Quantum Kinetic Theory I: A Quantum Kinetic Master Equation for Condensation of a weakly interacting Bose gas without a trapping potential

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A Quantum Kinetic Master Equation (QKME) for bosonic atoms is formulated. It is a quantum stochastic equation for the kinetics of a dilute quantum Bose gas, and describes the behavior and formation of Bose condensation. The key assumption in deriving the QKME is a Markov approximation for the atomic collision terms. In the present paper the basic structure of the theory is developed, and approximations are stated and justified to delineate the region of validity of the theory. Limiting cases of the QKME include the Quantum Boltzmann master equation and the Uehling-Uhlenbeck equation, as well as an equation analogous to the Gross-Pitaevskii equation.

I. INTRODUCTION

Recent observations of Bose-Einstein condensation (BEC) in a dilute gas of magnetically trapped alkali atoms \(^2\) and in excitonic systems \(^4\) has stimulated new theoretical efforts to describe the dynamics and signatures of weakly interacting Bose gases. In contrast to superfluid Helium, which for many years has been the only experimental example of BEC, these weakly interacting Bose gases are much more amenable to a theoretical analysis. Recent theoretical work has focused on a description of BEC in a trapping potential and dynamics of formation of a Bose condensate \(8\) to \(38\).

In this paper we want to develop techniques to describe the behavior and formation of the Bose condensate in which we will combine the simplicity of a quantum stochastic methods used in quantum optics \(40\) with a realistic treatment of the interatomic interactions which are known to play a major role in the dynamics of the condensing system \(41\). Such a description must necessarily involve aspects of a kinetic theory as well as quantum mechanics.

The first realistic formulation of kinetic theory was the Boltzmann Equation (BE) whose usefulness and success to this day is universally accepted. The so-called Quantum Boltzmann or Uehling-Uhlenbeck equation (QBE) \(42\) introduces corrections for quantum statistics into the Boltzmann collision term, but since it deals only with one-particle distribution functions we cannot expect this equation to give a realistic treatment of the quantum mechanical aspects which must occur in a Bose condensate.

A different description is provided by the time dependent Gross-Pitaevskii equation (GP equation) \(43\) which can be viewed as an equation for the condensate wave function (order parameter for the Bose condensate). This equation is clearly a simplified description in that it includes no quantum fluctuations, or thermal or irreversible effects, but it may well be valid in the situation of a large
number of condensate particles. Both of these equations contain essential aspects of the problem we are studying. However, in practice the process of creating a Bose condensate in a trap by means of evaporative cooling starts in a regime covered by a kinetic equation and finishes in a regime where the GP is thought to be valid. What is needed is unified description which covers the whole range — a true quantum kinetic theory. In this paper we will develop a *quantum kinetic master equation* (QKME) which is not a mere modification of the BE but extends its philosophy into quantum mechanics and derives a *quantum stochastic equation* of the kind similar to those derived in quantum optics.

The QKME which we derive is thus a consistent extension of the philosophy of the BE to a regime in which quantum mechanical effects are not a minor correction to classical results, but play a major role in the full description of the system.

In applying the QKME to the problem of Bose condensation, although quantum mechanics plays major role, the significant quantum aspects are restricted to a few modes, the remaining modes being able to be describe in a manner similar to the classical Boltzmann equation. This is a situation which is very familiar in quantum optics, where we very often find that it is necessary to describe a few optical modes fully quantum mechanically, while treating the rest of the systems as a heat bath. However, the methods necessary for quantum kinetic theory contain considerably more technical difficulty, largely because of the interaction between the atoms. The nearest optical analogy is multimode propagation in a medium with a strong nonlinear refractive index [44].

II. THE NEED FOR A QUANTUM KINETIC THEORY

Our goal is to derive a quantum kinetic master equation for a gas of $N$ weakly interacting Bose atoms. The master equation is formulated as an evolution equation for the $N$-atom density matrix, giving a quantum mechanical generalization of the Quantum Boltzmann equation. This provides a fully quantum mechanical description of the kinetics of a Bose gas, including the regime of Bose condensation. In particular, such an equation is capable of describing the formation of the Bose condensate. The quantum mechanical processes which must be included in this treatment are the atomic motion (transport) and coherent and incoherent interactions (collisions) between the atoms. In this section we give a qualitative overview over the main results to be derived in later sections.
A. Essential elements of the theory

There are three principal elements, as follows.

1. Coherent and incoherent dynamics

The derivation of a quantum master equation implies that the system dynamics can divided into into coherent and incoherent physical processes, where the incoherent dynamics is modeled as a quantum stochastic Markovian process. This builds on ideas, which have been developed and applied successfully in quantum optics as a method of describing coherent and incoherent processes simultaneously (e.g. in laser theory).

In a weakly interacting Bose gas, we will treat the collisions between the atoms resulting in a large momentum transfer as random and weak incoherent processes, responsible for the “noise” in the system. On the other hand, forward or near forward scattering is, if the wavelength is sufficiently long, largely a coherent process, giving rise to dispersive effects.

2. Dynamics of the condensate

The (coherent) dynamics of the Bose condensate is treated explicitly and separate from the description of the non-condensed modes which play the role of noise and feeding terms for the Bose condensate. Again, this is guided by laser theory where the coherent laser mode is separated from the weakly populated incoherent modes which are typically treated as a heat bath.

3. The “cell” description

The theory is formulated in terms of a quantum mechanical phase space description for with coarse grained position and momentum variables, based on division of phase space into “cells” of volume $\hbar^3$. This seems to be the most natural formulation, since collisions are best described in terms of momentum, whereas transport is best understood in terms of position. We will introduce this formulation by means of a wavelet description, which gives an exact description of the dynamics; approximations appear as a result of the procedure for describing the kinetics, and the conditions for the validity of our approximations then put some conditions on the precise nature of the cells chosen.

B. The scope of this paper

In developing the physical picture, there are three main stages through which we must proceed in order to achieve...
a full quantum kinetic theory applicable to the present experiments on Bose-Einstein condensation.

i) It is necessary first to develop the theory for the weakly interacting Bose gas with no trapping potential, whose stationary solution is well approximated by an ideal Bose gas.

ii) The next stage is to take account of the modifications (these may be very significant) to the dynamics, which are induced by the presence of a large proportion of atoms being in the condensate. This can be developed in terms of Bogoliubov quasiparticles [45,46], or more generally.

iii) Finally, we introduce the trapping potential. There are two extreme situations to consider. If the trap is very broad, then the situation is qualitatively not very different from the case of no trap, though the appropriate modifications can be quite intricate. In the case of a very tight trap, we have a completely different treatment, based on the kinetics of transitions between different trap levels. There will also be an intermediate regime, in which it is relevant to treat only the lower trap levels explicitly, while upper levels are thermalized.

This paper deals with i) only; ii) and iii) will be treated in our second paper QKII. Thus this paper develops all the basic ideas and methodology, while QKII will develop the refinements necessary to deal with strong condensation with and without a trapping potential.

1. The physical picture

This phase space description is one in which particles are represented as wave packets interacting with each other. From the point of view of wavepackets there are the following processes: **Transport**: that is the motion through space of a wavepacket. However we also understand that from a wavepacket point of view, transport is a process by which the wavepacket moves with unchanged shape—the wavepacket spreading inherent in the quantum mechanics of particle motion is not itself viewed as a part of transport. **Wavepacket spreading** occurs in addition to what one would normally call transport, and must contribute to the production of coherence which can arise in a Bose condensed system. It is purely quantum mechanical, but arises of course from exactly the same quantum mechanical source as transport, as defined here. Motion in a trap is readily included in these arguments to the extent the trapping potential can be considered as slowly varying. **Collisions**: here we mean localized events in which the momentum of wavepackets will change instantaneously, with a consequent change in the wavefunction. The localization cannot of course be exact, because wavepackets themselves are extended objects.
Quantum mechanics itself does not give any preferred size of the momentum space or coordinate space cells separately. Physically, we can characterize the choice of cells by a wavenumber Δ (or a cell size $l_c = \pi/\Delta$ (compare Fig. 1), and this will naturally provide a “cut” in momentum space; changes of momentum greater than $\hbar \Delta$ are seen as collisions, while smaller changes are seen as changes which take place in coordinate space. The value of Δ is constrained by two considerations.

(a) We want to have a description in terms of “energy levels” within a box inside each cell. This means that the wavefunction of a particular particle must maintain its coherence over the length $l_c$ of the cell. The coherence length which arises from collisions should normally be of the same order of magnitude as the mean free path $\lambda_{\text{mfp}} = v\tau$, where $v$ is the speed of the particle, and $\tau$ is the mean time between collisions. Thus this requirement yields the condition $l_c \ll \lambda_{\text{mfp}}$.

(b) We will be wanting to develop a Markovian description of collisions, which depends on the determination of a characteristic decoherence time, which is essentially the bandwidth of frequencies of particles in the system, that is, thermal correlation time $\hbar/2\pi kT$. This should be much less than the characteristic time for evolution of the phase-space density, and this yields the condition that the mean free path $\lambda_{\text{mfp}} \gg \lambda_T = \hbar/\sqrt{2mkT}$, which is the wavelength of a typical particle, known as the thermal wavelength.

(c) As well as the condition that the bandwidth of frequencies must be sufficiently large, we must also have a sufficient density of states to ensure that the correlation function inherent does indeed become very small for times greater than the correlation time. Essentially this requires that the maximum energy difference between cells should be much less than $kT$, leading to the requirement $l_c \gg l_T \equiv \hbar/\sqrt{2mkT}$, that is, the cells must be very much larger than the thermal wavelength.

(d) The method is based on a requirement that correlations which involve momentum differences greater than Δ are negligible. This means that the “collisions”, that is, processes which cause a momentum change larger than $|\Delta|$, are seen as inducing incoherence. The derivation of the QKME which we use does this by means of a projection formalism, and the condition for the validity of the procedure is found to be
\[ a \lambda_{\text{mfp}} \lambda_T \ll l_c^3 \]  

(1)

where \( a \) is the scattering length for the interaction between the particles.

(c) There is also a \textit{weak condensation condition} for the validity of the methods used in this paper, and this can be written in terms of the cell size \( l_c \), the scattering length \( a \), and the particle density \( \rho \) as \( l_c \gg \sqrt{\pi/8} a \rho \).

These criteria are easily met, for example in the experiment of [3] one finds that \( \lambda = 0.4619 \text{m} \), while the thermal wavelength is \( l_T = 4.8 \times 10^{-7} \text{m} \).

On the other hand in that experiment the trap itself has a size of the order of magnitude as \( l_T \). Thus to describe the behavior of the wavefunction within the trap, one would want \( l_c \) to be finer than this. This first paper does not deal with trapping potentials, but we will show how to overcome this difficulty in the QKII. The essence of the solution is that it is not necessary to have the same size cells for all ranges of momentum—they can be finer in space at the lower momentum ranges.

Figs. 2 and 3 illustrate the phase space description and the various physical processes. The figures show the phase space cells corresponding to different momentum bands \( \mathbf{K} \) with width \( \Delta \) and position cells \( \mathbf{r} \). A state of the system is given by specifying a set of occupation numbers \( \{ n(\mathbf{K}, \mathbf{r}) \} \) of the cells (Fig. 2). Transport and wave packet spreading corresponds to coherent quantum processes connecting cells in a given momentum band (horizontal arrows in Fig. 3a). Note that these coherent processes do not change a given momentum distribution \( N(\mathbf{K}) = (N(\mathbf{K}_1), N(\mathbf{K}_2), \ldots) \) with \( N(\mathbf{K}) = \sum_{\mathbf{r}} n(\mathbf{K}, \mathbf{r}) \) the number of atoms in a momentum band. In a similar way, coherent processes corresponding to a forward scattering, or motion in a slowly varying trapping potential give rise to smooth shifts between the cells of neighboring \( \mathbf{K} \) (Fig. 3a and b). Incoherent collision processes between two atoms, on the other hand, are associated with a “quantum jump like” momentum change \( \mathbf{K}_1, \mathbf{K}_2 \rightarrow \mathbf{K}_3, \mathbf{K}_4 \) between widely separated in momentum bands (however, essentially confined to within a single spatial cell \( \mathbf{r} \)) (see Fig. 3c). These transitions conserve momentum,

\[ \mathbf{K}_1 + \mathbf{K}_2 = \mathbf{K}_3 + \mathbf{K}_4 + \mathcal{O}(\Delta), \]  

(2)

up to an uncertainty \( \Delta \) associated with the width of the band, and energy

\[ E_1 + E_2 = E_3 + E_4 \quad (E_i = h^2 K_i^2/2m). \]  

(3)

Collisions cause transitions between different momentum distributions

\[ N(\mathbf{K}) = (\ldots, n_1, n_2, n_3, n_4, \ldots) \]

\[ \rightarrow N'(\mathbf{K}) = (\ldots, n_1 - 1, n_2 - 1, n_3 + 1, n_4 + 1, \ldots) \]  

(4)

which we write in the form

\[ N(\mathbf{K}) \rightarrow N'(\mathbf{K}) = N(\mathbf{K}) + \epsilon. \]  

(5)
C. The quantum kinetic master equation

The derivation of the master equation in Sec. IV C below assumes that the full quantum coherence is kept for different spatial configurations (occupation numbers of the phase space cells) within one $K$-band, and the assumption that atomic coherences between different momentum bands are eliminated in the Born and Markov approximation. The mathematical procedure of deriving a master equation in Sec. III is based on projecting the $N$-atom density operator $\rho$ on states associated with a given momentum distribution $N(K)$. For a given cell size there is a regime where this diagonally projected density matrix $v_N$ obeys a closed equation

$$\dot{v}_N(t) = -\frac{i}{\hbar} \left[ \sum_K \int d^3x \left( \frac{\hbar K}{2m} \right) \cdot j_K(x) + \sum_K \int d^3x \psi^\dagger_K(x) \left( -\frac{\hbar^2 \nabla^2}{2m} \right) \psi_K(x), v_N(t) \right]$$

$$- \frac{i}{2\hbar} \left[ \sum_{K_1 \neq K_2} (U(K_1, K_2, K_1, K_2) + U(K_1, K_2, K_2, K_1)) + \sum_{K_1} U(K_1, K_1, K_1, K_1), v_N(t) \right]$$

$$+ \frac{\pi}{\hbar} \sum_e \delta(\Delta E(e)) \{ 2U(e) v_{N-e}(t) U^\dagger(e) - U^\dagger(e) U(e) v_N(t) - v_N(t) U^\dagger(e) U(e) \}. \quad (6a)$$

The first line in (6a) describes atomic motion between the different phase space cells within a given $K$-band. The first term is a streaming term with current operator $j_K(x)$ (for a formal definition see (42 below), and the second term corresponds to wavepacket spreading (the field operator for a $K$-band will be defined in Eq. (eq1.16)). The second line is (coherent) forward scattering, and the last describes the redistribution by collisions according to a $U(e)$-operator, which is expressible in terms of the interaction potential, and is explicitly defined in (47). A detailed derivation of the equation will follow in Sec. IV below.

1. Wavefunction stochastic differential equation (SDE) interpretation

It is interesting to interpret (6a) from the point of view of evolution of a stochastic $N$-atom wavefunction where the wide angle collisions are described as quantum jumps [47]. Note that (6a) can be written in the form

$$\dot{v}_N(t) = -\frac{i}{\hbar} H_{\text{eff}} v_N(t) + \frac{i}{\hbar} v_N(t) H_{\text{eff}}^\dagger + 2\pi \frac{\hbar}{\hbar} \sum_e \delta(\Delta E(e)) U(e) v_{N-e}(t) U^\dagger(e). \quad (7)$$

Let us define an atomic state vector $|\psi_N(t)\rangle$ with $N(K)$ a given configuration of occupation numbers. In the time evolution of this state vector a collision is associated with an instantaneous jump

$$|\psi_{N+e}(t + dt)\rangle \propto U(e)|\psi_N(t)\rangle \quad (9)$$
Here the $U$-matrix plays the role of the jump operator, connecting configurations $N(K) \to N(K + e)$. The probability for a collision is in the time interval $(t, t + dt)$, given a normalized statevector $|\psi_N(K)(t)\rangle$ at time $t$, by

$$P_{(t,t+dt)} = \frac{2\pi}{\hbar} \sum_e \delta(\Delta E(e))|U(e)|^2 |\psi_N(t)\rangle^2 dt$$  \hspace{1cm} (10)

The time evolution between the collisions is governed by the nonhermitian Hamiltonian $H_{\text{eff}}$,

$$|\psi_N(K)(t)\rangle = e^{-iH_{\text{eff}}t/\hbar}|\psi_N(K)(0)\rangle.$$  \hspace{1cm} (12)

Physically, (12) describes the streaming and forward scattering between the jumps, and the nonhermitian is associated with loss due to collisions. Note that $H_{\text{eff}}$ preserves the distribution $N(K)$ (see Figs. 2a and b). A stochastic average over these quantum trajectories give the density matrix, $\rho_N(t) = \langle \langle |\psi_N(t)\rangle |\psi_N(t)\rangle |\psi_N(t)\rangle^2$.}

### D. Limiting cases

The Quantum Kinetic Master Equation (6a) includes as a limiting cases both the Quantum Boltzmann master equation and the Uehling-Uhlenbeck equation, as well as an equation analogous to the Gross-Pitaevskii equation. These results will be derived in Sec. V).

1. Quantum Boltzmann master equation

If we assume a single spatial cell, i.e. the size of the system equals the dimension of the system (compare Figs. 1 and 2), the transport terms trivially disappear and Eq. (6a) reduces (Sec. V) to an equation which we shall call the Quantum Boltzmann master equation:

$$\dot{w}_n = -\frac{\pi}{\hbar^2} \sum_{1234} \delta(\Delta E(1234))|T_{1234}|^2$$

$$\times \left\{ n_1 n_2 (n_3 + 1)(n_4 + 1)[w_n - w_{n+e}] + (n_1 + 1)(n_2 + 1)n_3 n_4 [w_n - w_{n-e}] \right\}.$$  \hspace{1cm} (13)

This is a rate equation connecting the occupation probabilities of a given configuration $n \equiv N$, $w_n$, where the factors $n_k + 1$ reflect quantum statistics for the collisional transition rates. It obviously has a limited validity, but it is attractive because of its simplicity and ease of simulation. [48].

2. Uehling-Uhlenbeck equation

For spatially inhomogeneous systems we derive from (6a) the Uehling-Uhlenbeck equation (Sec. V B). Let us
define a single particle distribution function \( f_{\mathbf{K}}(\mathbf{x}) \) where \( \mathbf{K} \) labels a momentum band and \( \mathbf{x} \) is a (continuous) spatial coordinate (for a precise definition see Eq. (12)). We interpret \( f_{\mathbf{K}}(\mathbf{x}) \) as a joint momentum position distribution function, similar to the Wigner function. Assuming a factorization of the \( N \)-atom distributions (an assumption not valid in the BEC regime) one obtains from \((6a)\) the kinetic equation

\[
\frac{\partial}{\partial t} f_{\mathbf{K}}(\mathbf{x}) \approx -\frac{\hbar \mathbf{K} \cdot \nabla \mathbf{x}}{m} f_{\mathbf{K}}(\mathbf{x}) + \frac{2|u|^2}{\hbar^2} \int \int \int d^3 \mathbf{K}_2 d^3 \mathbf{K}_3 d^3 \mathbf{K}_4 \\
\times \delta((\mathbf{K} + \mathbf{K}_2 - \mathbf{K}_3 - \mathbf{K}_4)) \delta(\omega + \omega_2 - \omega_3 - \omega_4) \\
\times \{ f_{\mathbf{K}}(\mathbf{x}) f_{\mathbf{K}_2}(\mathbf{x}) f_{\mathbf{K}_3}(\mathbf{x}) + 1 \} |f_{\mathbf{K}_4}(\mathbf{x}) + 1| \\
- \{ f_{\mathbf{K}}(\mathbf{x}) + 1 \} [f_{\mathbf{K}_2}(\mathbf{x}) + 1] f_{\mathbf{K}_3}(\mathbf{x}) f_{\mathbf{K}_4}(\mathbf{x}) \}
\]

(14)

which now includes a streaming term. The collisional term in Eq. (14) has been approximated as s-wave scattering.

3. Condensate master equation

Finally, to illustrate the kinetics of Bose condensation we will derive in Sec. (3) a simple approximation of the QKME based on the assumption that the density operator of the total system can be factorized into a condensate density operator \( \rho_0(t) \) for the \( \mathbf{K} = 0 \) Bose condensate band, and an operator for the non-condensed modes \( \mathbf{K} \neq 0 \) which is assumed to be in thermal equilibrium. We obtain the equation, which we shall call the condensate master equation:

\[
\dot{\rho}_0(t) = -\frac{i}{\hbar} \left[ \int d^3 \mathbf{x} \psi_0^\dagger(\mathbf{x}) \left( -\frac{\hbar^2 \nabla^2}{2m} \right) \psi_0(\mathbf{x}) + \frac{1}{2} \int d^3 \mathbf{x} \psi_0^\dagger(\mathbf{x}) \psi_0^\dagger(\mathbf{x}) \psi_0(\mathbf{x}) \psi_0(\mathbf{x}) , \rho_0 \right] \\
+ \left[ \frac{g(0)}{\hbar} \sum_{\mathbf{K} \neq 0} n_{\mathbf{K}} \right] \int d^3 \mathbf{x} \psi_0^\dagger(\mathbf{x}) \psi_0(\mathbf{x}) , \rho_0 \\
+ \int d^3 \mathbf{x} \int d^3 \mathbf{x'} G^{(-1)}(\mathbf{x} - \mathbf{x'}, T, \mu) \{ 2\psi_0(\mathbf{x}) \rho_0 \psi_0^\dagger(\mathbf{x'}) - \rho_0 \psi_0^\dagger(\mathbf{x'}) \psi_0(\mathbf{x}) - \psi_0^\dagger(\mathbf{x'}) \psi_0(\mathbf{x}) \rho_0 \} \\
+ \int d^3 \mathbf{x} \int d^3 \mathbf{x'} G^{(+)}(\mathbf{x} - \mathbf{x'}, T, \mu) \{ 2\psi_0^\dagger(\mathbf{x}) \rho_0 \psi_0(\mathbf{x'}) - \rho_0 \psi_0^\dagger(\mathbf{x'}) \psi_0(\mathbf{x}) - \psi_0(\mathbf{x'}) \psi_0^\dagger(\mathbf{x}) \rho_0 \},
\]

(15)

Here \( \psi_0(\mathbf{x}) \) refers to the atomic destruction operator for the \( \mathbf{K} = 0 \) band with the Bose condensate. The first line in Eq. (15) gives the dynamic of the Bose condensate including the nonlinear interaction term proportional to \( \psi_0^\dagger(\mathbf{x}) \psi_0^\dagger(\mathbf{x}) \psi_0(\mathbf{x}) \), and an interaction term of the atom in the Bose condensate with the above condensate particles with thermal occupation numbers \( g(0) \sum_{\mathbf{K} \neq 0} n_{\mathbf{K}} \) (where \( g(0) \) is a normalization factor to be defined in Eq. (27)). For zero temperature, and when the field operators \( \psi_0(\mathbf{x}) \) are replaced by c-numbers, Eq. (15) is, of course, equivalent to the Gross-Pitaevskii equation. For finite temperature, solutions of the corresponding Hartree Fock equations have been discussed in references (19)(20)(21). The
second and third line in Eq. (15) give dissipative loss and feeding terms for the condensate due collisions with the non-condensed atoms. The relevant collisions are of the form $K_1, K_2 \leftrightarrow K_3, K = 0$, where atoms are transferred to the Bose mode under conservation of momentum and energy. In Eq. (15) these transition rates are denoted to $G^{(\pm)}(x-x',T,\mu) \text{ (to be defined in Sec. 138); they involve the occupation numbers of the } K \neq 0 \text{ modes according to the given temperature and chemical potential.}$

4. Validity of the limiting cases

These three cases are all very simplified, and more realistic applications of the QKME will require much more care. But each one them illustrates a different aspect of the problem of quantum kinetics, which gives them great value as an aid to intuition.

III. DESCRIPTION OF THE SYSTEM

We consider a set of Spin-0 Bose particles, described by the Hamiltonian

$$H = H_0 + H_I + H_T,$$

in which

$$H_0 = \int d^3x \psi^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \psi(x)$$

and

$$H_I = \frac{1}{2} \int d^3x \int d^3x' \psi^\dagger(x) \psi^\dagger(x') u(x-x') \psi(x') \psi(x).$$

Thus, the operators $\psi(x)$ have the commutators

$$[\psi(x), \psi^\dagger(x')] = \delta(x-x'),$$

$$[\psi(x), \psi(x')] = [\psi^\dagger(x), \psi^\dagger(x')] = 0.$$ 

The potential function $u(x-x')$ is a c-number and is as usual not the true interatomic potential, but rather a short range potential—approximately a delta function—which reproduces the correct scattering length. This enables the Born approximation to be applied, and thus simplifies the mathematics considerably.

The term $H_T$ arises from a trapping potential, and is written as

$$H_T = \int d^3x V_T(x) \psi^\dagger(x) \psi(x).$$

In this paper we will restrict our considerations to the case of no trapping potential, so $V_T$ will be set equal to zero. The modifications necessary if there is a nonzero trapping potential will be dealt with in a future publication.

Thus, this is the standard second quantized theory of an interacting Bose gas of particles with mass $m$. 

10
A. Possible phase space descriptions

1. The Wigner function

The original work of Bose and Einstein [51] was conceived before the invention of quantum mechanics by Heisenberg and Schrödinger, and was based on a simple phase space description, in which both momentum and coordinate space were discretized to give phase space cells of volume $h^3$. The state of the system was then specified by the number of quanta in each phase space cell. The treatments in modern elementary textbooks use essentially the same arguments, but use a single large box in coordinate space, so that the discretizing comes about from the discrete energy levels in this box.

We will want to develop a formulation which is as close to the Boltzmann equation as is permitted by the quantum mechanical nature of the problem. This requires a phase-space description of the field $\psi(x)$. Although it might seem that the Wigner function provides the appropriate method, it is in fact impossible to write a phase-space Wigner function for a multiparticle system which manifestly exhibits the symmetry of the Bose wavefunction. A simple demonstration of this problem can be made for a two particle system whose Wigner function is obtained from the Fourier transforms with respect to $y_1, y_2$, of

$$\text{Tr}\{\psi(x_1 + y_1)\psi(x_2 + y_2)\psi^\dagger(x_1 - y_1)\psi^\dagger(x_2 - y_2)\rho_0\} = W(x_1, y_1, x_2, y_2),$$

(23)

where $\rho_0$ is the density operator of the vacuum. Thus, the Wigner function is (where $N$ is an appropriate normalization factor)

$$W(x_1, k_1, x_2, k_2) = N\int e^{2i(k_1 \cdot y_1 + k_2 \cdot y_2)} W(x_1, y_1, x_2, y_2) d^3y_1 d^3y_2.$$  

(24)

The Wigner function has the symmetry $1 \leftrightarrow 2$; but this is not the full Bose symmetry, which requires full symmetry under the independent exchanges:

$$x_1 + y_1/2 \leftrightarrow x_2 + y_2/2,$$

$$x_1 - y_1/2 \leftrightarrow x_2 - y_2/2.$$  

(25)

The Wigner function symmetry $1 \leftrightarrow 2$ is given by the simultaneous exchanges, not the independent exchanges. The problem obviously persists for all numbers of particles. Where the Wigner function has been used in kinetic theory [52], the Bose symmetry takes the form of a very complicated integral operator relation, whose use is very impractical. Although an exact evolution equation would preserve Bose symmetry, the absence of manifest Bose symmetry makes it extremely difficult to develop approximation methods which preserve Bose symmetry. In fact it is only in a very dilute gas limit, in which essentially only the one-particle Wigner function occurs that the Wigner function has been used, and for this of course Bose symmetry is not an issue.
2. Wavelet expansion of field operators

The most natural way to give a phase space description of a Bose gas is to follow the method of Bose and Einstein—that is, to divide space into cells of volume $\Delta V$, and for each cell to introduce a set of basis wavefunctions which vanish outside the cell, but are quantized within the cell. Unfortunately, even from the point of view of the non-interacting Hamiltonian (18), such wavefunctions have infinite energy, arising from the sharp transition from inside to outside the cell. This yields a wavefunction which is not twice differentiable, as required by (13), so that the spread in momentum $p$ is so large that the mean of $p^2$ is diverges.

To avoid this problem, the transition from inside the cell to outside it must be made smoother, and this is a problem which is like that which arises in the study of wavelets [53]. We introduce a set of wavelet functions (in one dimension)

$$v_K(x, r) = \frac{1}{\sqrt{4\pi \Delta}} \int_{K-\Delta}^{K+\Delta} e^{ik(x-r)} dk$$

$$\equiv \frac{e^{ik(x-r)}}{\sqrt{\pi \Delta}} \sin \frac{\Delta(x-r)}{x-r}.$$  \hfill (26)

If

$$r = n\pi/\Delta, \quad n = 0, \pm 1, \pm 2, ...$$ \hfill (27)

these functions have the property of orthogonality:

$$\int_{-\infty}^{\infty} dx v_K^*(x, r)v_K(x, r) = \delta_{KK'}\delta_{rr'}$$ \hfill (28)

and they are also complete. From the definition (26), it can be seen that $v_K(x, r)$ has momenta in the range $\Delta h (K-\Delta), \Delta h (K+\Delta)$, and from (27), it can be seen that wavefunction $v_K(x, r)$ is localized to a certain extent at the point $x = r \equiv n\pi/\Delta$.

These wavefunctions correspond to a complete set of phase cells; we see that if the uncertainties are defined as the intervals between the discrete values of the momenta and position, then

$$\delta x = \pi/\Delta \text{ and } \delta p = 2\Delta \hbar \Rightarrow \delta x \delta p = \hbar$$ \hfill (29)

However, the uncertainty as defined by a variance in $x$ is clearly infinite, reflecting the fact that the wavelet functions (26), (27) are not well localized. The quantities $\delta x$, $\delta p$ represent rather the spacing between the phase cells—not the uncertainties in $x$ and $p$. In terms of the variable $x$, these wavelet functions represent the smoothest possible functions we could choose, because by construction the momentum spread is bounded, so that the wavelet functions are in fact infinitely differentiable.

The field operators can now be expanded as (in an obvious three-dimensional generalization)
\[ \psi(x) = \sum_K \sum_r v_K^*(x, r) a(r, K) \] (31)

and the commutation relation for \( a(r, K) \) is

\[ [a(r, K), a^\dagger(r', K')] = \delta_{rr'} \delta_{KK'} . \] (32)

The states of the Bose gas are now specified by the eigenvalues of the number operators \( N(r, K) \), which is a truly quantum mechanical version of the original idea of Bose.

Notice that there is no need in this description for \( \Delta \) to be unique—one can choose a different value of \( \Delta \) for each \( K \)-band if one wishes, since momentum bands are orthogonal independently of their size.

3. Momentum resolved field operators

For many parts of our discussion, it is convenient to resolve field operators into only the different ranges of momentum; thus we write

\[ \psi(x) = \sum_K e^{-ik \cdot x} \psi_K(x) \] (33)

where

\[ \psi_K(x) = e^{iK \cdot x} \sum_r v_K^*(x, r) a(r, K) \] (34)

\[ = e^{iK \cdot x} \int D_K(x - x') \psi(x') \, d^3 x' \] (35)

where

\[ D_K(x - x') = e^{-iK \cdot (x - x')} g(x - x') \] (36)

where

\[ g(x) = \frac{1}{\pi^3} \left[ \frac{\sin \Delta x}{x} \right] \left[ \frac{\sin \Delta y}{y} \right] \left[ \frac{\sin \Delta z}{z} \right] . \] (37)

We also have the commutation relation

\[ [\psi_K(x), \psi_{K'}^\dagger(x')] = \delta_{KK'} g(x - x') . \] (38)

The resolution into momentum bands thus yields a rather nonlocal description. Notice also that we can write

\[ g(x - x') = \frac{1}{(2\pi)^3} \int_{-\Delta}^{\Delta} e^{ik \cdot (x - x')} \, d^3 k \]

\[ = \sum_r e^{-iK \cdot (x - x')} v_K(x, r) u_K^*(x', r), \] (39)

which is an expression of the completeness of the wavelet functions within a \( K \)-band, and is useful in some of the computations used in deriving the Uehling-Uhlenbeck equation in sect.\[\sqrt{\text{V}}\]
4. Free Hamiltonian in terms of momentum resolved field operators

Because the functions used in the expansion of \( e^{-iK \cdot x} \psi_K(x) \) are orthogonal to those used for \( e^{-iK' \cdot x} \psi_{K'}(x) \), it is obvious that

\[
\int d^3x \psi^\dagger_K(x) \psi_{K'}(x) e^{-i(K' - K) \cdot x} = 0 \quad \text{if} \quad K \neq K'.
\]

(40)

Using this fact, it is straightforward to show that

\[
H_0 = \sum_K \bar{\hbar}^2 K^2 \int d^3x \psi^\dagger_K(x) \psi_K(x) \quad (41a)
\]

\[
+ \sum_K \int d^3x \bar{\hbar} K \cdot j_K(x) \quad (41b)
\]

\[
+ \sum_K \int d^3x \psi^\dagger_K(x) \left( -\frac{\bar{\hbar}^2 \nabla^2}{2m} \right) \psi_K(x) \quad (41c)
\]

\[
\equiv H_a + H_b + H_c
\]

Here we have used a “probability current” for the momentum \( K \) defined in a way analogous to that normally employed

\[
j_K(x) \equiv -\frac{i\hbar}{2m} \left\{ \psi^\dagger_K(r) \nabla \psi_K(r) - \nabla \psi^\dagger_K(r) \psi_K(r) \right\}. \quad (42)
\]

The resolution into three parts has a simple interpretation. The resolution into a full wavelet description shows that we can write

\[
H_a = \sum_{K,r} \frac{\hbar^2 K^2}{2m} a^\dagger_{K}(r)a_{K}(r) \quad (43)
\]

corresponding to an energy \( \hbar^2 K^2 / 2m \) for each quantum at each phase space location \( K, r \). This is the Hamiltonian corresponding to the original ideas of Bose and Einstein.

The term \( H_b \) corresponds to transport, as shown by computing the commutator

\[
[H_b, \psi_K(x)] = i\hbar v_K \cdot \nabla \psi_K(x) \quad (44)
\]

where \( v_K = \hbar K / m \). This is obviously transport corresponding to the velocity appropriate to the central momentum of the momentum band \( K \).

Finally, the last term \( H_c \) corresponds to wavepacket spreading through

\[
[H_c, \psi_K(x)] = -\frac{\hbar^2}{2m} \nabla^2 \psi_K(x) \quad (45)
\]

Thus the wavelet description naturally gives the separation into the three parts fundamental to a phase space description of the processes.
5. Interaction Hamiltonian in terms of the momentum resolved field operators

It is trivial that the interaction part, \( H_I \), can be written

\[
H_I = \frac{1}{2} \sum_{K_1, K_2, K_3, K_4} U(K_1, K_2, K_3, K_4),
\]

in which

\[
U(K_1, K_2, K_3, K_4) = \int d^3x \int d^3x' e^{i(K_1 \cdot x + iK_2 \cdot x' - iK_3 \cdot x - iK_4 \cdot x')} \psi^\dagger_{K_1}(x) \psi^\dagger_{K_2}(x') u(x - x') \psi_{K_3}(x') \psi_{K_4}(x).
\]

Furthermore, it is easy to see that

\[
U(K_1, K_2, K_3, K_4) = 0
\]

unless

\[
K_1 + K_2 = K_3 + K_4 + O(\Delta)
\]

i.e., the quasimomentum \( K_1 \) is conserved to within something not much bigger than \( \Delta \).

IV. TREATMENT OF COLLISIONS

A. Eigenstates of \( H_a \) and its corresponding Liouvillian

Suppose we use the wavelet basis; then we can label the eigenstates of \( H_a \) (as given in (41a)) as \( |n⟩ \) where \( n \) is a vector of elements \( n_i \), the number of quanta belonging to the phase space wavelet \( i \), which has quantum number \((K_i, r_i)\). The eigenstates of the corresponding Liouvillian are given by the outer product \( |n⟩ ⟨m| \), and the eigenvalue is only zero if the energy of \( |n⟩ \) is the same as that of \( |m⟩ \).

B. Projectors

We will define a projector onto all eigenstates with the same number of quanta in each \( K \), irrespective of \( r \); thus we define

\[
p_N|n⟩ = |n⟩ \quad \text{if} \quad \sum_r n(K, r) = N(K) \quad \text{and} \quad K \neq 0;
\]

\[
= 0 \quad \text{otherwise.}
\]

This kind of projector identifies all configurations with the same distribution in \( K \), but ignores \( K = 0 \) and leaves undisturbed the distribution over \( r \).

Suppose now that \( \rho \) is the density operator for the system of particles; we define a projector on \( \rho \) by
\[ \mathcal{P}_N \rho = \rho_N \rho \rho_N \equiv v_N. \]  

(51)

Thus the projected \( \rho \) is an operator in position space, but acts only with a space that has the configuration \( N \) of particles over the momentum space cells—except any configuration of \( K = 0 \) particles is permitted (we call this \( K \) diagonal). It follows also that, for any \( \rho \)

\[
\mathcal{P}_N H_b \rho = H_b \mathcal{P}_N \rho \\
\mathcal{P}_N H_c \rho = H_c \mathcal{P}_N \rho
\]  

(52a, 52b)

and that for \( H_a \) there is the stronger result

\[ [H_a, \mathcal{P}_N \rho] = 0 \]  

(53)

which is true by construction.

The thrust of this paper is now to develop a closed equation of motion for the projected parts of \( \rho(t) \), namely \( v_N(t) \), and to show that we can use these parts to represent the physics in which we are interested. Thus we will be making the approximation

\[ \rho(t) \approx \sum_N v_N(t), \]  

(54)

which will require the assumption that we can neglect the remainder: thus

\[ w(t) \equiv \left( 1 - \sum_N \mathcal{P}_N \right) \rho(t) \approx 0. \]  

(55)

A density operator of the form (54) will be called \( K \)-diagonal. For such \( K \)-diagonal density operators, the algebra in deriving the equations of motion is considerably simplified by results like

\[ \mathcal{P}_M \{ \psi_K^\dagger(x) \psi_K'(x') v_N \} = 0 \]

unless \( K = K' \) and \( M = N \).  

(56)

Notice however that in this equation, we do not require that \( x = x' \); thus the designation \( K \)-diagonal is appropriate. Another kind of identity is

\[ \mathcal{P}_M \{ \psi_K^\dagger(x) v_N \psi_K(x') \} = 0 \]

unless \( K = K' \) and \( M = N + b \).  

(57)

where \( b \) is a vector in the same space as \( M \) and \( N \), and whose only non-zero component is \( b(K) = 1 \), so that \( M \) and \( N \) are identical apart from the change \( M(K) = N(K) + 1 \).

There are many other relations like these, but all are essentially of the same kind, that the \( K \)-diagonal property is preserved only by matching a creation field operator with a destruction field operator with the same \( K \), though not necessarily the same \( x \), either on the same or the other side of the density operator. If the matching is done on the same side, the configuration \( N \) is preserved, if the matching is done on opposite sides the configuration changes.
C. Derivation of the quantum kinetic master equation

The equation of motion for the density operator is
\[
\dot{\rho} = -\frac{i}{\hbar} [H_a + H_b + H_c, \rho] - \frac{i}{\hbar} [H_I, \rho]
\]
(58)

\[
= \mathcal{L}_a \rho + \mathcal{L}_b \rho + \mathcal{L}_c \rho + \mathcal{L}_2 \rho.
\]
(59)

We define the Laplace transform
\[
\tilde{\rho}(s) = \int_0^\infty e^{-st} \rho(t) dt
\]
(60)
and correspondingly
\[
\tilde{v}_N(s) = \mathcal{P}_N \tilde{\rho}(s)
\]
(61)
\[
\tilde{w}(s) = \mathcal{Q} \tilde{\rho}(s) \equiv \left[ 1 - \sum_N \mathcal{P}_N \right] \tilde{\rho}(s),
\]
(62)
so that
\[
sv_N(s) - v_N(0)
\]
\[
= (\mathcal{L}_b + \mathcal{L}_c) \tilde{v}_N(s) + \mathcal{P}_N \mathcal{L}_2 \left\{ \sum_M \tilde{v}_M(s) + \tilde{w}(s) \right\}
\]
(63)
and
\[
sw(s) - w(0)
\]
\[
= \{\mathcal{L}_a + \mathcal{L}_b + \mathcal{L}_c\} \tilde{w}(s) + \mathcal{Q} \mathcal{L}_2 \left\{ \sum_M \tilde{v}_M(s) + \tilde{w}(s) \right\}.
\]
(64)

We assume \(w(0) = 0\), that is the state that is already \(K\)-diagonal. This assumption cannot be made without some justification, which we shall postpone to Sect. IV D 3. Obviously we can choose any initial condition we wish; the justification required is that when we solve the equations of motion it will be possible to show that \(w(t)\) rapidly becomes negligible, and negligible at all times, so that any time can be chosen as an initial time.

From this we can then readily derive
\[
sv_N(s) - v_N(0) = (\mathcal{L}_b + \mathcal{L}_c) \tilde{v}_N(s) + \mathcal{P}_N \mathcal{L}_2 \sum_M \tilde{v}_M(s)
\]
\[
+ \mathcal{P}_N \mathcal{L}_2 [s - \mathcal{L}_a - \mathcal{L}_b - \mathcal{L}_c - \mathcal{Q} \mathcal{L}_2]^{-1} \mathcal{Q} \mathcal{L}_2 \sum_M \tilde{v}_M(s).
\]
(65)

This equation is exact; the physical content comes into the assumptions concerning what parts can be considered to be negligible. We invert the Laplace transform in (65), and consider the parts separately.

1. Streaming and Quantum Terms

These are the names we use for \(\mathcal{L}_b\) and \(\mathcal{L}_c\) as defined in (59), (41b, 41c). They keep the same form with no approximations.
2. The Forward Scattering Terms

The term $\mathcal{P}(\mathbf{N}) \mathcal{L}_2 \sum_M \hat{v}_M(s)$ can be simplified by noting that $v_M(s)$ is $K$-diagonal, and that $\mathcal{P}(\mathbf{N})$ projects onto a $K$-diagonal density operator. Since $\mathcal{L}_2$ is a commutator; i.e.,

$$\mathcal{L}_2 \sum_M v_M(s) = -\frac{i}{\hbar} \sum_M [H_1, v_M(s)]$$  \hspace{1cm} (66)

this can only yield a $K$-diagonal term from those parts of $H_1$ which do not change the $K$-distribution; that is, the terms in $H_1$ given by $H_F$, which we define as

$$H_F \equiv \frac{1}{2} \sum_{K_1 \neq K_2} U(K_1, K_2, K_1, K_2) + \frac{1}{2} \sum_{K_1 \neq K_2} U(K_1, K_2, K_2, K_1) + \frac{1}{2} \sum_{K_1} U(K_1, K_1, K_1, K_1).$$  \hspace{1cm} (67)

This thus gives only transitions between the same $K$ distribution, and this can be regarded as forward scattering. These forward scattering terms give rise to the so-called mean field effects, that is the average effect on the motion of one particle of the interaction with all other particles.

3. The Collision Terms

We now introduce a Born approximation, which amounts to the neglect of $\mathcal{L}_b + \mathcal{L}_c + Q\mathcal{L}_2$ in the $|\cdot|^{-1}$ term in (65), leaving a contribution to $\dot{v}_N(t)$ given by

$$\sum_M \mathcal{P}_N \mathcal{L}_2 \int_0^t d\tau \exp \{ \mathcal{L}_a \tau \} Q\mathcal{L}_2 v_M(t - \tau).$$  \hspace{1cm} (68)

Notice however that $Q\mathcal{L}_2$ contains terms which depend on $\psi_0, \psi_0^\dagger$, and when there is significant condensation these terms can become very large. Thus this approximation is valid only in the case of weak condensation. This means that we approximate the free evolution operator by discretizing the eigenvalues to those corresponding to the centers of the momentum bands. This leads to an approximate measure of the validity of the neglect of the terms $Q\mathcal{L}_2$ in comparison to the term retained, $\mathcal{L}_a$, which is given by requiring that the modification by the presence of any condensate to the excitation spectrum should be negligible for energy greater than $\hbar^2 \Delta^2/2m$. Using the Bogoliubov theory, this leads to the conclusion that we must have the condition on the cell size

$$l_c = \frac{\pi}{\Delta} \gg \frac{\pi \hbar}{\sqrt{2m \rho u}} = \frac{\sqrt{\pi}}{8a \rho}$$  \hspace{1cm} (69)
where $\rho$ is the density of particles. We now want to make a Markov approximation, which involves two steps. Firstly we neglect the $\tau$ dependence in the last term, and secondly we let the upper limit in the integral become infinite. For this approximation to be valid there must be a smooth distribution over the available energy states, so that when we sum over all $M$, the resultant range of $\tau$ in which the integrand is non-zero is very much smaller then the characteristic time over which $v_M(t)$ evolves. This is a requirement on the kind of $v_M(t)$ being considered.

Now define the vector in the space of $M, N$, called $e(1234)$ which can be written

$$e(1234)_{K_1} = e(1234)_{K_2} = -e(1234)_{K_3} = -e(1234)_{K_4} = 1.\quad (70)$$

and all other components are zero, and let

$$\hbar\omega_K = \frac{\hbar^2 K^2}{2m} \quad (71)$$

We also introduce the notation

$$\Delta\omega_e = \omega_4 + \omega_3 - \omega_1 - \omega_2, \quad (72)$$

Before we examine the range of validity of the Markov conditions, we can see that using them (68) now becomes

$$-\frac{1}{4\hbar^2} \mathcal{P}_N \sum_{1234} \{ \left[ U(1'2'3'4'), \right. \left. \int_0^\infty d\tau \exp(i\Delta\omega_e\tau) \right] \mathcal{Q}[U(4321), \sum_M v_M(t)] \}. \quad (73)$$

Since the state $v_M(t)$ is $K$-diagonal, and we project onto $K$-diagonal states, we must have

$$1 = 1', 2 = 2' \text{ or } 1 = 2', 2 = 1'$$

and

$$3 = 3', 4 = 4' \text{ or } 3 = 4', 4 = 3'$$

but since the operator $U(1234)$ is symmetric in $(12)$ and $(34)$ this simply gives 4 times the result obtained from setting $(1234) = (1'2'3'4')$.

Notice that no “forward scattering terms” arise in (73). These have already been explicitly separated from the scattering terms and included in the term $H_F$ defined in (71), and are eliminated from (73) by the $\mathcal{Q}$ projection operator.

We can now carry out the time integral so that (73) becomes

$$-\lim_{\epsilon \to 0} \sum_e \left\{ \frac{U_e U_e^\dagger v_N + v_N U_e^\dagger U_e - U_e v_N - e U_e^\dagger - U_e^\dagger v_N + e U_e}{\hbar^2 (\epsilon + i\Delta\omega_e)} \right\}. \quad (74)$$
Here we have used $U(1234) = U(4321)$. We now use
\[ \frac{1}{z + i\epsilon} \rightarrow P \frac{1}{z} - i\pi\delta(z) \] (75)
and rearrange, so that (74) becomes
\[ -\frac{i}{\hbar} \sum_e P \frac{1}{\Delta\omega_e} [U_e U^\dagger_e, v_N] + \frac{\pi}{\hbar^2} \sum_e \delta(\Delta\omega_e) \{ 2U_e v_{N-e}(t)U^\dagger_e - U^\dagger_e U_e v_N - v_N U^\dagger_e U_e \}. \] (76)

As is usual, we find a level shift term, which is a commutator, and a purely dissipative term. Adding together (76), (66), (59), we get the full Quantum Kinetic Master Equation (QKME)
\[ \dot{v}_N(t) = -\frac{i}{\hbar} \sum_K \int d^3x \left( \frac{\hbar K}{2m} \cdot j_K(x), v_N(t) \right) \] (77a)
\[ -\frac{i}{\hbar} \sum_K \int d^3x \psi_K^\dagger(x) \left( -\frac{\hbar^2 \nabla^2}{2m} \right) \psi_K(x), v_N(t) \] (77b)
\[ -\frac{i}{2\hbar} \sum_{K_1 \neq K_2} (U(K_1, K_2, K_1, K_2) + U(K_1, K_2, K_2, K_1)) + \sum_{K_1} U(K_1, K_1, K_1, K_1), v_N(t) \] (77c)
\[ -\frac{i}{\hbar^2} \sum_e P \frac{1}{\Delta\omega(e)} [U(e) U^\dagger(e), v_N(t)] \] (77d)
\[ + \frac{\pi}{\hbar^2} \sum_e \delta(\Delta\omega(e)) \{ 2U(e) v_{N-e}(t) U^\dagger(e) - U^\dagger(e) U(e) v_N(t) - v_N(t) U^\dagger(e) U(e) \}. \] (77e)

D. Approximations

1. Weak condensation condition

Approximations only occur in the derivation of the collision and level shift terms. The major approximation is the neglect of $L_b + L_c + QL_2$ compared to $L_a$. We choose $\Delta$ so that eigenvalues of $L_a$ (apart from zero eigenvalues) are substantially larger than typical measures of the size of $QL_2$ on the particular states involved. Since the projectors $P_N$ do not affect the $K = 0$ composition of the states, the operator $QL_2$ includes the term $(u/2) \int d^3x \psi_0^\dagger \psi_0^\dagger \psi_0 \psi_0$, which can become very large when there is significant condensation, hence this approximation will only be valid in the case of weak condensation, the condition for which is given by (69); that is
\[ l_c = \frac{\pi}{\Delta} \gg \frac{\pi \hbar}{\sqrt{2m\rho u}} \]
\[ = \frac{\pi}{\sqrt{8\rho u}} \] (78)

We will deal with the issues of strong condensation in a subsequent paper.
2. The Markov Approximation

The Markov approximation is really a kind of perturbative result. The change from the integral \( \int_0^t d\tau \rightarrow \int_0^{\infty} d\tau \) requires the assumption that the terms that turn up have a broad spectrum of frequencies which are almost continuous. The frequencies which do turn up are of the form \( \omega_n \), and the range of these is of the order \( kT/\hbar \), while a typical separation between the frequencies corresponding to adjacent transitions with a typical magnitude of momentum \( \sqrt{2mkT} \) is of order of magnitude \( \Delta \sqrt{2kT/m} \), which is the inverse of the time required for a particle to traverse a cell at a typical thermal velocity.

The condition that we can regard the frequency spectrum as almost continuous is that the separation between the frequencies is very much less than their range, that is, the density of states is sufficiently high. Quantitatively, this leads to

\[
l_c \gg \lambda_T \equiv \hbar/\sqrt{2mkT}. \tag{79}
\]

If the density operators \( v_N \) are such that the contributions from sums over the different \( e \) are all smoothly varying functions of the contributing frequencies, then the time dependence given by summing up over all transitions in (73) will drop off over a characteristic time given by the inverse of the bandwidth, i.e., \( \hbar/kT \), and this time must be very much less than the typical time scale of evolution of the the distribution, which is of the order of magnitude of the time between collisions. This leads to the requirement on the mean free path \( \lambda_{mfp} \)

\[
\lambda_{mfp} \gg \lambda_T. \tag{80}
\]

Finally, the QKME itself gives a level broadening, which is implicitly small compared to the distance between levels. The condition for this must be that there is little likelihood of a collision as a particle traverses a single cell, which means of course that

\[
\lambda_{mfp} \gg l_c \tag{81}
\]

All these conditions can be consistently satisfied.

Coming back now to the quantum kinetic master equation we see that the summations \( \sum_e \) are over the discrete momentum ranges \( K_1, K_2, K_3, K_4 \), and the energy conservation delta function is sharp. This sharpness is really an artifact which arises from the extension of the upper limit of the time integral to infinity. This integral can be cut off at any time very much larger than the characteristic decay time of the kernel, \( \hbar/kT \). This means that the delta function can be taken as being broadened correspondingly, and it is easy to see that this broadening can encompass a significant number of momentum bands. Nevertheless, this broadened delta function can be written as an exact delta function if the remainder of the integrand is smooth, and the sums written as integrals using the continuum approximation \( \sum \rightarrow \int d^3K \).
However, we have already assumed this smoothness in establishing the validity of the Markov approximation so this procedure is consistent with the Markov approximation.

3. The neglect of \( w(0) \)

We will assume \( w(0) = 0 \), and then make an estimate of the size of \( w(t) \) and find under what conditions that it is negligible for all future times. From (64) it follows, on inverting Laplace transforms, that

\[
w(t) = \int_0^t \exp \{ (L_a + L_b + L_c + Q\mathcal{L}_2)(t - t') \} \sum_M v_M(t') dt'.
\]

(82)

We can now approximate this by keeping \( L_a \), as in the derivation of the QKME, and replacing the effect of the all the other terms, including the interactions, by a phenomenological decay term, so that we write approximately

\[
w(t) \approx \int_0^t e^{\{ (L_a - \gamma)(t - t') \} \sum_M v_M(t') dt'.
\]

(83)

\[
= -\frac{i}{\hbar} \sum_e \sum_M e^{(i\Delta\omega_e - \gamma)(t - t')} [U(e), v_M(t')] dt'.
\]

(84)

As in the QKME derivation, we make the replacement \( v_M(t') \rightarrow v_M(t) \), and now we can do the integration over \( t' \) to get approximately

\[
w(t) \approx -\frac{i}{\hbar} \sum_e \sum_M \frac{1}{\gamma - i\Delta\omega_e} [U(e), v_M(t)].
\]

(85)

For any given \( M \) and \( e \) we get a specific non-\( K \)-diagonal term. The largest of these will occur when \( \Delta\omega_e = 0 \). To estimate their size, we go to the definition (47) of \( U(e) \). Substituting the expansion on wavelet functions into this equation, and assuming the approximation \( u(x) = u\delta(x) \), we find that the largest terms that occur are of the form

\[
\int d^3x / v_{K_1}(x, r) e^{iK_1 \cdot x} v_{K_2}(x, r) e^{iK_2 \cdot x} \times v_{K_3}^*(x, r) e^{-iK_3 \cdot x} v_{K_4}^*(x, r) e^{-iK_4 \cdot x} \times a^d(K_1, r) a^d(K_2, r) a(K_3, r) a(K_4, r)
\]

(86)

in which all wavelet functions refer to the same cell. Using the definitions of the wavelet functions, the coefficient of the operator part in this equation can be estimated to be of order of magnitude \( 1/l_c^3 \). The effect of the creation and destruction operators is of order of magnitude 1, so we can now estimate the size of the term in \( w(t) \) compared to those in \( v_M(t) \) to be of order of magnitude given by
\[ w(t) \approx \frac{a}{\lambda_{\text{mfp}} l_c^3} \]
\[ \times \sum_{e,M,r} [a^\dagger (K_1, r) a^\dagger (K_2, r) a(K_3, r) a(K_4, r), v_M(t)]. \] (87)

The size of the initial coefficient can be made clearest by taking \( \gamma \) to be given by \( \nu_T/\lambda_{\text{mfp}} \), in terms of which the coefficient can be simplified, leading to the condition for the validity of the neglect of non-\( K \)-diagonal terms:

\[ \frac{a \lambda_{\text{mfp}} \lambda_T}{l_c^3} \ll 1. \] (88)

This condition can be satisfied simultaneously with the two other conditions (79) and (80). For example, for sodium at \( T = 2\mu \text{K} \), the scattering length is \( a = 4.9 \text{nm} \), leading to

\[ \lambda_{\text{mfp}} = 0.42 \text{m} \] (89)
\[ \lambda_T = 4.8 \times 10^{-7} \text{m} \] (90)
\[ a = 4.9 \times 10^{-9} \text{m} \] (91)
\[ (a \lambda_{\text{mfp}} \lambda_T)^{1/3} \approx 10^{-5} \text{m} \] (92)

Thus if \( l_c \) is chosen in the range somewhat greater than \( 10^{-5} \text{m} \) this kind of treatment will be valid.

The condition (89) is best viewed as a condition on the condensate density \( \rho \); insertion of the sodium data into it gives the requirement that \( \rho \ll 10^{18} \text{m}^{-3} \), which can be satisfied, but will not always be satisfied in current experiments. In fact this density corresponds to about one atom per cube of volume \( \lambda_T^3 \) using the above data, which indicates that for an accurate treatment of condensation, the weak condensation assumption will be invalid in this case.

It should be borne in mind that all of the above has been in the absence of a trapping potential—the question will be revisited in our forthcoming paper dealing with strong condensation.

4. Born Approximation

The derivation of the collision terms relies on the Born approximation, and the collision rates appearing in the QKME (6a) are proportional to the Born scattering cross section. This implies that the potential should be weak, i.e. a small perturbation on the energy scale associated with the momentum coarse graining. In derivations of the quantum Boltzmann equation it is shown [5] that in a binary collision approximation, which assumes a low density but not necessarily a weak potential (\( \rho a^3 \ll 1 \)), the Born amplitude should be replaced by the two particle \( T \)-matrix element (proportional to the scattering amplitude \( a \) in low energy s-wave scattering). Essentially the same situation should pertain in this case and this means that we replace the exact interatomic potential with one for which the Born approximation is valid, and whose scattering length is the same as that of the exact potential.
However, a proof of this assertion in our formulation is at present lacking.

5. Level shifts

What are normally called “collisional level shifts” appear in our formalism in two guises. There are the forward scattering terms which generate $H_F$, as defined in (67), and there are the higher order terms which from the derivation of the collisional terms in (77d). In the weak condensation situation which we want to treat in this paper, we expect the density to be so low that these can be ignored, but in our forthcoming work it will not be possible to do so without more careful justification.

E. Stationary Solution

Let us assume the level shift term is small—negligible in fact. Then it is clear, since none of the other terms can actually change the eigenvalue of $H_a$, (the total coarse grained kinetic energy) or the total number of particles, that any function of

$$H_a = \sum_{r,\mathbf{K}} \frac{\hbar^2 \mathbf{K}^2}{2m} a_{\mathbf{K}}^\dagger(r)a_{\mathbf{K}}(r)$$

and

$$N = \sum_{r,\mathbf{K}} a_{\mathbf{K}}^\dagger(r)a_{\mathbf{K}}(r)$$

will provide a stationary solution—clearly microcanonical, canonical, and grand canonical versions will exist.

Thus the result is the statistical mechanical result—but coarse grained in momentum space—the size $\Delta$ of the momentum coarse graining to be such that $H_I$ is negligible compared with it on the states of interest.

1. Correlation Functions in the Stationary Solution

Since the stationary solution can be written as a function of $H_a$ and $N$, the correlation functions of the wavelet creation and destruction operators can be written as

$$\langle a_{\mathbf{K}}^\dagger(r)a_{\mathbf{K}'}(r') \rangle = \bar{N}_{\mathbf{K} \cdot \mathbf{K}'} \delta_{r,r'}.$$  

Assuming the grand canonical form

$$\rho_s(T,\mu) = \exp\left\{-(H_a - \mu N)/kT\right\},$$

which is of quantum Gaussian form, we can easily see that

$$\bar{N}_{\mathbf{K}}(T,\mu) = \left[\exp\left(\frac{\hbar \omega_{\mathbf{K}} - \mu}{kT}\right) - 1\right]^{-1}.$$
The field operator correlation function is then
\[ \langle \psi_K^\dagger(x)\psi_{K'}(x') \rangle = \delta_{KK'}g(x-x')\bar{N}_K(T,\mu) \] (98)
and similarly
\[ \langle \psi_K(x)\psi_{K'}^\dagger(x') \rangle = \delta_{KK',K'}g(x-x')[1 + \bar{N}_K(T,\mu)]. \] (99)

V. SIMPLEST APPLICATIONS OF THE QUANTUM KINETIC MASTER EQUATION

The situation in which something like the “molecular chaos” assumption of Boltzmann is valid is always of great interest, and it guides the intuition of most physicists in kinetic theory. We will consider in this section two simplified versions of the QKME which are valid in this situation, and one equation which permits the existence of coherent effects, which cannot arise in a molecular chaos regime.

The Uehling-Uhlenbeck equation, sometimes called the quantum Boltzmann equation, is a simple modification of the Boltzmann equation in which the phase space effects arising from quantum statistics are included. This equation will be derived by assuming the distribution is not very different from equilibrium, and by factorizing higher order correlation functions.

The situation in which we eliminate all dependence on position is obviously an extreme simplification, and corresponds to the system being composed of only one spatial cell. However, in this situation the QKME reduces to a stochastic master equation of great simplicity and intuitive appeal. This equation does not appear ever to have been treated in the literature, so we have given it the name “quantum Boltzmann master equation”.

Finally, a very simplified quantum mechanical master equation for the \( K = 0 \) band can be derived by assuming all other bands are thermalized. This equation will be called the “condensate Master equation”, and we are able to give an appealing description of the initiation of the condensation process, and of the growth of the condensate as long as the weak condensation condition is valid.

A. The quantum Boltzmann master equation

A very simple stochastic master equation can be derived by assuming that \( l = \pi/\Delta \) is equal to the size of the whole system, so that \( r \) takes on only one value. In this case we find that the \( K \)-bands are all one-dimensional, so that all the commutator terms, (77a–77d) are zero. Since in this case there is really no difference between \( n \) and \( N \), we can write
\[ v_n(t) = |n\rangle\langle n|w_n(t) \] (100)
so that \( w_n(t) \) is the occupation probability of the state \( n \).

We then derive what we will call the quantum Boltzmann master equation

\[
\dot{w}_n = -\frac{\pi}{\hbar^2} \sum_{1234} \delta(\omega_4 + \omega_3 - \omega_2 - \omega_1) |U_{1234}|^2 \\
\times \left\{ n_1 n_2 (n_3 + 1)(n_4 + 1) [w_n - w_{n+e}] \\
+ (n_1 + 1)(n_2 + 1)n_3 n_4 [w_n - w_{n-e}] \right\} 
\]  

(101)

For clarity of argument we will also write (100) in the form

\[
\dot{w}(n) = \sum_{1234} \left\{ t_{1234}^+(n-e)w(n-e) - t_{1234}^+(n)w(n) \right\} \\
+ \sum_{1234} \left\{ t_{1234}^-(n+e)w(n+e) - t_{1234}^-(n)w(n) \right\} 
\]  

(102)

where \( t_{1234}^\pm(n) = 0 \) unless \( \omega_1 + \omega_2 = \omega_3 + \omega_4 \), and if this is satisfied

\[
t_{1234}^+(n) = \gamma_{1234}(n_1 + 1)(n_2 + 1)n_3 n_4 \\
t_{1234}^-(n) = \gamma_{1234} n_1 n_2 (n_3 + 1)(n_4 + 1) 
\]  

(103)

and

\[
\gamma_{1234} = \frac{\pi |U_{1234}|^2}{\hbar^2}. 
\]  

(104)

1. The Boltzmann master equation

If we drop the terms \( 1 + n_i \) in the quantum Boltzmann master equation we get an equation called the Boltzmann Master Equation, which has been previously considered by Van Kampen [54] and Gardiner [55] based on stochastic arguments. The equation we have given includes no streaming terms, since we have only one spatial cell, and thus our treatment assumes that the energy levels are discretely spaced. This means that our normalization volume is so small that the broadening of the levels which arises from collisions is significantly less than the spacing between levels.

2. Stationary solutions

Apart from the ambiguities caused by conserved quantities, the solutions of equations like (101) are unique. There is a consistent detailed balance stationary solution, in which

\[
t_{1234}^+(n-e)w_s(n-e) = t_{1234}^-(n)w_s(n) 
\]  

(105)

and from this we see, using the explicit form (103) of \( t^\pm \), that
\[ \frac{w_s(n-e)}{w_s(n)} = \frac{t_{1234}(n)}{t_{1234}(n-e)} = 1 \]  \hspace{1cm} (106)

so that for all \( n \) able to be connected by a collision \( 1+2 \leftrightarrow 3+4 \),

\[ w_s(n) = \text{constant}. \]  \hspace{1cm} (107)

Thus \( w_s(n) \) is a function only of conserved quantities, total kinetic energy, momentum and the total number of particles. We can thus choose the grand canonical solution given by

\[ w_s(n) \propto \exp \left( -\frac{E - \mu N - u \cdot P}{kT} \right) \]  \hspace{1cm} (108)

where \( E \) is the total kinetic energy, \( N \) the total number of particles, and \( P \) the total momentum of the particles, while \( u \) is the mean velocity of the system. The stationary distribution is in this case factorizable

\[ w_s(n) = \prod_i \left( e^{-\frac{\bar{h} \omega_i - \mu - \bar{h} K_i \cdot u}{kT}} \right)^{n_i} \]  \hspace{1cm} (109)

3. Factorized equation for the mean occupation numbers

We can straightforwardly derive the equation for \( \langle n_a \rangle = \sum_n n_a w(n) \)

\[ \langle \dot{n}_a \rangle = 4 \sum_{234} \gamma_{a234} \left\{ -\langle n_a n_2(n_3+1)(n_4+1) \rangle \right. \\
+ \langle (n_a+1)(n_2+1)n_3n_4 \rangle \left\} \]  \hspace{1cm} (110)

If we assume that the averages inside this equation can be factorized, which should be valid if we are not too far from equilibrium, and for compactness set \( \langle n_i \rangle \rightarrow n_i \), we get (without the streaming terms) the Uehling-Uhlenbeck equation [42]:

\[ \dot{n}_a = 4 \sum_{234} \gamma_{a234} \left\{ -n_a n_2(n_3+1)(n_4+1) \right. \\
+ \langle (n_a+1)(n_2+1)n_3n_4 \rangle \left\} \]  \hspace{1cm} (111)

The quantum Boltzmann master equation is a very simple equation whose simulation is entirely feasible, and results of such simulations will be presented elsewhere. However, as shown by our derivation, it is expected that it will not give an accurate description of situations in which there is significant condensation. Nevertheless it could well give valuable insights into the region just below the threshold of condensation, which will be investigated in QKIII.
B. The Uehling-Uhlenbeck equation

We will now show that we can derive from the quantum kinetic master equation (77a–77e) the more conventional kinetic equation known as the Uehling-Uhlenbeck equation [42]. This equation is essentially the same as (111), but with streaming terms added as well, which in our derivation will arise naturally out of the streaming terms of the QKME. For this we consider the one particle distribution function to be defined as

\[
\frac{2\pi}{\Delta} \sum_{N} \operatorname{Tr}\left\{ \rho \psi_{K}^{\dagger}(x) \psi_{K}(x) \right\} \tag{112}
\]

\[
\frac{2\pi}{\Delta} \sum_{N} \operatorname{Tr}\left\{ v_{N} \psi_{K}^{\dagger}(x) \psi_{K}(x) \right\}. \tag{113}
\]

Notice that the definitions (31,34) imply that

\[
\psi(x) = \sum_{K} e^{-iK \cdot x} \psi_{K}(x) \tag{114}
\]

so that the usual probability density function is, because the \( v_{N} \) are \( K \)-diagonal,

\[
\frac{2\pi}{\Delta} \sum_{N} \operatorname{Tr}\left\{ \rho \psi_{K}^{\dagger}(x) \psi(x) \right\} = \sum_{K} f_{K}(x) \tag{115}
\]

so that \( f_{K}(x) \) can be viewed as a phase space density per phase space volume \( h^{3} \).

1. Streaming terms

We consider the various terms in the quantum kinetic master equation. The term arising from (77d) is obtained by considering

\[
\left[ \psi_{K}(x), \int d^{3}y \, j_{K}(y) \right] \tag{116}
\]

which can be written

\[
\left[ \psi_{K}(x), \int d^{3}y \, \psi_{K}^{\dagger}(y) \left( -\frac{i\hbar}{m} \right) \nabla \psi_{K}(y) \right] \tag{117}
\]

\[
= \int d^{3}y \, g(x - y) \left( -\frac{i\hbar}{m} \right) \nabla y \psi_{K}(y) \tag{118}
\]

and now integrating by parts,

\[
\tag{118} = -\frac{i\hbar}{m} \nabla x \left( \int d^{3}y \, g(x - y) \psi_{K}(y) \right) \tag{119}
\]

but the integral is simply the projection of \( \psi_{K}(y) \) on to the \( K \) subspace; thus

\[
\tag{118} = -\frac{i}{\hbar m} \nabla \psi_{K}(x). \tag{120}
\]

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Using this kind of technique, it is straightforward to show that the contributions to $\dot{f}_K(x)$ from (77a, 77e) become

$$\dot{f}_K(x)|_a = \frac{\hbar K}{m} \cdot \nabla_x f(K, x) \quad (121)$$

$$\dot{f}_K(x)|_b = \left( \frac{\pi}{\Delta} \right)^3 \nabla \cdot J_K(x) \quad (122)$$

where

$$J_K(x) = \frac{i\hbar}{2m} \left\langle \psi^\dagger_K(x) \nabla \psi_K(x) - [\nabla \psi^\dagger_K(x)] \psi_K(x) \right\rangle. \quad (123)$$

The term (121) is the usual Boltzmann streaming term. The term (122) is a purely quantum mechanical term arising from the spreading of the wavepacket.

In order to get some idea of the significance of this and some terms to come, we make a local equilibrium ansatz, in which we write

$$\langle \psi^\dagger_K(x) \psi_K'(x') \rangle = g(x - x') f_K \left( \frac{x + x'}{2} \right) \delta_{K, K'}. \quad (124)$$

This is a natural generalization of (98) to a slightly non-equilibrium situation, and since $g(0) = (\pi/\Delta)^3$, it is consistent with (112). Using this form we find quite straightforwardly that $J_K(x) = 0$. The extent to which this term does not vanish must be related to the extent to which the mean momentum in the band $(K - \Delta, K + \Delta)$ is different from $\hbar K$, and this difference is of order of magnitude $\Delta$, which will only be appreciable for very small $K$, and in particular for $K = 0$.

### 2. Forward scattering terms

If we work out the mean value of the commutator, we find for the term arising from (77d)

$$-\frac{i}{\hbar} \left\{ 2 \int d^3x' \sum_{K'} \langle \psi^\dagger_K(x') \psi^\dagger_{K'}(x') \psi_{K'}(x') \psi_K(x) \rangle g(x - x') \right. \right.$$

$$\left. -2 \int d^3x' \langle \psi^\dagger_K(x) \psi^\dagger_{K'}(x') \psi_K(x') \psi_{K'}(x) \rangle g(x - x') \right\}. \quad (125)$$

If $g(x - x')$ was a perfect delta function, this term would vanish, thus the degree to which it does not vanish depends on the smoothness of the averages as functions of $x, x'$. Using the local equilibrium ansatz (124), and a Gaussian factorization assumption on the four point correlations, it is easy to show that this term vanishes, and is therefore presumably very small when the state is close to equilibrium. Thus we can say $\dot{f}_K(x)|_c \approx 0$. 29
3. Collision terms

In evaluating the contribution from (124) we will get a number of terms, of which a typical one is proportional to

\[-\sum_{K_2, K_3, K_4} \int d^3y \, d^3y' \, g(x - y') \langle \psi_K(x) \psi_{K_2}(y') \psi_{K_3}(y') \psi_{K_4}(y') \rangle \psi_{K_4}(y) \psi_{K_2}(y) \psi_{K_4}(x) \ \times \delta(\omega_K + \omega_{K_2} - \omega_{K_3} - \omega_{K_4}) e^{i(K + K_2 - K_3 - K_4) \cdot (y - y')} . \]

(126)

If we factorize as in local equilibrium, and use (124), we get terms like

\[-\sum_{K_2, K_3, K_4} \int d^3y \, d^3y' \, g(x - y') \langle \psi_{K}(x) \psi_{K_2}(y') \rangle \int d^3y \, g(y) \langle \psi_{K_3}(y) \psi_{K_4}(y) \rangle \psi_{K_4}(x) \ \times \delta(\omega_K + \omega_{K_2} - \omega_{K_3} - \omega_{K_4}) e^{i(K + K_2 - K_3 - K_4) \cdot (y - y')} . \]

(127)

Assuming the functions are relatively smooth, so that we can set (because of the peaked nature of \(g(x - y')\), \(g(x - y)\) and \(g(y - y')\))

\[\frac{x + y}{2} \approx \frac{y' + y}{2} \approx x\]

(128)

we get

\[-\sum_{K_2, K_3, K_4} f_K(x) f_{K_2}(x) \int d^3y \, g(y') \langle \psi_{K_3}(y) \rangle \langle \psi_{K_4}(y) \rangle \psi_{K_4}(x) \ \times \delta(\omega_K + \omega_{K_2} - \omega_{K_3} - \omega_{K_4}) \]

\[\times \int d^3y \, g(y') \langle g(y') \rangle \langle g(y - y') \rangle^3 e^{i(K + K_2 - K_3 - K_4) \cdot (y - y'')} . \]

(129)

The last factor is in fact able to be evaluated exactly, and the result is a momentum conservation function \(M_\Delta(K + K_2 - K_3 - K_4)\), where

\[M_\Delta(Q) = \left(\frac{\Delta}{\pi}\right)^3 \prod_{i=1}^{3} \delta(Q_i, \Delta) \cdot \delta(Q_i, -\Delta) . \]

(130)

Thus “momentum” \(K\) is not exactly conserved, since the quantity \(K\) in \(\psi_K(x)\) represents only the midpoint of the range of possible momenta; it is possible for three momenta, each from such a range, to add up to a value either within the range, or in either of the ranges above or below. The exact proportions of each are shown by the calculation to be \(\frac{3}{2} : \frac{1}{2} : \frac{1}{2}\). However, assuming that \(f_K(x)\) are smooth functions of \(K\) on the scale of \(\Delta\), we can ignore the slight spreading, and make the transfer from a summation to an integration: This yields

\[-\sum_{K_2, K_3, K_4} \left(\frac{\Delta}{\pi}\right)^3 M_\Delta(K + K_2 - K_3 - K_4) \rightarrow \frac{1}{(2\pi)^3} \int d^3K_2 \int d^3K_3 \int d^3K_4 \delta(K + K_2 - K_3 - K_4) . \]

(131)

so that this form eventually becomes
Here we have made the approximation
\[ u(x - x') = u\delta(x - x') \]  
(133)

Taking all terms into account we eventually get a term
\[
\dot{f}(K, x) |_{e} = \bar{\hbar} K \cdot \nabla_x f(K, x) + \frac{2|u|^2}{\hbar^2} \int d^3K_2 \int d^3K_3 \int d^3K_4 \delta(K + K_2 - K_3 - K_4)\delta(\omega + \omega_2 - \omega_3 - \omega_4) \times \{f(K, x)f(K_2, x)[f(K_3, x) + 1][f(K_4, x) + 1] - [f(K, x) + 1][f(K_2, x) + 1][f(K_3, x)f(K_4, x)] \}
\]

(134)

which is the collision term of the equation known as the Uehling-Uhlenbeck equation.

4. Summary

In the situation that we have an approximate local equilibrium, and that multifield correlation functions can be factorized as if the density operator is Gaussian, we derive the Uehling-Uhlenbeck equation as an approximate kinetic equation.

\[
\frac{\partial f}{\partial t}(K, x) \approx \frac{\bar{\hbar} K \cdot \nabla_x f(K, x)}{m} + \frac{2|u|^2}{\hbar^2} \int d^3K_2 \int d^3K_3 \int d^3K_4 \delta(K + K_2 - K_3 - K_4)\delta(\omega + \omega_2 - \omega_3 - \omega_4) \times \{f(K, x)f(K_2, x)[f(K_3, x) + 1][f(K_4, x) + 1] - [f(K, x) + 1][f(K_2, x) + 1][f(K_3, x)f(K_4, x)] \}
\]

(135)

In situations of interest for Bose Condensation it would no longer be valid to make the factorizations necessary for the collision term as above, nor factorization in the local equilibrium assumption \cite{124).

C. Equations for the condensate density operator

Let us now assume that the scattering of non-condensate modes is strong, and that we are only interested in the behavior of the condensate. We can then assume that the total density operator can be factored into a thermal non-condensate part, and a condensate density operator \( \rho_0(t) \) as a first approximation at least. Thus

\[
\rho(t) = \sum_N \nu_N(t) \rightarrow \rho_B(\mu, T) \otimes \rho_0(t)
\]

(136)

This situation is not that employed in current experiments, where the condensate grows by taking atoms out of the bath of warmer atoms, but is given for illustrative purposes only—it describes the situation in which the condensate mode is put in contact with a bath composed of all the atoms in the other modes, which are held at a given temperature and chemical potential. More realistic treatments of condensate growth are left to a later paper.
We trace over the non-condensate modes and the assumption that the non-condensate is thermalized will mean that all terms not involving condensate operators in the QKME will be vanish. The only non-vanishing dissipative terms will involve matched $\psi_0^\dagger$ and $\psi_0$ operators, so that we arrive at the condensate master equation:

$$\dot{\rho}_0(t) = -\frac{i}{\hbar} \left[ \int d^3x \psi_0^\dagger(x) \left( -\frac{\hbar^2\partial^2}{2m} \right) \psi_0(x) + \frac{1}{2} U(0000), \rho_0(t) \right] - \frac{i}{\hbar} (ug(0)) \sum_{K \neq 0} \bar{n}_K \left[ \int d^3x \psi_0^\dagger(x) \psi_0(x), \rho_0 \right]$$

$$+ \int d^3x \int d^3x' G^{(-)}(x - x', T, \mu) \{2\psi_0(x)\rho_0 \psi_0^\dagger(x') - \rho_0 \psi_0^\dagger(x') \psi_0(x) - \psi_0^\dagger(x') \psi_0(x) \rho_0 \}$$

$$+ \int d^3x \int d^3x' G^{(+)}(x - x', T, \mu) \{2\psi_0^\dagger(x)\rho_0 \psi_0(x') - \rho_0 \psi_0(x') \psi_0^\dagger(x) - \psi_0(x') \psi_0^\dagger(x) \rho_0 \}, \quad (137)$$

in which the quantities $G^{(\pm)}$ are given by

$$G^{(+)}(x - x', T, \mu) = Tr_B \left\{ \sum_{123} \frac{\pi}{\hbar^2} Z^\dagger(1, 2, 3, x)Z(1, 2, 3, x')\rho_B(T, \mu) \right\}$$

$$G^{(-)}(x - x', T, \mu) = Tr_B \left\{ \sum_{123} \frac{\pi}{\hbar^2} Z(1, 2, 3, x)Z^\dagger(1, 2, 3, x')\rho_B(T, \mu) \right\}. \quad (138)$$

with the definition

$$Z(K_1, K_2, K_3, x) = u e^{-i(K_1 + K_2 - K_3) \cdot x} \psi_{K_1}(x) \psi_{K_2}(x) \psi_{K_3}^\dagger(x) \quad (139)$$

Using thermal averages we find

$$G^{(+)}(x - x', T, \mu) = \frac{4\mu^2}{\hbar^2} \left\{ \sum_{123} [g(x - x')]^3 e^{i(K_1 + K_2 - K_3) \cdot (x - x')} \bar{n}_{K_1} \bar{n}_{K_2} \bar{n}_{K_3} \delta(\omega_1 + \omega_2 - \omega_3) \right\}$$

$$G^{(-)}(x - x', T, \mu) = \frac{4\mu^2}{\hbar^2} \left\{ \sum_{123} [g(x - x')]^3 e^{i(K_1 + K_2 - K_3) \cdot (x - x')} (\bar{n}_{K_1} + 1)(\bar{n}_{K_2} + 1) \bar{n}_{K_3} \delta(\omega_1 + \omega_2 - \omega_3) \right\} \quad (140)$$

Suppose we now set, as in (97)

$$\bar{n}_K = \left( e^{(\hbar \omega_K - \mu)/kT} - 1 \right)^{-1}, \quad (K \neq 0) \quad (141)$$

then it follows that

$$\bar{n}_{K_1} \bar{n}_{K_2} (1 + \bar{n}_{K_3}) = e^{\mu/kT}(\bar{n}_{K_1} + 1)(\bar{n}_{K_2} + 1) \bar{n}_{K_3}, \quad (142)$$

so that

$$G^{(+)}(x - x', T, \mu) = e^{\mu/kT} G^{(-)}(x - x', T, \mu). \quad (143)$$

1. Quantum stochastic differential equation form

We can write a Quantum stochastic differential equation (QSDE) equivalent to the master equation (137) by using the methods in Chap.5 of [11]. This equation takes the form
\[ i\hbar \frac{\partial \psi_0(y,t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m} \nabla^2 \psi_0(y,t) - \left( u g(0) \sum_{\mathbf{K} \neq 0} \bar{n}_\mathbf{K} \right) \psi_0(y,t) + u \int d^3 x g(x-y) \psi_0^\dagger(x,t) \psi_0(x,t) \psi_0(x,t) \right\} \\
\quad + \int d^3 x \int d^3 x' g(x'-y) \{ G^{(+)}(x-x',T,\mu) - G^{(-)}(x-x',T,\mu) \} \psi_0(x,t) \}
\]
\[ + \int d^3 x g(x-y) \, dW(x,t) \tag{144} \]
in which \(dW(x,t)\) is a quantum white noise increment which satisfies the conditions
\[ dW(x,t) dW^\dagger(x',t) = 2G^{(-)}(x-x',T,\mu) \tag{145a} \]
\[ dW^\dagger(x,t) dW(x',t) = 2G^{(+)}(x-x',T,\mu) \tag{145b} \]
\[ dW(x,t) dW(x',t) = 0 \tag{145c} \]
\[ dW^\dagger(x,t) dW^\dagger(x',t) = 0 \tag{145d} \]

2. Gain and loss

In order to get some idea of the predictions of the master equation (137) we can write equations for the averages
\[ \langle \psi_0(y) \rangle \equiv \phi(y), \tag{146} \]
\[ \langle \psi_0^\dagger(y) \psi_0(y) \rangle \equiv \rho(y). \tag{147} \]
These become
\[ \frac{\partial \phi(y)}{\partial t} = -\frac{i}{\hbar} \left\{ -\frac{\hbar^2}{2m} \nabla^2 \phi(y) - \left( u g(0) \sum_{\mathbf{K} \neq 0} \bar{n}_\mathbf{K} \right) \phi(y) + u \int d^3 x g(x-y) \psi_0^\dagger(x) \psi_0(y) \psi_0(x) \right\} \\
\quad + \int d^3 x \int d^3 x' g(x'-y) \{ G^{(+)}(x-x',T,\mu) - G^{(-)}(x-x',T,\mu) \} \phi(x) \]
\[ \frac{\partial \rho(y)}{\partial t} = -\nabla \cdot \mathbf{j}(y) + \int d^3 x \{ G^{(+)}(y-x,T,\mu) - G^{(-)}(y-x,T,\mu) \} \\
\quad \times \langle \psi_0^\dagger(x) \psi_0(y) + \psi_0^\dagger(y) \psi_0(x) \rangle + 2 \int d^3 x \, G^{(+)}(x,T,\mu) g(x). \tag{148} \]
Here \(\mathbf{j}(y)\) is the probability current. The equation (148) for \(\phi(y)\) is a rather familiar non-linear Schrödinger equation form, but contains the second line as well, which is an explicit gain-loss term. We can use the relation (143) to write this in the form
\[ \int d^3 x \int d^3 x' g(x'-y) (e^{\mu/kT} - 1) G^{(+)}(x-x',T,\mu) \phi(y) \tag{149} \]
and clearly when \(\mu = 0\), this vanishes.

If we consider spatially homogeneous solutions, then we can write \(\phi(x) \to \phi\), and we find
\[ \frac{\partial \phi}{\partial t} = -\frac{i}{\hbar} \left( u g(0) \sum_{\mathbf{K} \neq 0} \bar{n}_\mathbf{K} \right) \phi - \frac{i}{\hbar} u \int d^3 x g(x-y) \psi_0^\dagger(x) \psi_0(x) \psi_0(x) \]
\[ + \phi(e^{\mu/kT} - 1) \frac{u^2}{2\hbar^2 \pi^5} \int d^3 K_1 \int d^3 K_2 \bar{n}_{K_1} \bar{n}_{K_2} (1 + \bar{n}_{K_1+K_2}) \delta(\omega_{K_1+K_2} - \omega_{K_1} - \omega_{K_2}) \]. \tag{150}
3. Stationary solutions.

If \( \mu < 0 \), as must be the case above the condensation temperature, the last part clearly represents a loss term. There will be no growth of a non zero \( \phi \) value. If we assume a Gaussian solution, we can write

\[
\langle \psi_0^\dagger(y) \psi_0(y) \psi_0(y) \rangle \rightarrow 2 \phi \langle \psi_0^\dagger(y) \psi_0(y) \rangle \tag{151}
\]

and it is clear that the only stationary solution will be \( \phi = 0 \).

Similarly, we can get an approximate closed equation from (148) by assuming

\[
\langle \psi_0^\dagger(x) \psi_0(y) \rangle = \frac{g(x-y)}{g(0)} \bar{\rho}, \tag{152}
\]

which assumes the equilibrium shape \( g(0) \) of the correlation function. This leads to

\[
\frac{\partial \bar{\rho}}{\partial t} = 2 \int d^3x G^+(y-x,T,\mu) g(x-y) \left\{ (e^{\mu/kT} - 1) \bar{\rho} / g(0) + 1 \right\} \tag{153}
\]

We then find the stationary solution

\[
\bar{\rho} = \frac{g(0)}{1 - e^{\mu/kT}} = \frac{l^{-3}}{1 - e^{\mu/kT}}, \tag{154}
\]

which gives the total mean number per volume as \( l^3 \) as \( 1/(1-e^{\mu/kT}) \), the usual statistical mechanical result when \( \mu < 0 \). When \( \mu = 0 \) there is no longer a stationary state of Eq. (148); \( \bar{\rho} \) will grow indefinitely. However there is still no gain, so no coherent phase appears. Of course in practice \( \mu \) is not exactly zero, so indefinite growth will not occur.

Thus we see that the ideal Bose condensate result arises purely out of noise; that no coherent phase appears at all. This result is only valid in the weak condensation limit; we will see in a subsequent paper that higher order terms can lead to an effective gain, and that a non-zero stationary value of \( \phi \) can arise.

4. Gain and a coherent phase arising from a modified distribution of energies in the non-condensate

It is of interest to see whether we could produce a non-zero value of \( \phi \) by manipulating the nature of the energy distribution of the non-condensate. If we do assume that the non-condensing modes are in a non-equilibrium stationary state, so that instead of \( \rho_B(T,\mu) \) we have an arbitrary density operator \( \rho_{nc} \), the gain in (148) becomes
\[
\frac{u^2}{2\hbar^2 \pi^5} \int d^3 K_1 d^3 K_2 \delta(\omega_{K_1} + \omega_{K_2} - \omega_{K_1 + K_2}) \left\{ \tilde{n}_{K_1} \tilde{n}_{K_2} [1 + \tilde{n}_{K_1 + K_2}] - [1 + \tilde{n}_{K_1}] [1 + \tilde{n}_{K_2}] \tilde{n}_{K_1 + K_2} \right\}.
\]

(155)

We can get gain if (but not only if) every team in the \( \{} \) is positive. Assuming that \( \tilde{n}(K) \) is only a function of \( \omega_K \), this will happen when

\[
\frac{\tilde{n}(\omega_1)}{1 + \tilde{n}(\omega_1)} \frac{\tilde{n}(\omega_2)}{1 + \tilde{n}(\omega_2)} \frac{1 + \tilde{n}(\omega_1 + \omega_2)}{\tilde{n}(\omega_1 + \omega_2)} > 1
\]

or, defining

\[
F(\omega) = \log \left\{ \frac{\tilde{n}(\omega)}{1 + \tilde{n}(\omega)} \right\}
\]

(156)

(157)

\[
F(\omega_1) + F(\omega_2) > F(\omega_1 + \omega_2).
\]

(158)

This is the condition that \( F(\omega) \) is a convex downwards function as in the solid line in the diagram. For example,

\[
F(\omega) = \frac{-\hbar \omega - \lambda \omega^2}{kT}
\]

(159)

gives

\[
F(\omega_1) + F(\omega_2) - F(\omega_1 + \omega_2) = \frac{2\lambda \omega_1 \omega_2}{kT} > 0
\]

(160)

and the net gain is

\[
\frac{u^2}{2\hbar^2 \pi^5} \int d^3 K_1 d^3 K_2 \delta(\omega_{K_1} + \omega_{K_2} - \omega_{K_1 + K_2}) \times \exp \left( \frac{2\lambda \omega_{K_1} \omega_{K_2}}{kT} \right) \tilde{n}_{K_1} \tilde{n}_{K_2} [1 + \tilde{n}_{K_1 + K_2}].
\]

(161)

VI. CONCLUSIONS

Quantum kinetic theory is both a genuine kinetic theory and a genuine quantum theory. The kinetic aspect arises from the decorrelation between different momentum bands, and this is essentially our version of the molecular chaos condition. However, because each \( K \)-band has a range of momenta within it, from which coherences are not eliminated, there is still the possibility of long wavelength quantum coherence. In practice such coherence is not expected to be of significance except in the Bose condensate, but the formulation we have developed enables a correct formulation of the method by which incoherence can be transferred into the condensate.

We have formulated quantum kinetic theory in terms of the Quantum Kinetic Master Equation for bosonic atoms. It is a quantum stochastic equation for the kinetics of a dilute quantum degenerate bose gas, and it is valid in the regime of Bose condensation, as well as in regimes where no condensation takes place.

The QKME is a genuine \( N \)-atom equation, which is intermediate between the full description in terms of the complete density matrix and the familiar kinetic equations for single particle distribution functions (like the quantum Boltzmann equation). It contains as limiting cases both the Uehling-Uhlenbeck (or quantum Boltzmann equation) and the Gross-Pitaevskii equation.

The key assumption in deriving the QKME is a Markov approximation for the atomic collision terms. This is valid to the extent we are interested in a situation where in addition to the Bose condensate we have a thermal fraction of atoms which effectively acts like a heat bath with a (short) thermal correlation time \( \hbar/kT \), which is taken as zero in the Markov approximation.

The present paper has developed the basic structure of the theory, has stated and justified the approximations which are needed, and has thus delineated the region of validity of the theory. Extensions to include a trapping potential and to account for a large fraction of condensed atoms giving rise to Bogoliubov type excitation spectrum are essentially technical, because the basic formulation carries through with little conceptual change, although the
equations which are appropriate in these cases are significantly changed. These aspects, which are essential for the application of the QKME method to realistic experiments, will be dealt with in QKII.

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\( K = 0 \)

\( \pi / \Delta \)

\( r \)

Fig. 1
Fig. 3
\[ (x)u(|r-x|) \quad v_K(x,r) \]