \quad (B6)
$$

and Eq. (B2) turns into

$$
\langle N_k \rangle(N - N_0, T) = \frac{Z^{(k)}_\perp(N - N_0)}{Z_\perp(N - N_0)} \sum_{N_k=0}^{(N-N_0)} N_k \exp \left[ -\left( \beta \epsilon_k + \alpha^{(k)}_\perp(N - N_0, T) \right) N_k \right] . \quad (B7)
$$
It remains to apply the same procedure to the partition function $Z_{\perp}(N-N_0)$. Using the decomposition in Eq. (B7) and applying Eq. (124), one finds that

$$Z_{\perp}(N-N_0) = Z_{\perp}^{(k)}(N-N_0) \sum_{N_k=0}^{(N-N_0)} \exp \left[ -\left( \beta \epsilon_k + \alpha_{\perp}^{(k)}(N-N_0,T) \right) N_k \right].$$  \hspace{1cm} (B8)

Setting Eq. (B8) into Eq. (B1), the expectation value of particle number occupations of a particular non-condensate single particle state $|\Psi_k\rangle$, given that $(N-N_0)$ particles are in the non-condensate, is given by

$$\langle N_k \rangle_{(N-N_0),T} = \frac{1}{\exp \left[ \beta \epsilon_k + \alpha_{\perp}^{(k)}(N-N_0,T) \right] - 1}.$$  \hspace{1cm} (B9)

We now use that the parameter $\alpha_{\perp}^{(k)}(N-N_0,T)$ is approximately independent of the state $k$ [24], i.e. the change of non-condensate single particle number occupations during condensation is described by one single parameter, $\alpha^{(k)} \approx \alpha_{\perp}(N-N_0,T)$, which is determined by the constraint of particle number conservation, as spelled out by the implicit equation

$$\sum_{k\neq 0} \langle N_k \rangle_{(N-N_0),T} = \sum_{k\neq 0} \frac{1}{\exp \left[ \beta \epsilon_k + \alpha_{\perp}(N-N_0,T) \right] - 1} = (N-N_0).$$  \hspace{1cm} (B10)

As evident from Eq. (B1), and the fact that each subspace of $(N-N_0)$ particles is in a thermal state, the parameter $\alpha_{\perp}(N-N_0,T)$ can be interpreted as the ratio of the non-condensate chemical potential for a state of $(N-N_0)$ atoms, to the thermal energy $\beta^{-1}$. Hence, from the definition in Eq. (124), we see that $\alpha_{\perp}(N-N_0,T)$ is, upon a constant, nothing more than the derivative of the Helmholtz free energy, $\alpha_{\perp}(N-N_0,T) = -\beta^{-1}\ln Z_{\perp}(N-N_0)$ of the $(N-N_0)$ particles in the non-condensate [25], related to $\mu_{\perp}(N-N_0,T)$ by

$$\alpha_{\perp}(N-N_0,T) = -\beta \mu_{\perp}(N-N_0,T),$$  \hspace{1cm} (B11)

which introduces the non-condensate chemical potential $\mu_{\perp}(N-N_0,T)$.

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