Dynamics of thermal Bose fields in the classical limit

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We develop an approximate formalism suitable for performing simulations of the thermal dynamics of interacting Bose gases. The method is based on the observation that when the lowest energy modes of the Bose field operator are highly occupied, they may be treated classically to a good approximation. We derive a finite temperature Gross-Pitaevskii equation for these modes which is coupled to an effective reservoir described by quantum kinetic theory. We discuss each of the terms that arise in this Gross-Pitaevskii equation, and their relevance to experimental systems. We then describe a simpler projected Gross-Pitaevskii equation that may be useful in simulating thermal Bose condensates. This classical method could be applied to other Bose fields.

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I. INTRODUCTION

The achievement of Bose-Einstein condensation (BEC) in a dilute gas offers the possibility of studying the dynamics of a quantum field in the laboratory. In principle it presents an opportunity to directly compare computational predictions with experimental results; however carrying out dynamical calculations of thermal quantum fields is an extremely difficult problem that generally requires severe approximations to be made.

The most successful finite temperature theories of BEC are based on second-order perturbation theory, and are limited to the case of thermal equilibrium away from the region of critical fluctuations. These theories have allowed the accurate determination from first principles of quantities such as excitation frequencies and damping rates of Bose-condensed systems. However, their extension to dynamical situations is computationally difficult.

At very low temperatures when most of the atoms are in the condensate, the Gross-Pitaevskii equation (GPE) has proved remarkably successful in numerically modelling BEC experiments. The time-dependent GPE has the form

\[ i\hbar \frac{\partial \psi(x)}{\partial t} = \hat{H}_{sp}\psi(x) + U_0|\psi(x)|^2\psi(x), \]

where \( U_0 = 4\pi\hbar^2a/m \) is the effective interaction strength at low momenta, \( a \) is the s-wave scattering length, and \( m \) is the particle mass. \( \hat{H}_{sp} \) is the single particle Hamiltonian

\[ \hat{H}_{sp} = -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}(x), \]

where \( V_{\text{trap}}(x) \) is the external confining potential of the system. The GPE can be derived by a number of different approaches (e.g. a number-conserving approach), but a direct method is to take the mean mean value of the equation of motion for the Bose field operator and assume that the quantum fluctuations can be neglected. This procedure effectively assumes that the field is well approximated by a coherent state.

It has been argued that the GPE can also describe the dynamics of a Bose-Einstein condensate at finite temperature for the reason that in the limit that all the low-lying modes of the system are highly occupied (\( N_k \gg 1 \)), the classical fluctuations of the field operator \( \hat{\Psi}(x,t) \) will be much larger than the quantum fluctuations. It is therefore reasonable to neglect the quantum fluctuations, and thus all highly-occupied modes may be well approximated by a coherent wave function. This is analogous to the situation in laser physics where the highly occupied laser modes can be well described by classical equations. Despite this proposal appearing in the literature in 1991, very few numerical calculations have been performed. The first was by Damle et al., who calculated the approach to equilibrium of a near-ideal superfluid using the GPE. Subsequently, Marshall et al. performed two-dimensional simulations of evaporative cooling of a thermal Bose field in a trap. More recently, papers by Stoof and Bijlsma and Sinatra et al. have used classical methods in dynamical calculations of thermal one-dimensional Bose-Einstein condensates. Goral et al. have performed dynamical calculations that treat several modes of a 3D homogeneous Bose gas classically. Their method, while not specifically employing the GPE, is similar to the approach we suggest here and for which we have presented our own numerical results in reference.
quantum field equations have also been successful in the calculation of the dynamics of the electroweak phase transition [18].

The major advantage of using the GPE to describe thermal dynamics is simply that, while it is still a major computational task, it is possible to numerically solve the equation for realistic systems in a reasonable amount of time. In addition, the GPE is non-perturbative and it should be possible to study the region of the BEC phase transition, where perturbation theory often fails.

There are, however, a number of problems associated with the use of the GPE to represent the entire Bose field at finite temperature. It is a classical equation, and so in equilibrium it will satisfy the equipartition theorem—all modes of the system will have an occupation of \( N_k = k_B T / \epsilon_k \). Thus, if we couple the GPE to a heat bath and numerically solve the equation with infinite accuracy, we will observe an ultra-violet catastrophe. Also, we can see that the higher the energy of any given mode, the lower its occupation will be in equilibrium and at a sufficiently high energy the criterion \( N_k \gg 1 \) will no longer be satisfied. For these low occupation modes a form of kinetic equation is more appropriate. The solution to both of these problems is to introduce a cutoff in the modes represented by the GPE.

In this paper we develop an approximate formalism in which the low-lying modes of the system are described non-perturbatively by the GPE, coupled to a thermal bath described by a quantum Boltzmann equation. We derive a finite temperature Gross-Pitaevskii equation (FTGPE), and discuss the terms that couple the part of the field operator represented by a coherent wave function to the thermal bath. In particular we show how a description of loss via elastic collisions arises naturally in the formalism.

Several other authors have developed formalisms for non-equilibrium dynamics using quite different theoretical methods—we mention Gardiner and Zoller [19–21], Proukakis et al. [22], Stoof [23,24], Zaremba et al. [25], Walser et al. [26], and finally Sinatra et al. [27]. The work we present here has elements in common with several of these. In particular, the average of the quantum Langevin equation written down in the formalism of Stoof [23,24] would correspond to the FTGPE we derive in section IV.

This paper is organized as follows. In section II we write down and discuss the Hamiltonian which is our starting point. In section III we outline how we decompose the field operator into a coherent and incoherent region, and in section IV we derive a finite temperature Gross-Pitaevskii equation that forms the main result of this paper. In section V we discuss the terms that arise in the FTGPE, their relation to experiments, and their approximate form in terms of occupations numbers of incoherent region modes. We discuss a simple finite temperature equation which we call the projected GPE in section VI and finally conclude in section VII.

II. HAMILTONIAN

We begin with the usual second quantized many-body Hamiltonian for a system of identical, structureless bosons with pair-wise interactions

\[
\hat{H} = \hat{H}_0 + \hat{H}_I,
\]

\[
\hat{H}_0 = \int d^3x \, \hat{\Psi}^\dagger(x, t) \hat{H}_{sp} \hat{\Psi}(x, t),
\]

\[
\hat{H}_I = \frac{1}{2} \int d^3x \int d^3x' \, \hat{\Psi}^\dagger(x, t) \hat{\Psi}^\dagger(x', t) V(x - x') \hat{\Psi}(x', t) \hat{\Psi}(x, t).
\]

The non-interacting part of the Hamiltonian, \( \hat{H}_0 \), corresponds to an ideal gas and can be diagonalized exactly by the eigenvectors of \( \hat{H}_{sp} \). The quantity \( \hat{H}_I \) describes two-body interactions via the interatomic potential \( V(x) \). The field operator \( \hat{\Psi}(x, t) \) annihilates a single boson of mass \( m \) at position \( x \) and time \( t \), and obeys the equal-time commutation relations

\[
\left[ \hat{\Psi}(x, t), \hat{\Psi}^\dagger(x', t) \right] = \left[ \hat{\Psi}^\dagger(x, t), \hat{\Psi}^\dagger(x', t) \right] = 0,
\]

\[
\left[ \hat{\Psi}(x, t), \hat{\Psi}^\dagger(x', t) \right] = \delta(x - x').
\]

The field operator is normalised such that

\[
\int d^3x \, \hat{\Psi}^\dagger(x, t) \hat{\Psi}(x, t) = \hat{N},
\]

where \( \hat{N} \) is the particle number operator of the system.
A. Basis set representation

It is useful to expand the field operator on a basis set

\[ \hat{\Psi}(x, t) = \sum_n \hat{a}_n(t) \phi_n(x), \]  

where \( \phi_n(x) \) is a mode function, and \( \hat{a}_n(t) \) annihilates a particle in mode \( n \) at time \( t \). These operators obey the equal-time commutation relations

\[ [\hat{a}_m, \hat{a}_n] = 0, \]

\[ [\hat{a}_m, \hat{a}_n^\dagger] = \delta_{mn}, \]

where we have dropped the time labels for clarity. If we substitute equation (9) into the Hamiltonian (3) and take the set \( \{ \phi_n \} \) to be the eigenvectors of \( \hat{H}_{sp} \), we find

\[ \hat{H} = \sum_n \hbar \omega_n \hat{a}_n^\dagger \hat{a}_n + \frac{1}{2} \sum_{pqmn} \langle pq | V | mn \rangle \hat{a}_p^\dagger \hat{a}_q \hat{a}_m \hat{a}_n, \]

where we have defined the symmetrized matrix element

\[ \langle pq | V | mn \rangle = \frac{1}{2} \int d^3x \int d^3x' \phi_p^*(x) \phi_q^*(x') V(x - x') \phi_m(x') \phi_n(x), \]

\[ + \frac{1}{2} \int d^3x \int d^3x' \phi_p^*(x) \phi_q^*(x') V(x - x') \phi_n(x') \phi_m(x). \]

whose use significantly reduces the length of the equations of motion we later derive. Equation (13) represents both direct and exchange collisions, which are physically indistinguishable for identical bosons.

The Heisenberg equation of motion for the individual mode operator \( \hat{a}_p \) is therefore

\[ i\hbar \frac{d\hat{a}_p}{dt} = \hbar \omega_p \hat{a}_p + \sum_{qmn} \langle pq | V | mn \rangle \hat{a}_q^\dagger \hat{a}_m \hat{a}_n, \]

and we can define slowly-varying operators

\[ \hat{a}_p = \hat{a}_p e^{i\omega_p t}, \]

so that the equation of motion for the annihilation operator becomes

\[ i\hbar \frac{d\hat{a}_p}{dt} = \sum_{qmn} \langle pq | V | mn \rangle \hat{a}_q^\dagger \hat{a}_m \hat{a}_n e^{i(\omega_p + \omega_q - \omega_m - \omega_n)t}. \]

B. Effective low-energy Hamiltonian

The Hamiltonian described above contains spatial integrals over the bare interatomic potential between two atoms, \( V(x) \). However, it is well-known that at low temperatures the scattering of neutral atoms in three dimensions can be described by the \( s \)-wave scattering length \( a \). This parameter is often introduced into the theory by replacing the real interatomic potential by the contact potential

\[ V(x - x') \rightarrow U_0 \delta(x - x'), \quad U_0 = \frac{4\pi \hbar^2 a}{m}. \]

The interaction strength \( U_0 \) can be shown to arise from the increase in kinetic energy of a two-particle wave function, when an excluded region of radius \( a \) is introduced corresponding to a hard sphere interaction potential \( U_0 \). The contact potential approximation, however, can lead to ultraviolet divergences in theories of BEC if it is simply
substituted into the Hamiltonian (3). This is not surprising, as the delta-function potential can scatter high-energy atoms just as effectively as low-energy atoms. Physically this is unrealistic, as momentum transfer between atoms will vanish at high momenta \((k > 1/\alpha)\). The contact potential is a low-energy approximation, and care must be taken when summing over high energy states.

The ultraviolet renormalization of the theory can be achieved by introducing the two-body T-matrix into the Hamiltonian, resulting in a high-momentum cutoff \(K\) to the the states considered \[4\]. This procedure is valid as long as the condition \(K\alpha \ll 1\) is satisfied for the entire gas. We will consider the issue of ultraviolet divergence further in section \[V A\].

### III. Projection Operator

The aim of this paper is to represent the highly occupied modes of the field operator \(\hat{\Psi}(x)\) by a wave function \(\psi(x)\). It is reasonable to neglect the quantum fluctuations of these modes, and therefore \(\psi(x)\) represents a classical field. To achieve our goal we divide our representation of the field operator into two separate regions. The first, in which the condition \(N_k \gg 1\) is satisfied, we call the coherent region \(C\). The other which contains the remainder of the field, is denoted the incoherent region \(I\).

We define the coherent region projection operator

\[
\hat{P} = \sum_{\nu \in C} |\nu\rangle\langle\nu|,
\]

where the region \(C\) is determined by the requirement that \(\langle a_\nu^\dagger a_\nu \rangle \gg 1\), and the set \(|\nu\rangle\) defines some basis in which the field operator is approximately diagonal near the cutoff. This condition is imposed simply so that in equilibrium the quantity \(\langle a_\nu^\dagger a_\nu \rangle\) has a well-defined average at the boundary of \(C\) that can be interpreted as a mode occupation number. The position of the cutoff is a choice that must be made before any calculation, and is required for the construction of the initial wave function.

Operating on the field operator with \(\hat{P}\) gives

\[
\hat{P}\hat{\Psi}(x) = \sum_{\nu \in C} \phi_\nu(x) \int d^3x' \phi_\nu^*(x') \hat{\Psi}(x'),
\]

\[
= \sum_{\nu \in C} \hat{a}_\nu \phi_\nu(x),
\]

\[
\equiv \hat{\psi}(x).
\]

such that \(\hat{\psi}(x)\) is the field operator for the coherent region. We now introduce the orthogonal projector \(\hat{Q} = \hat{1} - \hat{P}\) and define

\[
\hat{Q}\hat{\Psi}(x) = \sum_{k \notin C} \hat{a}_k \phi_k(x),
\]

\[
\equiv \hat{\eta}(x).
\]

The quantity \(\hat{\eta}(x)\) is the field operator for the incoherent region and represents an effective thermal bath. Quantum fluctuations are important for these modes—in fact we will later assume that \(\langle \hat{a}_k \rangle \approx 0\) for the large majority of \(k \notin C\).

The full field operator is

\[
\hat{\Psi}(x) = [\hat{P} + \hat{Q}]\hat{\Psi}(x),
\]

\[
= \hat{\psi}(x) + \hat{\eta}(x),
\]

\[
= \sum_{\nu \in C} \hat{a}_\nu \phi_\nu(x) + \sum_{k \notin C} \hat{a}_k \phi_k(x),
\]

where we indicate indices within \(C\) by Greek subscripts, and outside \(C\) by Roman subscripts. We shall follow this convention throughout the body of this paper.

As an example of the size of the regions we consider a \(^{87}\)Rb gas in a harmonic trap with a geometric mean trap frequency of \(\bar{\omega} = 2\pi \times 100\) Hz. For a condensate of \(10^6\) atoms at a temperature of 640 nK (and hence a total number of trapped atoms of about \(5 \times 10^6\)), we find that a quantum level with energy \(\epsilon - \mu \approx 15\hbar\bar{\omega}\) has a mean occupation of \(\langle N \rangle \approx 10\), so this would be an appropriate boundary for the coherent region. In comparison, the remainder of the gas spans energies up to about \(E = 1500\hbar\bar{\omega}\), meaning that the incoherent region contains many more quantum states and is much larger than the coherent region.
IV. EQUATIONS OF MOTION

A. Hamiltonian

We now substitute the decomposition of equation (21) into the Hamiltonian (3). We assume for \( k \notin C \) that \( \phi_k(x) \) is an eigenstate of \( \hat{H}_{sp} \), and so \( \hat{H}_0 \) simplifies to

\[
\hat{H}_0 = \sum_{\alpha\beta} \langle \alpha | \hat{H}_{sp} | \beta \rangle \hat{a}_\alpha \hat{a}_\beta + \hbar \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k.
\]  

(22)

For the interaction part of the Hamiltonian we have

\[
\hat{H}_I = \frac{1}{2} \sum_{\alpha\beta\chi\sigma} \langle \alpha\beta | V | \chi\sigma \rangle \hat{a}_\alpha \hat{a}_\beta \hat{a}_\chi \hat{a}_\sigma
\]  

(23a)

\[
+ \sum_{\alpha\beta\chi n} \langle \alpha\beta | V | \chi n \rangle \hat{a}_\alpha \hat{a}_\beta \hat{a}_n \hat{a}_n + h.c.
\]  

(23b)

\[
+ \frac{1}{2} \sum_{\alpha\beta mn} \langle \alpha\beta | V | mn \rangle \hat{a}_\alpha \hat{a}_\beta \hat{a}_m \hat{a}_n + h.c.
\]  

(23c)

\[
+ 2 \sum_{\alpha j\chi n} \langle \alpha j | V | \chi n \rangle \hat{a}_\alpha \hat{a}_j \hat{a}_n \hat{a}_n
\]  

(23d)

\[
+ 2 \sum_{\alpha j mn} \langle \alpha j | V | mn \rangle \hat{a}_\alpha \hat{a}_j \hat{a}_m \hat{a}_n + h.c.
\]  

(23e)

\[
+ \frac{1}{2} \sum_{kj mn} \langle kj | V | mn \rangle \hat{a}_k \hat{a}_j \hat{a}_m \hat{a}_n.
\]  

(23f)

where the symmetrized matrix element \( \langle kj | V | mn \rangle \) is defined in equation (13), and \( h.c. \) stands for hermitian conjugate. Using (22) and (23) we now derive the Heisenberg equations of motion for the operators in each region.

B. Coherent region

The evolution of a mode of the coherent part of the field operator is given by

\[
i\hbar \frac{d\hat{a}_\alpha}{dt} = \sum_{\beta} \langle \alpha | \hat{H}_{sp} | \beta \rangle \hat{a}_\beta
\]  

(24a)

\[
+ \sum_{\beta\chi\sigma} \langle \alpha\beta | V | \chi\sigma \rangle \hat{a}_\alpha \hat{a}_\beta \hat{a}_\chi \hat{a}_\sigma
\]  

(24b)

\[
+ \sum_{\alpha q\chi\sigma} \langle \alpha q | V | \chi\sigma \rangle \hat{a}_\alpha \hat{a}_q \hat{a}_\chi \hat{a}_\sigma
\]  

(24c)

\[
+ 2 \sum_{\beta mn} \langle \alpha\beta | V | mn \rangle \hat{a}_\alpha \hat{a}_\beta \hat{a}_m \hat{a}_n
\]  

(24d)

\[
+ \sum_{\beta mn} \langle \alpha\beta | V | mn \rangle \hat{a}_\alpha \hat{a}_m \hat{a}_n
\]  

(24e)

\[
+ 2 \sum_{\alpha q\sigma} \langle \alpha q | V | m\sigma \rangle \hat{a}_\alpha \hat{a}_q \hat{a}_m \hat{a}_\sigma
\]  

(24f)

\[
+ \sum_{qmn} \langle \alpha q | V | mn \rangle \hat{a}_q \hat{a}_m \hat{a}_n.
\]  

(24g)

in which the coupling to the incoherent region is made explicit. We now begin to introduce our approximations. The condition that a mode is in the coherent region \( C \) is that the population \( \langle \hat{a}_\nu^\dagger \hat{a}_\nu \rangle \gg 1 \), which allows us to neglect the
FIG. 1. Representation of the degree of coherence in the different regions of the Bose field. The shading indicates schematically the coherence of the field. The classical region of the field in indicated by $C$, and the incoherent region by $I$. The states in $I$ near the boundary of $C$ will be partially coherent.

Quantum fluctuations of the projected field operator $\hat{\psi}(x)$. Thus we assume that the region $C$ is well approximated by a mode function given by the mean value

$$\psi(x) \equiv \langle \hat{\psi}(x) \rangle,$$

and we can expand the wave function on our basis functions as

$$\psi(x) = \sum_{\nu \in C} \langle \hat{a}_\nu \rangle \phi_{\nu}(x),$$

$$= \sum_{\nu \in C} c_\nu \phi_{\nu}(x).$$

We obtain the finite temperature GPE by taking the mean value of equation (24). In this procedure we expand the coherent region operators as $\hat{a}_\nu = c_\nu + \hat{\delta}_\nu$, and then neglect the terms involving the quantum fluctuations $\hat{\delta}_\nu$. A typical term simplifies as follows

$$\langle \sum_{q \chi \sigma} \langle \alpha q | V | \chi \sigma \rangle \hat{a}_q^\dagger \hat{a}_\chi \hat{a}_\sigma \rangle \rightarrow \sum_{q \chi \sigma} \langle \alpha q | V | \chi \sigma \rangle \langle \hat{a}_q^\dagger \rangle c_\chi c_\sigma$$

$$= \sum_q \langle \alpha q | V | \psi \psi \rangle \langle \hat{a}_q^\dagger \rangle,$$

where the matrix element is time dependent as the wave function $\psi$ is not a stationary state.

The incoherent region $I$ is, for the most part, best represented by number states. However, this is not always the case. In particular the states within $I$ but near the boundary of the two regions will be partially coherent, as is illustrated in figure 1. The expectation value $\langle \hat{a}_q^\dagger \rangle$ in this transitional region will not be zero, and so terms such as (27) are retained in our equations. This is different from other mean field theories in which all coherence is absorbed into the GPE. In systems that are partially condensed, however, the effect of these terms will be small, as the transition region will be narrow compared to the full width of the incoherent region.

The full equation of motion for a coherent region mode obtained by taking the mean value of all terms in equation (24) is

$$i\hbar \frac{dc_\alpha}{dt} = \langle \alpha | \hat{H}_{sp} | \psi \rangle$$

$$+ \langle \alpha \psi | V | \psi \psi \rangle$$

$$+ \sum_q \langle \alpha q | V | \psi \psi \rangle \langle \hat{a}_q^\dagger \rangle$$

$$+ 2 \sum_m \langle \alpha \psi | m \psi \rangle \langle \hat{a}_m \rangle$$

$$= \langle \alpha | \hat{H}_{sp} | \psi \rangle$$

$$+ \langle \alpha \psi | V | \psi \psi \rangle$$

$$+ \sum_q \langle \alpha q | V | \psi \psi \rangle \langle \hat{a}_q^\dagger \rangle$$

$$+ 2 \sum_m \langle \alpha \psi | m \psi \rangle \langle \hat{a}_m \rangle.$$
+ \sum_{mn} \langle \alpha | V | mn \rangle \langle \hat{a}_m \hat{a}_n \rangle 
\tag{28c}
\hline
+ 2 \sum_{qm} \langle \alpha | V | m\bar{\psi} \rangle \langle \hat{a}_q \hat{a}_m \rangle 
\tag{28f}
\hline
+ \sum_{qm} \langle \alpha | V | mn \rangle \langle \hat{a}_q \hat{a}_m \hat{a}_\alpha \rangle. 
\tag{28g}
\end{align}

We can convert this expression to the spatial representation by applying the operation \( \sum_{\alpha \in C} \langle \alpha | \rangle \langle \alpha | \) to both sides. Using the contact potential approximation and recognizing \( \sum_{\alpha \in C} \langle \alpha | \rangle \langle \alpha | \) as our projector of \( \hat{\psi}(x) \), this procedure results in an equation we call the finite temperature Gross-Pitaevskii equation (FTGPE)

\[
\begin{align}
\hat{h} \frac{\partial \hat{\psi}(x)}{\partial t} &= \hat{H}_{sp} \hat{\psi}(x) + U_0 \hat{P} \left\{ |\psi(x)|^2 \psi(x) \right\} 
+ U_0 \hat{P} \left\{ 2|\psi(x)|^2 \langle \hat{\eta}(x) \rangle + \psi(x)^2 \langle \hat{\eta}^\dagger(x) \rangle \right\} 
+ U_0 \hat{P} \left\{ \psi^* (x) \langle \hat{\eta}(x) \rangle \hat{\eta}(x) \rangle + 2\psi(x) \langle \hat{\eta}^\dagger(x) \rangle \psi(x) \rangle \right\} 
+ U_0 \hat{P} \left\{ \langle \hat{\eta}^\dagger(x) \rangle \hat{\eta}(x) \rangle \hat{\eta}(x) \rangle \right\},
\end{align}
\]

where \( \hat{\eta}(x) \) is defined by \( \langle x | \rangle \). The FTGPE constitutes the main result of this work, and the remainder of this paper is devoted to discussing the physics of this equation.

The only approximation that has been made in the derivation of the FTGPE is that the modes it represents must be highly occupied. No perturbative techniques have been used, and therefore the equation should be valid as long as the condition \( N_k \gg 1 \) is satisfied. As a corollary, we expect the FTGPE could be used to study the region of the phase transition in certain circumstances.

The FTGPE describes the full dynamics of the region \( C \) and its coupling to an effective thermal bath \( \hat{\eta}(x) \). The initial wave function for the coherent region will be made up of a sum over a basis with amplitudes with random phases as is appropriate for a thermal system \( \langle x | \rangle \). Despite the fact that the FTGPE is completely unitary and reversible, we expect that it will evolve general initial states of \( \psi(x) \) to an equilibrium determined by the temperature and chemical potential of the field \( \hat{\eta}(x) \). This is because deterministic nonlinear systems exhibit chaotic, and hence ergodic, behavior if more than a few degrees of freedom are present \( \langle x | \rangle \). In fact, we have shown in reference \( \langle x | \rangle \) that a simplified form of the FTGPE that we discuss in section \( \langle x | \rangle \) can indeed describe evolution towards equilibrium.

Each of the lines of the FTGPE represents collision processes involving a different number of coherent region states. We describe them briefly here and then discuss them in more detail in section \( \langle x | \rangle \).

The terms on the first line of the FTGPE \( \langle x | \rangle \) represent purely coherent region dynamics. The first term describes the free evolution of the wave function \( \psi \), while the second represents evolution due to two particles from \( C \) colliding, with both particles remaining inside the coherent region.

The terms on the second line of the FTGPE \( \langle x | \rangle \) we refer to as the linear terms. These describe two coherent atoms interacting, resulting in one remaining in \( C \) and one escaping to the incoherent region (and the reverse process) and are depicted in figure \( \langle x | \rangle \). These are stimulated processes as the terms contain three coherent region labels, and they result in the transfer of some coherence to the bath \( \hat{\eta}(x) \) (see figure \( \langle x | \rangle \)). However, because the coherent region is much smaller than the incoherent region these terms can often be neglected in comparison with the third and fourth lines.

The third line of the FTGPE \( \langle x | \rangle \) will usually be more important than the second. The first term, which we call the anomalous term, represents the collision of two coherent atoms with two incoherent atoms resulting as in figure \( \langle x | \rangle \). If the region \( C \) represents only a single condensate in thermal equilibrium then this term cannot conserve energy and therefore it cannot describe real processes.\(^1\) However, it can describe \textit{virtual} processes and thus contributes to the appearance of both the two-body and many-body \( T \)-matrices.

The second term of the third line of the FTGPE \( \langle x | \rangle \) represents a coherent atom colliding with an incoherent atom, with one atom remaining in each region after the interaction as in figure \( \langle x | \rangle \). In equilibrium this process represents the mean field of the incoherent region acting on \( C \), and can be added to the \( |\psi(x)|^2 \) term of \( \langle x | \rangle \). Away from equilibrium this term also describes \textit{scattering} processes, identical to those described in the model of condensate growth developed in references \( \langle x | \rangle \).

\(^1\)When the coherent region is made up of two or more condensates then the first term of \( \langle x | \rangle \) can describe real processes as we discuss in section \( \langle x | \rangle \).
Finally the fourth line (29d) represents the collision of two incoherent atoms in which one is transferred to the coherent region $C$ as depicted in figure 2(d). This is the growth process described in references [30,31], and is the main contribution to the transfer of population between the coherent and incoherent regions.

C. Incoherent region

The coherence of the majority of levels outside of $C$ is negligible, and therefore most of the incoherent region is approximately diagonal in the number state representation. The energy of the quantum levels is large enough that the mean field of the wave function $\psi$ does not significantly affect this region, and so we assume that $H_I$ is a small perturbation to $H_0$. Therefore quantum kinetic theory can accurately describe the evolution of the majority of this part of the quantum field, with the appropriate modifications to treat the coupling to the coherent region.

We can derive an equation of motion for the incoherent region using similar techniques to those used in the derivation of the quantum Boltzmann equation (QBE) and employing two major approximations—the random phase approximation (RPA) and Wick’s theorem [32]. We demonstrate this approach in appendix A where we derive QBE from the field theory equations. We also use these methods to simplify the thermal terms of the FTGPE as we discuss in the next section. The kinetic equation for the incoherent region is not the main topic of this paper; however, for completeness we write it down and discuss the terms that arise in appendix D.

V. DETAILED ANALYSIS OF THE COUPLING TERMS OF THE FTGPE

In this section we interpret in detail the meaning of, and find expressions for, the terms involving mean values of combinations of the bath operator $\hat{\eta}(x)$ on the right-hand side of the FTGPE, equation (29). As the incoherent region is best represented by the number occupation of the quantum levels, it is appropriate to express these mean values in terms of the occupation numbers and to do so we are guided by kinetic theory.
Expressions are required for the quantities \( \langle \hat{\eta} \rangle, \langle \hat{\eta}^\dagger \rangle, \langle \hat{\eta}\hat{\eta} \rangle, \) and \( \langle \hat{\eta}^\dagger\hat{\eta} \rangle \). These can be derived from the equation of motion for the corresponding combinations of creation and annihilation operators for the incoherent region. The equations we begin with are rather long, and we write them out fully in appendix \( \text{A} \).

We then follow the general procedure used to derive the QBE (see appendix \( \text{A} \)). First we approximately integrate the starting equations for the combinations of creation and annihilation operators, before taking the mean value and employing Wick’s theorem and the RPA to simplify the resulting terms such that they depend explicitly on populations \( n_p = \langle \hat{a}_p^\dagger\hat{a}_p \rangle \). These expressions are then substituted back into \( \langle \hat{\eta} \rangle, \langle \hat{\eta}^\dagger \rangle, \) etc, and then into the FTGPE. Each of the terms requires slightly different treatment, and we provide key details in the following subsections.

A. The linear terms

The two terms involving \( \langle \hat{\eta}(x) \rangle \) or \( \langle \hat{\eta}^\dagger(x) \rangle \) in equation \( \text{(29)} \) describe the collision of two coherent atoms, where one particle remains in the region \( C \) and the other is transferred to the incoherent region (along with the reverse process). In systems where there is significant population in the incoherent region, these terms will not be very large in comparison to the terms of higher order in \( \hat{\eta} \) due to the requirements of energy conservation and the relatively small size of the region \( C \).

Beginning with equation \( \text{(27)} \), eliminating the free evolution via the transformation \( \hat{a}_p = \hat{a}_p e^{i\omega_p t} \), taking the mean value, and using Wick’s theorem and the RPA, the only terms that survive are the principal part (the first term on the right-hand side). The relevant term in the FTGPE in basis form \( \text{(28d)} \) is thus

\[
\text{(30)}
\]

We can also drop the last term in this equation using the rotating wave approximation, as the components of \( \psi \) will be oscillating at frequencies smaller than \( \omega_p \). Thus the result is

\[
\text{(31)}
\]

In order to find an approximate solution for equation \( \text{(31)} \), we assume that we can expand the coherent region wave function in a basis that is approximately diagonal—essentially a quasiparticle basis. We write

\[
\psi(x) = \sum_\sigma \tilde{c}_\sigma \xi_\sigma(x) e^{-i\omega_\sigma t},
\]

\[
\text{(32)}
\]

where the coefficients \( \tilde{c}_\sigma = c_\sigma e^{i\omega_\sigma t} \). The equation of motion for \( \hat{a}_p \) becomes

\[
\text{(33)}
\]

where we have introduced the notation

\[
\omega_{pqmn} \equiv \omega_p + \omega_q - \omega_m - \omega_n.
\]

If the set \( \{ \xi_\sigma \} \) is a good basis for the coherent region, then the exponential term contains most of the time dependence of equation \( \text{(33)} \). We can therefore take everything else outside the integral, and use the standard result

\[
\frac{1}{x + i\epsilon} = P \left( \frac{1}{x} \right) - i\pi \delta(x),
\]

\[
\text{(35)}
\]

to find an approximate solution to equation \( \text{(33)} \). Incorporating the free evolution in the solution, we find

\[
\langle \hat{a}_p \rangle = \sum_{\beta\chi\sigma} \left\{ \frac{c_\beta^* c_\chi c_\sigma \langle p\beta|V|\chi\sigma \rangle}{\hbar\omega_{p\beta\chi\sigma}} - i\pi c_\beta^* c_\chi c_\sigma \langle p\beta|V|\chi\sigma \rangle \delta(\hbar\omega_{p\beta\chi\sigma}) \right\}.
\]

\[
\text{(36)}
\]

Since we are mainly interested in the kinetic processes that can occur, we neglect the energy shift described by the principal part (the first term on the right-hand side). The relevant term in the FTGPE in basis form \( \text{(28d)} \) is thus...
\[ \frac{\hbar}{i} \frac{dc_{n}}{dt} = -2\pi i \sum_{p\nu} (\alpha \kappa | V | p\nu) c_{p\nu}^{*} \sum_{\beta \chi} c_{\beta \chi}^{*} \langle p\beta | V | \chi \sigma \rangle \delta (\hbar \omega_{p\beta \chi \sigma}), \]

where we have expanded all the condensate wave functions as in (32). We note that equation (35) contains only coherent region amplitudes \{c_{n}\} because the processes we have included are all stimulated.

A situation where the terms discussed in this section may become important is for experiments in which a Bose condensate near \( T = 0 \) is disturbed by a sudden change in its scattering length by the use of a Feshbach resonance. Such experiments have been carried out by Donley et al. using \(^{85}\text{Rb}\) at JILA [33]. The change in scattering length causes the collision processes represented by the linear terms of the FTGPE to become energetically allowed. This description of the physics is identical to the argument by Duine and Stooft that the loss observed can be explained via elastic collisions due to an imaginary part of the many-body T-matrix [34]. We will address this issue further in a future paper.

### B. The anomalous term

We now consider the term involving \( \langle \hat{\eta} \hat{\eta} \rangle \) on the third line of the FTGPE (29c). Expanding this quantity in the incoherent region basis gives

\[ \langle \hat{\eta} \hat{\eta} \rangle = \sum_{mn} \phi_{m} \phi_{n} \langle \hat{a}_{m} \hat{a}_{n} \rangle e^{-i(\omega_{m} + \omega_{n})t}. \]

To find an expression for \( \langle \hat{a}_{m} \hat{a}_{n} \rangle \) we use the equation of motion for this quantity given as equation (32). Eliminating the free evolution, taking the mean value, expanding the coherent region wave function in the approximately diagonal basis according to equation (32), and finally using Wick’s theorem and the RPA we obtain

\[ \frac{i\hbar}{\partial t} \langle \hat{a}_{m} \hat{a}_{n} \rangle = \sum_{\chi \sigma} \hat{e}_{\chi} \hat{e}_{\sigma} \langle mn | V | \chi \sigma \rangle e^{i\omega_{m}n_{x}x_{t}} (1 + n_{m} + n_{n}) + \sum_{kj} \langle mn | V | k\sigma \rangle \langle \hat{a}_{k} \hat{a}_{j} \rangle e^{i\omega_{m}n_{x}x_{t}} (1 + n_{m} + n_{n}). \]

The first line of this equation describes two particles scattering from the coherent region into states \( m \) and \( n \). The second line would usually be ignored in the RPA, as it is of higher order than the first line. However the matrix element of this line describes particles from \((m, n)\) scattering into \((k, j)\) and then onto other states. This offers the possibility of ladder diagrams, such that the two particles could scatter back into the coherent region without interacting with a third atom. We retain this term in equation (39) as the mean value it contains is of the same form as the that on the left-hand side. Because of this, equation (39) has the form of a Lippmann-Schwinger equation in the time domain, and we will see that this is where the T-matrix appears in the formalism.

To solve this equation we start by considering the first line only, as it is the lowest order term. Once again, most of the time dependence is contained within the exponential, and so we find the solution is

\[ \langle \hat{a}_{m} \hat{a}_{n} \rangle = \sum_{\chi \sigma} \hat{e}_{\chi} \hat{e}_{\sigma} \langle mn | V | \chi \sigma \rangle (1 + n_{m} + n_{n}) e^{i\omega_{m}n_{x}x_{t}} \left( \frac{\varepsilon_{\chi} + \varepsilon_{\sigma} - \varepsilon_{m} - \varepsilon_{n}}{\varepsilon_{\chi} + \varepsilon_{\sigma} - \varepsilon_{m} - \varepsilon_{n}} \right) - i\pi \sum_{\chi \sigma} \hat{e}_{\chi} \hat{e}_{\sigma} \langle mn | V | \chi \sigma \rangle \delta (\varepsilon_{\chi} + \varepsilon_{\sigma} - \varepsilon_{m} - \varepsilon_{n}). \]

For a single condensate near thermal equilibrium, the energy delta-function can never be satisfied as it requires two low-energy, coherent atoms from within the coherent region to collide and result in two high-energy, incoherent atoms. We will return to this point later in the section. We assume that the full solution of equation (29) is of the same form as (40) but with the interaction potential \( V \) replaced by a T-matrix \( T^{\text{up}} \)

\[ \langle \hat{a}_{m} \hat{a}_{n} \rangle = \sum_{\chi \sigma} c_{\chi} c_{\sigma} \frac{\langle mn | T^{\text{up}} | \chi \sigma \rangle}{\varepsilon_{\chi} + \varepsilon_{\sigma} - \varepsilon_{m} - \varepsilon_{n}}. \]

This is a solution of equation (39) if the operator \( T^{\text{up}} \) obeys

\[ T^{\text{up}}(z) = V + \sum_{kj} V | k\sigma \rangle \frac{1 + n_{k} + n_{j}}{z - \varepsilon_{m} - \varepsilon_{n}} \langle k\sigma | T^{\text{up}} | z \rangle, \]

\[ \text{where we have set} \quad \varepsilon_{z} = \varepsilon_{\chi} + \varepsilon_{\sigma} - \Delta E \]

and

\[ \Delta E = \sum_{kj} V | k\sigma \rangle \frac{1 + n_{k} + n_{j}}{z - \varepsilon_{m} - \varepsilon_{n}} \langle k\sigma | V | z \rangle. \]
where we have identified the parameter \( z = \epsilon_x + \epsilon_\sigma + i\delta \) as the incoming energy of the two particles in the collision. The small imaginary part \( i\delta \) in this parameter generates the delta function term in \([40]\). Equation \([12]\) is the definition of a restricted many-body T-matrix as the indices \( k, j \) are defined to be outside the coherent region.

The many-body T-matrix describes collisions in the presence of a medium. It takes into account the fact that the virtual states that two particles pass through in the collision may be occupied, and the scattering rate enhanced by a factor of \((1 + n_k + n_j)\). However, as the states \( k, j \) are in the incoherent region the populations are generally small, and if we can approximate \( n_k = n_j = 0 \) we recover the definition of a restricted two-body T-matrix.

If we now substitute the solution equation \([27]\) into the basis set FTGPE equation \([28]\), we find from the terms \([28b]\) and \([28e]\)

\[
\frac{ih}{dt} \frac{dc_\alpha}{dt} = \ldots + \sum_{\chi \sigma} c_\chi c_\sigma \langle \alpha | V | \chi \sigma \rangle + \sum_{mn} \langle \alpha | V | mn \rangle \sum_{\chi \sigma} c_\chi c_\sigma \frac{\langle mn | T^{up} | \chi \sigma \rangle}{\epsilon_\chi + \epsilon_\sigma - \epsilon_m - \epsilon_n}.
\]

\[
= \sum_{\chi \sigma} c_\chi c_\sigma \langle \alpha | V | mn \rangle \sum_{\chi \sigma} \frac{\langle mn | T^{up} | \chi \sigma \rangle}{\epsilon_\chi + \epsilon_\sigma - \epsilon_m - \epsilon_n} | \chi \sigma \rangle,
\]

\[
\equiv \langle \alpha | T^{up} | \psi \rangle.
\]

Thus the anomalous term introduces the restricted T-matrix into coherent region collisions, and it is appropriate to approximate this T-matrix by a contact potential \([4]\). With this treatment of the anomalous term we have carried out the ultra-violet renormalization of the theory.

It is useful to make two additional points. First, the T-matrix that enters our equations is not the full two-body T-matrix as the sum over intermediate states only includes levels in the incoherent region. Thus the contact potential we use in our calculations should be

\[
T^{up} \to \tilde{U}_0 \delta(\mathbf{x} - \mathbf{x}'),
\]

where \( \tilde{U}_0 \neq U_0 \). The remainder of the terms that would ‘upgrade’ \( \tilde{U}_0 \) to \( U_0 \) are included directly in the simulation of the coherent region using the FTGPE, and so all T-matrix effects are actually included in the formalism.

In practice we find these two quantities are related in the homogeneous limit \([3]\) by

\[
\tilde{U}_0 = \frac{U_0}{1 - U_0 \alpha_K},
\]

where \( \alpha_K \) is defined by

\[
\alpha_K = \frac{1}{(2\pi)^3} \int_0^K d^3k \frac{m}{\hbar^2 k} = \frac{mK}{2\pi^2 \hbar^2},
\]

and \( K \) is the wave vector of the cutoff between the coherent and incoherent region. Thus as long as the condition \( U_0 \alpha_K \ll 1 \), or equivalently \( K a \ll 1 \) is satisfied, we are justified in setting \( \tilde{U}_0 \approx U_0 \). As in any calculation the coherent region will be rather small, and experimentally measured scattering lengths for alkali atoms are generally not known with an accuracy of better than 10%, this approximation is well justified in the homogeneous case. It seems reasonable to expect the same condition should hold true in a trap.

The second point is that the remaining terms of the FTGPE still have the interatomic potential rather than the T-matrix in their matrix elements. It turns out that it is reasonable to use the contact potential approximation in these, although we have not explicitly upgraded the matrix elements to T-matrices. For further details we refer the reader to references \([33, 4, 22, 36]\).

1. Elastic loss in condensate collisions

In section \( \ref{Elastic loss in condensate collisions} \) we stated that the delta function in the solution of the anomalous term \([40]\) could not be satisfied for a system with only one condensate near thermal equilibrium. The situation is different when we consider the collision of two condensates, where the T-matrix can have an imaginary part.

In the formalism described here the coherent region \( C \) is defined such that it contains only the modes of the gas whose occupation number satisfies \( N_k \gg 1 \). If we consider a condensate that has been formed in a harmonic trap, but then quickly released into free space, we can analyse the wave function in terms of a plane-wave basis. The region \( C \) will typically be defined by a small spherical or ellipsoidal region in \( k \)-space about a central wave-vector \( \mathbf{K} \). For
a condensate released at rest we have \( \mathbf{K} = 0 \), but by applying a Bragg-pulse to the condensate on release, it can be split into two equal parts—one at rest and one with a momentum \( \hbar \mathbf{K} / 2 \). In the centre-of-mass frame, the two condensates have momenta \( -\hbar \mathbf{K}/2 \) and \( +\hbar \mathbf{K}/2 \) respectively.

Now consider this system analysed in the plane-wave basis. If \( \hbar \mathbf{K} \) is large compared to the momentum width of the two condensates, then the region \( \mathcal{C} \) will be made up of two distinct parts of \( k \)-space, as depicted in figure 3. This means that in the collision of the two condensates it is possible for an atom from each to collide, and then scatter into any spatial direction while energy is still conserved. A large number of these collisions will take both particles outside the region \( \mathcal{C} \), as depicted in figure 3. As these processes cause scattering of both particles into modes that are otherwise empty (and are hence spontaneous), they cannot be represented by the GPE (1) (see appendix B for further explanation). However, these collisions can be represented in the FTGPE via the anomalous term \( \langle \hat{\eta} \hat{\eta} \rangle \). Unlike the case of a single condensate, the delta function part of equation (40) can now be satisfied, and therefore real transitions can occur.

We can also see that if the relative momenta of the two condensates is not large, then the two parts of the region \( \mathcal{C} \) will overlap and most of the circumference of the dashed circle in figure 3 will lie within \( \mathcal{C} \). This means that the GPE can describe condensate collisions at low momenta for which spontaneous collisions can be neglected. However, at high relative momenta other methods, such as described here, are required.

The process of elastic loss is a form of spontaneous Beliaev damping. An analogous phenomenon for a trapped BEC is, for example, when a high energy coherent collective excitation is generated in a ground state condensate. The coherent region is again divided into two parts, and the excitation can interact with the ground state condensate and spontaneously decay into two lower energy quasiparticles.

2. Four-wave mixing

In an elegant experiment, the Phillips group at NIST demonstrated the atom-optical equivalent of four-wave mixing with Bose-Einstein condensates [38]. After releasing a condensate from a trap, two separate Bragg pulses were applied in succession such that the BEC split into three distinct parts, each with a different momentum (two moving and one at rest in the lab frame). For appropriately chosen momentum values, a fourth condensate was observed to appear.

This experiment can be understood by considering figure 3, but now with a third condensate at the tip of the arrow at the top of the dashed circle. While the entire dashed region is still available in collisions between atoms from the first two condensates, the presence of third condensate stimulates transitions into this particular mode, resulting in the formation of a condensate at the tip of the downward pointing arrow.

The ordinary GPE (1) can describe the formation of the fourth condensate as this is a stimulated collision process [39,40]. However, the new condensate that appears is entangled with the atoms that are scattered into the third condensate as the colliding atoms are necessarily correlated. This correlation cannot be described by the ordinary GPE, and other methods are required [41]. We emphasize that such effects can be described by the anomalous term in the FTGPE.
C. The scattering term

We now consider the term containing $\langle \hat{q}^\dagger \hat{q} \rangle$ in the third line of the FTGPE (29a). To find an explicit expression for this quantity, we first eliminate the free evolution of equation (C3), before taking the mean value and making use of Wick’s theorem and the RPA to find the equation of motion

$$i\hbar \frac{\partial \langle \hat{a}_m^\dagger \hat{a}_n \rangle}{\partial t} = 2 \sum_{\chi \sigma} \hat{c}_\chi^* \hat{c}_{\sigma} \langle \chi m | V | \sigma n \rangle (n_m - n_n) e^{i \omega_{\chi m \sigma} t}.$$  \hspace{1cm} (47)

The solution of equation (47) differs slightly from that of the anomalous and linear terms we considered earlier. We previously made the assumption that the approximate solutions were zero at time $t = -\infty$, but this is not the case here. The diagonal term ($m = n$) of $\langle \hat{a}_m^\dagger \hat{a}_n \rangle$ is the average number of particles in mode $n$. For a system at finite temperature in which the incoherent region begins with some population, this will have a non-zero initial value, and appears in the solution of equation (47) as a constant of integration. We find

$$\langle \hat{a}_m^\dagger \hat{a}_n \rangle = -2\pi i \sum_{\chi \sigma} \hat{c}_\chi^* \hat{c}_{\sigma} \langle \chi m | V | \sigma n \rangle (n_m - n_n) \delta(\hbar \omega_{\chi m \sigma} + n_m \delta_{mn}),$$  \hspace{1cm} (48)

where in the spatial representation of the FTGPE the term involving the Kronecker delta function represents the mean field of the incoherent region acting on the coherent region wave function. We have neglected the principal part in the solution as it is dominated by the energy conserving processes.

In the basis set representation of the FTGPE the corresponding term (28a) is therefore

$$i\hbar \frac{dc_{\alpha}}{dt} = \ldots + 2 \sum_{m \beta} n_m c_{\beta} \langle \alpha m | V | m \beta \rangle$$  \hspace{1cm} (49)

$$-4\pi i \sum_{m n \beta} c_{\beta} \langle \alpha m | V | n \beta \rangle \sum_{\chi \sigma} \hat{c}_\chi^* \hat{c}_{\sigma} \langle \chi m | V | \sigma n \rangle (n_m - n_n) \delta(\hbar \omega_{\chi m \sigma} + n_m \delta_{mn}).$$

The processes it describes are analogous to the scattering term that was introduced in the model of condensate growth in references [30,31]. It represents an incoherent particle colliding with a coherent particle, with the coherent particle moving between levels within the region $C$. In the presence of a condensate this process is recognized as Landau damping, and in references [30,31] it was shown to have an important effect in the onset of condensate growth. However in simulations closer to equilibrium when a condensate is already present, the off-diagonal part of this term is unlikely to be large as the forward and backward rates will be similar.

D. The growth term

Finally, we consider the term involving $\langle \hat{q}^\dagger \hat{q} \rangle$ on the fourth line of the FTGPE (29g) which we identify as the growth term. This will generally be the most important term involving the field $\hat{q}$ in the FTGPE, as it will be responsible for the majority of particle exchange between the coherent and incoherent regions. While the linear terms and the anomalous terms can be important in certain circumstances near $T = 0$, in most situations at finite temperature they are small in comparison with the growth term because of the size difference between the coherent and incoherent regions.

To find an explicit expression for this term we begin with the equation of motion for $\hat{a}_q^\dagger \hat{a}_m \hat{a}_n$, equation (C4). Eliminating the free evolution, taking the mean value and making use of Wick’s theorem and the RPA leaves us with

$$i\hbar \frac{\partial \langle \hat{a}_q^\dagger \hat{a}_m \hat{a}_n \rangle}{\partial t} = 2 \sum_{\chi} \hat{c}_\chi \langle mn | V | q \chi \rangle e^{i \omega_{mnq} t} \{n_q (1 + n_m + n_n) - n_m n_n \}. $$  \hspace{1cm} (50)

As this can represent energy conserving processes, the approximate solution is

$$\langle \hat{a}_q^\dagger \hat{a}_m \hat{a}_n \rangle = 2\pi i \sum_{\chi} \hat{c}_\chi \langle mn | V | q \chi \rangle \delta(\hbar \omega_{mnq}) \{n_m n_n - n_q (1 + n_m + n_n) \}. $$  \hspace{1cm} (51)

Substituting equation (51) into the basis set version of the FTGPE we find the term corresponding to equation (28g) becomes
\[ i\hbar \frac{dc_\alpha}{dt} = \ldots + 2\pi i \sum_{qmn} c_\alpha \langle \alpha q|V|mn\rangle \langle mn|V|q\rangle \delta(\hbar \omega_{mnq}) \times \{ n_m n_n - n_q(1 + n_m + n_n) \}. \quad (52) \]

We can understand the physical meaning of this result by comparing it with the equivalent quantum Boltzmann rate for the growth of a coherent region level with population \( N_\alpha \) (see equation A14). Making the approximation that \( (1 + N_\alpha) \approx N_\alpha \), we find

\[ \frac{dN_\alpha}{dt} \propto \sum_{qmn} (1 + N_\alpha)(1 + n_q)n_m n_n - N_\alpha n_q(1 + n_m)(1 + n_n), \]

\[ \approx \sum_{qmn} N_\alpha [n_m n_n - n_q(1 + n_m + n_n)], \quad (53) \]

and we can see that the right-hand sides of \( (52) \) and \( (53) \) are similar.

Equation \( (52) \) is very similar to the growth part of the description of condensate formation of reference [30]. However, rather than describing the rate of change of an occupation number of a quasiparticle level, it describes the growth in amplitude of a basis component making up the coherent region wave function \( \psi \). To calculate this term for inclusion in the FTGPE requires both a reasonably good basis and corresponding energies for the coherent region, along with a method of calculating or approximating the matrix elements that appear in equation \( (52) \). While this is not difficult in principle, in practice they need to be calculated at each time step in the evolution of the FTGPE. This issue will be treated in future numerical work.

VI. THE PROJECTED GROSS-PITAEVSKII EQUATION

The finite temperature Gross-Pitaevskii equation contains all the necessary elements for a complete description of a condensed Bose gas, given that the occupation number conditions are satisfied. However, it is somewhat complicated to implement numerically. Some insight can be gained by neglecting all the terms coupling the coherent region to the effective bath \( \hat{\eta} \), and considering the equation of motion for the coherent region region alone—the first line of equation \( (29) \). We call this the projected Gross-Pitaevskii equation (PGPE)

\[ i\hbar \frac{\partial \psi(x)}{\partial t} = \hat{H}_{sp}\psi(x) + U_0 \hat{P} \{ |\psi(x)|^2 \psi(x) \}, \quad (54) \]

and we have studied solutions of this in reference [17]. Although it is not immediately evident, the PGPE does conserve normalization and energy, and this can be easily understood by considering the effective Hamiltonian as we discuss further in appendix E.

The projected GPE describes a microcanonical system, whereas in the full FTGPE the region \( C \) will fluctuate in energy and number of particles. However, if the region \( C \) contains sufficiently many modes, then fluctuations in energy and particle number in the grand canonical ensemble would be small. Hence we would expect an equilibrium state of the projected GPE to be similar to that of the finite temperature GPE coupled to a bath \( \hat{\eta}(x) \) with the appropriate chemical potential and temperature.

The projected GPE by itself cannot capture the entire physics of the Bose field at finite temperature. Indeed, in any system in which there is a significant thermalized coherent region that may be modelled by this equation, there will be a much larger incoherent region whose effects will be important. Nonetheless, we showed in reference [17] that the GPE without any additional terms can describe evolution of general configurations of the coherent region \( C \) towards an equilibrium that can be parameterized by a temperature.

The detailed non-equilibrium dynamics of the system will depend on the exchange of energy and particles between \( C \) and the bath. However, we expect that for modelling many experiments at finite temperature the projected GPE alone may be sufficient. It is well known from kinetic theory that particles mainly interact with others of similar energy. If the presence of the bath is important, then it could be well approximated by a constant temperature and chemical potential, along the lines of the formalism outlined in reference [20] and used in the model of condensate growth in references [30,31]. This issue will be considered further elsewhere.
VII. CONCLUSIONS AND PROSPECTS

In this paper we have derived an approximate formalism for calculating the dynamics of a thermal Bose gas in the highly-occupied limit. We have derived a non-perturbative finite temperature Gross-Pitaevskii equation that describes the evolution of the wave function of the coherent region \( C \), and identified and discussed the physical meaning of each of the terms that arise. In particular we have indicated how the anomalous term introduces the T-matrix in coherent region collisions, and that this can describe elastic particle loss in condensate collisions at large relative momenta. The terms analogous to the scattering and growth processes of reference \([30]\) have also been discussed.

While the formalism discussed here leaves out the possibility of quantum correlation effects in BECs, it should nevertheless provide a basis for the description of many experimentally accessible features that can not be described by the ordinary Gross-Pitaevskii equation. An important aim of our development has been to produce a numerically tractable formalism, and the first step in a practical implementation has been made in reference \([17]\) where it was shown that the projected GPE will evolve a generalized random initial distribution to an equilibrium described by a temperature. The next step is to include some of the additional terms of the FTGPE described in section \(V\).

We can also expect the FTGPE to describe the phase transition region, as long as the condition \( N_k \gg 1 \) is satisfied for the coherent region modes. The physics of phase transitions is generally classical in nature, being dominated by large fluctuations at long wavelengths. This of course is what the GPE describes, and in fact it has been used as a model of phase transitions in other areas of condensed matter physics. The GPE has the same energy functional as that used in the classical renormalization group theory of the superfluid phase transition, and it is therefore reasonable to expect the same approximations to be valid for the case of BEC. Our formalism, which couples the GPE to a kinetic treatment of the thermal particles, provides a non-perturbative dynamical finite temperature theory of BEC. This can then be used to study the region of the phase transition where perturbative approaches fail, and indeed where no other techniques are available.

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APPENDIX A: DERIVATION OF THE QUANTUM BOLTZMANN EQUATION

In this appendix we give a derivation of the quantum Boltzmann equation, which gives an accurate description of the time evolution of a Bose gas well above the transition temperature. In this regime the mean time between particle collisions is long compared to the duration of a collision, so the eigenstates of \( H_0 \) provide a good basis and the interaction part of the Hamiltonian \( H_I \) can be treated as a perturbation. This is the method by which incoherent region terms are treated in this paper.

The operators \( \hat{a}_p \) have no mean value above the transition temperature, and so we want an equation of motion for the mean number of particles in mode \( p \), \( \langle \hat{n}_p \rangle = \langle \hat{a}_p^\dagger \hat{a}_p \rangle \). From equation (16) we find

\[
\frac{d\hat{n}_p}{dt} = -\frac{i}{\hbar} \sum_{qmn} \langle pq|V|mn\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_m \hat{a}_n e^{i(\omega_p+\omega_q-\omega_m-\omega_n)t} + h.c.,
\]

(A1)

where \( h.c. \) is the hermitian conjugate. In order to find a closed expression for the evolution of \( \hat{n}_p \), we begin by finding an equation of motion for the quantity \( \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_m \hat{a}_n \) which appears on the right-hand side of equation (A1). However, this new equation for four operators contains terms involving six operators, and the equations of motion for six operators involve eight operators and so on. We proceed by truncating this series at the first iteration, approximately solving the equation for \( \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_m \hat{a}_n \), and substituting the result back into equation (A1).

One way to derive an equation of motion for \( \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_m \hat{a}_n \) would be to commute it with the Hamiltonian. An equivalent method (which will be useful for other purposes later) is simply to use the chain rule. We can formally write the solution as

\[
\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_m \hat{a}_n = \int_{-\infty}^{t} dt' \frac{d}{dt'} (\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_m \hat{a}_n),
\]

(A2)
\[ \rho_{ij} = \text{the occupation of any individual level. In fact, it is most useful to take the ensemble average, which can be written as} \]

\[ \langle \hat{A} \rangle = \text{Tr}(\hat{\rho} \hat{A}), \]

where \( \hat{\rho} \) is the density matrix of the system, and Tr denotes the trace operation. We are left to calculate quantities such as \( \langle \hat{a}_i^{\dagger} \hat{a}_j \hat{a}_m \hat{a}_n \rangle \). To do so, we assume that our system is sufficiently near thermal equilibrium that we can use Wick's theorem [32]. This states that for any system with a Hamiltonian that is a quadratic form in creation and annihilation operators, the ensemble average of any product of these is simply the contraction of all possible pairings of the operators. For example we have
On substituting these relations into equation (A6) the final result is
\[ \langle \hat{a}_i^\dagger \hat{a}_j \rangle = \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle + \langle \hat{a}_i^\dagger \hat{a}_j \rangle = \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle + \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle. \]  

(A8)

This relation is exact at thermal equilibrium, and should be a very good approximation nearby.

We now make use of a further approximation, known as the random phase approximation (RPA), which states that if the density matrix for the system is diagonal then
\[ \langle \hat{a}_i^\dagger \hat{a}_j \rangle = \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle = 0, \quad \langle \hat{a}_i^\dagger \hat{a}_j \rangle = n_i \delta_{ij}. \]  

(A9)

This will be an excellent approximation when there is no condensate present, as the interaction Hamiltonian \( \hat{H}_I \) is only a small perturbation to the ideal gas Hamiltonian \( \hat{H}_0 \). Thus we have
\[ \langle \hat{a}_i^\dagger \hat{a}_j \rangle = n_m n_n (\delta_{im} \delta_{jm} + \delta_{im} \delta_{jn}), \]  

(A10)

\[ \langle \hat{a}_i^\dagger \hat{a}_j \hat{a}_l \hat{a}_m \rangle = n_i n_m n_j n_l \delta_{il} \delta_{jm} \delta_{mn} \delta_{pl} \]  

(A11)

On substituting these relations into equation (A6) the final result is
\[ \frac{dn_p}{dt} = \frac{4\pi}{\hbar^2} \sum_{qmn} |\langle pq|V|mn\rangle|^2 \delta(\omega_p + \omega_q - \omega_m - \omega_n) \times \left[ (n_p + 1)(n_q + 1)n_m n_n - n_p n_q (n_m + 1)(n_n + 1) \right] \]  

(A12a)

\[ + \frac{8\pi}{\hbar^2} \sum_{qmn} \langle pq|V|mn\rangle \langle mn|V|mq\rangle n_p n_m (n_n - q) \delta(\omega_n - \omega_q) \]  

(A12b)

\[ + \frac{8\pi}{\hbar^2} \sum_{qmn} \langle pq|V|qn\rangle \langle mn|V|mp\rangle n_q n_m (n_n - p) \delta(\omega_n - \omega_p). \]  

(A12c)

The first part of this expression (A12a) is the standard quantum Boltzmann equation; however, the lines of (A12b) and (A12d) do not appear in most definitions of the QBE. We would like to note the following about these terms:

1. The scattering processes described by the matrix elements in these terms involves a third particle, and hence these collision terms are of higher order than those described by (A12a).

2. If we calculate the matrix elements using the contact potential approximation in the homogeneous limit, then these terms become
\[ (A12b) \rightarrow \frac{8\pi U_0^2}{\hbar^2 \Omega^2} \sum_{qmn} \delta(k_q - k_n)^2 n_p n_m (n_n - q) \delta(\omega_n - \omega_q), \]  

(A13a)

\[ (A12d) \rightarrow \frac{8\pi U_0^2}{\hbar^2 \Omega^2} \sum_{qmn} \delta(k_p - k_n)^2 n_q n_m (n_n - p) \delta(\omega_n - \omega_p). \]  

(A13b)

The delta functions in momentum are equivalent to Kronecker delta functions in the quantum labels for the system, and hence these terms vanish.

3. For an ergodic system where the occupation of a level depends only on its energy, these terms are again identically zero.

4. The delta functions in frequency depend on only two of the particle indices, rather than four as for equation (A12d). This means there will be far fewer matches for (A12b) and (A12d), and therefore these can be considered surface terms that become small in the thermodynamic limit.

We are therefore justified in neglecting these terms, and are left with the usual quantum Boltzmann equation
\[ \frac{dn_p}{dt} = \frac{4\pi}{\hbar} \sum_{qmn} |\langle pq|V|mn\rangle|^2 \delta(\epsilon_p + \epsilon_q - \epsilon_m - \epsilon_n) \times \left( (n_p + 1)(n_q + 1)n_m n_n - n_p n_q (n_m + 1)(n_n + 1) \right). \]  

(A14)
Validity

We summarize the validity conditions for the QBE as:

1. The Markov approximation must be valid such that correlations induced by collisions are unimportant.
2. The system should close enough to equilibrium such that the factorization of Wick’s theorem is valid.
3. There must be a good basis such that the RPA is valid. In our derivation we have assumed that \( \tilde{H}_f \) should be a perturbation to the system for this to hold. However, if the average effect of \( \tilde{H}_f \) can be absorbed into \( \tilde{H}_0 \) to form an effective Hamiltonian with a good basis, then the QBE derivation may still be valid. It must be noted, however, that the Markov approximation may not be valid in this regime as the mean collision time will be much reduced.

APPENDIX B: THE GPE KINETIC EQUATION

It is interesting to consider the kinetic equation that would result if we assume that the GPE is a good description of the system of interest. We expand the time dependent wave function as

\[
\psi(x, t) = \sum_k \hat{c}_k \phi_k(x) e^{-i\omega_k t},
\]

where the \( \{ \hat{c}_k \} \) are slowly varying. Substituting equation \( B1 \) into the time-dependent GPE \( I \) and performing the operation \( \int d^3x \phi^*_k(x) \) on both sides results in the basis set representation of the GPE

\[
\frac{i\hbar}{2} \frac{d\hat{c}_k}{dt} = \sum_{qmn} \langle pq|V|mn\rangle \hat{c}_q^* \hat{c}_m \hat{c}_n e^{i(\omega_q + \omega_m - \omega_n)t}. \tag{B2}
\]

We note that equation \( B2 \) is identical in form to the basis set equation of motion for the Bose field \( I \) but for the replacement \( \hat{a}_k \leftrightarrow \hat{c}_k \). In fact, equation \( B2 \) could be derived directly from equation \( I \) by expanding the annihilation operators as \( \hat{a}_k = c_k + \hat{\delta}_k \) and then neglecting the quantum fluctuation terms \( \hat{\delta}_k \).

We can now carry out the same procedure on \( B2 \) as was applied to equation \( I \) in the derivation of the QBE. The only difference is that we are now manipulating \( c \)-numbers rather than operators, and so any terms arising from commutators in the previous treatment will not appear. This means that the terms of the form \( \hat{a}_k^\dagger \hat{a}_k \hat{a}_l^\dagger \hat{a}_l \) will disappear from equation \( A4 \), leaving only terms involving six \( c \)-numbers. Writing \( n_p \) for \( \hat{c}_p^\dagger \hat{c}_p \), the resulting GPE kinetic equation is

\[
\frac{dn_p}{dt} = \frac{4\pi u_0^2}{\hbar} \sum_{qmn} |\langle pq|mn\rangle|^2 \delta(\epsilon_p + \epsilon_q - \epsilon_m - \epsilon_n) \times \left\{ (n_p + n_q)n_m n_n - n_p n_q(n_m + n_n) \right\} \tag{B3}
\]

which is exactly the same form as the QBE \( A14 \) except that the spontaneous collision terms are excluded. This equation was first considered by Svistunov in a study of the formation of a condensate in a weakly-interacting Bose gas \( I \).

Some of the approximations made in the derivation of the GPE kinetic equation may not hold in the presence of a condensate. In particular, the assumption of correlations being unimportant on the scale of the collision time is unlikely to be valid. The GPE kinetic equation does, however, give us an understanding of the collision processes that are described by the full GPE.

From equation \( B3 \) we can see that the GPE contains stimulated collision processes only. To understand this, consider the collision \( p + q \rightarrow m + n \). This process will only be represented by the GPE if one of the levels \( (m, n) \) is already occupied. This is in contrast to the QBE, for which the term in the curly brackets of equation \( A14 \) can be written

\[
\left\{ (1 + n_p + n_q)n_m n_n - n_p n_q(1 + n_m + n_n) \right\}. \tag{B4}
\]

Thus, due to the neglect of the quantum nature of the modes, the GPE can only accurately describe the evolution and interaction of modes which satisfy \( n_p \gg 1 \), such that \( (1 + n_p + n_q) \approx (n_p + n_q) \).
APPENDIX C: INCOHERENT REGION EQUATIONS

In this appendix we write out the Heisenberg equations of motion for all the operator combinations that appear in the basis set version of the FTGPE (28). The single operator term is

\[ i\hbar \frac{d\hat{a}_p}{dt} = \hbar \omega_p \hat{a}_p + \langle p \psi | V | \psi \rangle + \sum_{q} \langle p q | V | \psi \psi \rangle \hat{a}_q^\dagger \]

\[ + 2 \sum_{m} \langle p \psi | V | m \psi \rangle \hat{a}_m \]

\[ + \sum_{mn} \langle p \psi | V | m n \rangle \hat{a}_m \hat{a}_n \]

\[ + 2 \sum_{q m} \langle p q | V | m \psi \rangle \hat{a}_q^\dagger \hat{a}_m \]

\[ + \sum_{q mn} \langle p q | V | m n \rangle \hat{a}_q^\dagger \hat{a}_m \hat{a}_n. \]  

The equation of motion for \( \hat{a}_p^\dagger \) is simply the hermitian conjugate of (C1). The other equations of motion can be found either by calculating the commutator with the Hamiltonian, or using the chain rule. We have

\[ i\hbar \frac{d(\hat{a}_m \hat{a}_n)}{dt} = \hbar (\omega_m + \omega_n) \hat{a}_m \hat{a}_n + \langle m \psi | V | \psi \rangle \hat{a}_n + \langle n \psi | V | \psi \rangle \hat{a}_m \]

\[ + \sum_{k} \left[ \langle k n | V | \psi \rangle \hat{a}_k^\dagger \hat{a}_m + \langle k m | V | \psi \rangle \hat{a}_k^\dagger \hat{a}_n \right] \]

\[ + 2 \sum_{k} \left[ \langle n \psi | V | k \psi \rangle \hat{a}_k \hat{a}_m + \langle m \psi | V | k \psi \rangle \hat{a}_k \hat{a}_n \right] \]

\[ + \sum_{k j} \left[ \langle m \psi | V | k j \rangle \hat{a}_n \hat{a}_k \hat{a}_j + \langle n \psi | V | k j \rangle \hat{a}_m \hat{a}_k \hat{a}_j \right] \]

\[ + 2 \sum_{k j} \left[ \langle k m | V | j \psi \rangle \hat{a}_k \hat{a}_j \hat{a}_n + \langle k n | V | j \psi \rangle \hat{a}_k \hat{a}_j \hat{a}_m \right] \]

\[ + \sum_{k j} \langle m n | V | k j \rangle \hat{a}_k \hat{a}_j \]

\[ + \sum_{q k j} \left[ \langle m q | V | k j \rangle \hat{a}_q^\dagger \hat{a}_n \hat{a}_k \hat{a}_j + \langle n q | V | k j \rangle \hat{a}_q^\dagger \hat{a}_m \hat{a}_k \hat{a}_j \right], \] 

\[ i\hbar \frac{d(\hat{a}_m^\dagger \hat{a}_n)}{dt} = \hbar (\omega_n - \omega_m) \hat{a}_m^\dagger \hat{a}_n \]

\[ + \langle n \psi | V | \psi \rangle \hat{a}_m^\dagger \hat{a}_n - \langle \psi \psi | V | m \psi \rangle \hat{a}_n \]

\[ + \sum_{k} \left[ \langle k n | V | \psi \rangle \hat{a}_k^\dagger \hat{a}_m^\dagger \hat{a}_n - \langle \psi \psi | V | k m \rangle \hat{a}_k \hat{a}_n \right] \]

\[ + 2 \sum_{k} \left[ \langle n \psi | V | k \psi \rangle \hat{a}_m^\dagger \hat{a}_k - \langle k \psi | V | m \psi \rangle \hat{a}_k^\dagger \hat{a}_n \right] \]

\[ + \sum_{k j} \left[ \langle n \psi | V | k j \rangle \hat{a}_m^\dagger \hat{a}_k \hat{a}_j - \langle k j | V | m \psi \rangle \hat{a}_k^\dagger \hat{a}_j \hat{a}_n \right], \]
same methods as in the derivation of the QBE in appendix A and the techniques outlined in section V. We find

\[ + 2 \sum_{kj} \left[ \langle kn | V | j \rangle \hat{a}_m \hat{a}_j - \langle j \psi | V | km \rangle \hat{a}_j \hat{a}_n \right] \]

\[ + \sum_{qkj} \left[ \langle qn | V | kj \rangle \hat{a}_m \hat{a}_j \hat{a}_q \hat{a}_n - \langle kj | V | qn \rangle \hat{a}_j \hat{a}_q \hat{a}_n \right], \]

\[ (C3f) \]

and

\[ i\hbar \frac{d(\hat{a}_m \hat{a}_n)}{dt} = i\hbar \left[ \hat{a}_n \frac{d(\hat{a}_m \hat{a}_n)}{dt} + \frac{d(\hat{a}_j \hat{a}_m \hat{a}_n)}{dt} \right] \]

\[ = \hbar (\omega_m + \omega_n - \omega_q) \hat{a}_j \hat{a}_m \hat{a}_n \]

\[ + \langle m \psi | V | \psi \rangle \hat{a}_j \hat{a}_m \hat{a}_n + \langle n \psi | V | \psi \rangle \hat{a}_q \hat{a}_m \hat{a}_n \]

\[ + \langle mn | V | \psi \psi \rangle \hat{a}_q \hat{a}_m \hat{a}_n \]

\[ + \sum_{k} \left[ \langle kn | V | \psi \rangle \hat{a}_j \hat{a}_m \hat{a}_n \right] \]

\[ + 2 \sum_{k} \left[ (\langle n \psi | V | k \rangle \hat{a}_q \hat{a}_m \hat{a}_n + \langle m \psi | V | k \rangle \hat{a}_q \hat{a}_m \hat{a}_n \right] \]

\[ + \langle kn | V | q \psi \rangle \hat{a}_q \hat{a}_m \hat{a}_n \]

\[ + \sum_{kj} \left[ \langle m \psi | V | kj \rangle \hat{a}_q \hat{a}_m \hat{a}_j \right] \]

\[ + 2 \sum_{kj} \left[ \langle kn | V | j \rangle \hat{a}_q \hat{a}_j \hat{a}_m \right] \]

\[ + \langle kj | V | q \rangle \hat{a}_q \hat{a}_j \hat{a}_m \]

\[ (C4g) \]

\[ (C4h) \]

\[ (C4i) \]

\[ (C4j) \]

\[ (C4k) \]

\[ + \sum_{kj} \left[ \langle km | V | j \rangle \hat{a}_q \hat{a}_j \hat{a}_m \right] \]

\[ + \sum_{kj} \left[ \langle mn | V | kj \rangle \hat{a}_j \hat{a}_m \hat{a}_k \hat{a}_j \right] \]

\[ + \sum_{kj} \left[ \langle mr | V | kj \rangle \hat{a}_q \hat{a}_j \hat{a}_m \hat{a}_k \right] \]

\[ + \langle kj | V | rq \rangle \hat{a}_q \hat{a}_j \hat{a}_m \hat{a}_n \]

\[ (C4o) \]

APPENDIX D: INCOHERENT REGION KINETIC EQUATION

In this section we present the kinetic equation of motion that can be derived for the incoherent region, using the same methods as in the derivation of the QBE in appendix A and the techniques outlined in section V. We find

\[ \frac{dn_p}{dt} = \frac{2\pi}{\hbar} \sum_{\alpha\beta} \langle pq | V | \alpha \beta \rangle^2 \delta(\hbar \omega_{pq\alpha\beta}) |c_\alpha c_\beta|^2 (n_p + n_q + 1) \]

\[ + \frac{8\pi}{\hbar} \sum_{\alpha\beta \gamma} \langle \alpha \beta | V | \gamma \rangle^2 \delta(\hbar \omega_{p\alpha\beta\gamma}) |c_\alpha c_\beta c_\gamma|^2 (n_\gamma - n_p) \]

\[ + \frac{4\pi}{\hbar} \sum_{\alpha \beta \gamma} \langle \alpha \beta | V | \gamma \rangle^2 \delta(\hbar \omega_{p\alpha\gamma\gamma}) \]

\[ \times |c_\alpha|^2 \left( n_\gamma n_n - n_p (1 + n_m + n_n) \right) \]

\[ (D1a) \]

\[ (D1b) \]

\[ (D1c) \]
\[
\begin{aligned}
&+ \frac{8 \pi}{\hbar} \sum_{\alpha q m} \langle pq | V | m \alpha \rangle^2 \delta(h \omega_{pq m}) \\
&\quad \times |c_{\alpha}|^2 \{(n_p + n_q + 1)n_m - n_p n_q\} \\
&+ \frac{4 \pi}{\hbar} \sum_{q m n} \langle pq | V | m n \rangle^2 \delta(h \omega_{pq m n}) \\
&\quad \times \{(1 + n_p)(1 + n_q)n_m n_n - n p n_q (1 + n_m)(1 + n_n)\}.
\end{aligned}
\] (D1d)

We can recognize each of these terms from our previous discussions:

1. The term (D1a) is from the anomalous term, and is only non-zero when we consider the collision of multiple condensates.

2. The line (D1b) describes the scattering processes.

3. The two terms (D1c) and (D1d) are due to the forward and backward growth terms of the coherent region.

4. The line (D1e) is simply the QBE for the incoherent region.

It may seem surprising that there is no contribution from the linear terms discussed in the previous section. This is because the rates for each of the forward and backward processes contain only stimulated terms and so they cancel. The kinetic equation for the incoherent region is thus the usual QBE but with additional couplings to the coherent region whose physical meanings can be understood from the corresponding terms in section V.

**APPENDIX E: CONSERVATION OF NORMALIZATION IN THE PGPE**

The PGPE conserves normalization and energy because the effective projected Hamiltonian is hermitian. The nonlinear term of the GPE can be considered to describe interactions between two particles, and as such there can be collisions in which two coherent atoms collide and one is ejected from the coherent region. However, the projector excludes these terms from the equation of motion which we now demonstrate.

Consider the equation of motion in a basis set. By substituting \( \psi(x) = \sum_{k \in C} c_k \phi_k(x) \) into equation (54) and performing the operation \( \int d^3x \phi_p(x) \) on both sides we find

\[
i \hbar \frac{dc_p}{dt} = \hbar \omega_p c_p + U_0 \hat{P} \sum_{q m n \in C} c_q^* c_m c_n \langle pq | mn \rangle.
\] (E1)

If the state \( p \in C \) then all four labels are from the coherent region and there is no transfer of population outside the region. For \( p \notin C \) the matrix element \( \langle pq | mn \rangle \) is not zero necessarily, and therefore it seems collisions between states from within the coherent region can transfer population outside of \( C \). However, we should not be considering the equations of motion for amplitudes \( p \notin C \) in the first place, as they not in the definition of the wave function \( \psi(x) \).

The projection operation is therefore performed implicitly by the basis set representation.

Numerically solving the GPE using a basis set method requires a triple summation over indices, which is a very time-consuming operation. This suggests that we should instead use the spatial representation of equation (54), where the nonlinear term is local. However, any spatial grid that is fine enough to provide a good representation of all the states within \( C \) will also be able to represent modes outside the region \( C \). From equation (E1) we can see that this will cause population to be transferred outside of \( C \), and so in this case we need to consider the projection operation explicitly.

Another method of approaching this issue is to assume that all modes in the problem can be represented by the GPE, but artificially choose part of the system to be the coherent region. Thus the field operator can be written as

\[
\hat{\Psi}(x) \approx \psi(x) + \eta(x),
\] (E2)

where both fields are classical. Substituting this into the interaction part of the Hamiltonian (8) and using the contact potential approximation, we have

\[
\hat{H}_1/U_0 = \hat{H}_4 + \hat{H}_3 + \hat{H}_2 + \hat{H}_1 + \hat{H}_0,
\] (E3)

\[
\hat{H}_4 = \frac{1}{2} \psi^* \psi^* \psi \psi,
\] (E4)
TABLE I. Classical FTGPE divided into terms representing physical processes involving \( n \) coherent states

| No. of coherent states | \( \hbar \frac{\partial \psi}{\partial t} = \mathcal{P} \times \ldots \) | \( \hbar \frac{\partial \eta}{\partial t} = \mathcal{Q} \times \ldots \) |
|------------------------|------------------------------------------------|------------------------------------------------|
| 4                      | \( \frac{|\psi|^2}{\eta} \)                      | 0                                               |
| 3                      | \( +2|\psi|^2 \eta + \eta^* \psi^2 \)           | \( +|\psi|^2 \eta \)                            |
| 2                      | \( +2\psi|\eta|^2 + \psi^* \eta^2 \)           | \( +2\psi^2 |\eta|^2 + \psi^* \eta^2 \)             |
| 1                      | \( +|\eta|^2 \eta \)                            | \( +|\eta|^2 \eta \)                            |
| 0                      | \( +0 \)                                         | \( +0 \)                                         |

where we have dropped all space and time labels for clarity, and have divided the Hamiltonian into five terms depending on the number of coherent region fields they contain. Considering the Hamiltonian in this form we can easily interpret each of the terms. Each \( \psi^* \) creates a particle in the coherent region, and each \( \psi \) removes a particle from the coherent region. The \( \eta^* \) and \( \eta \) perform the same operation outside the region \( C \). This allows us to identify which processes each of the terms in the Hamiltonian contribute to the equations of motion for both \( \psi \) and \( \eta \).

We can now derive equations of motion for \( \psi \) and \( \eta \) by using functional differentiation. We find

\[
\hbar \frac{\partial \psi}{\partial t} = \mathcal{P} \frac{\partial H}{\partial \psi^*}, \quad \hbar \frac{\partial \eta}{\partial t} = \mathcal{Q} \frac{\partial H}{\partial \eta^*}.
\]

(E9)

As an example, let us consider the contribution to these equations for all interactions involving three coherent and one incoherent state described by \( H_3 \). We find from (E5) and (E9)

\[
\hbar \frac{\partial \psi}{\partial t} \sim \mathcal{P} \left( 2|\psi|^2 \eta + \eta^* \psi^2 \right),
\]

(E10)

\[
\hbar \frac{\partial \eta}{\partial t} \sim \mathcal{Q} \left( |\psi|^2 \psi \right).
\]

(E11)

The results of carrying out this operation for all particle processes are summarized in table I. The equations of motion for the system will together conserve both energy and normalization if all terms in any row of the table are included, as this correctly accounts for all forward and backward processes of the same order. We have confirmed this numerically by carrying out coupled simulations of \( \psi \) and \( \eta \) and including only some of these terms.

We can now see that if we want an equation describing interactions involving four coherent states, but neglecting all processes involving incoherent particles, then this is simply the PGPE.

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[1] Anderson M, Ensher JR, Matthews MR, Wieman CE and Cornell EA 1995 Science 269 198
[2] Davis KB, Mewes M-O, Andrews MR, van Druten NJ, Durfee DS, Kurn DM and Ketterle W 1995 Phys. Rev. Lett. 75 3969
[3] Bradley CC, Sackett CA, Tollet JJ and Hulet R 1995 Phys. Rev. Lett. 75 1687; Sackett CA, Tollet JJ and Hulet R 1997 Phys. Rev. Lett. 79 1170
[4] Morgan SA 2000 J. Phys. B 33 3847
[5] Fedichev PO and Shlyapnikov GV 1998 Phys. Rev. A 58 3146
[6] Giorgini S 2000 Phys. Rev. A 61 063615
[7] Gardiner CW 1997 Phys. Rev. A 56 1414
[8] Svistunov BV 1991 J. Moscow Phys. Soc. 1 373
