Excitations of Bose-Einstein Condensates at Finite Temperatures

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Abstract

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Recent experimental observations of collective excitations of Bose condensed atomic vapours have stimulated interest in the microscopic description of the dynamics of a Bose-Einstein condensate confined in an external potential.

We present a finite temperature field theory for collective excitations of trapped Bose-Einstein condensates and use a finite-temperature linear response formalism, which goes beyond the simple mean-field approximation of the Gross-Pitaevskii equation. The effect of the non-condensed thermal atoms we include using perturbation theory in a quasiparticle basis. This presents a simple scheme to understand the interaction between condensate and non-condensed atoms and enables us to include the effect the condensate has on collision dynamics.

At first we limit our treatment to the case of a spatially homogeneous Bose gas. We include the effect of pair and triplet anomalous averages and thus obtain a gapless theory for the excitations of a weakly interacting system, which we can link to well known results for Landau and Beliaev damping rates. A gapless theory for trapped systems with a static thermal component follows straightforwardly.

We then investigate finite temperature excitations of a condensate in a spherically symmetric harmonic trap. We avoid approximations to the density of states and thus emphasise finite size aspects of the problem. We show that excitations couple strongly to a restricted number of modes, giving rise to resonance structure in their frequency spectra. Where possible we derive energy shifts and lifetimes of excitations. For one particular mode, the breathing mode, the effects of the discreteness of the system are sufficiently pronounced that the simple picture of an energy shift and width fails. Experiments in spherical traps have recently become feasible and should be able to test our detailed quantitative predictions.

To my family.

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Contents

CHAPTER 1

GENERAL INTRODUCTION

Ever since Bose-Einstein condensation (BEC) was linked to the macroscopic quantum phenomena like superfluidity and superconductivity it has been an active area of research for theoretical and experimental physicists alike. Over the years the concept of BEC has emerged to be connected with a variety of fields within physics, ranging from low temperature gases and liquids to elementary particle and astro physics [1].

For many years signatures of BEC were observed experimentally only in strongly interacting systems, such as liquid helium. The strong interactions of these systems, however, complicated their study and often masked genuine properties of the condensate itself. It was not until July 1995 that BEC was observed in a weakly interacting system. At JILA, Boulder, Colorado, a dilute metastable vapour of atomic rubidium, confined in a magneto-optical trap, was cooled down using a combination of laser and evaporative cooling techniques. Below a temperature of around 170 nK atoms began to accumulate in the ground state of the trap, merging together to form a single entity, amplifying the quantum nature of the atoms to a macroscopic scale [2]. The announcement of this first successful experiment triggered intense activity in the communities of atomic physics, condensed matter physics, and quantum optics and by now, a few years later, the experimental and

[1] A. Griffin, D. W. Snoke, and S. Stringari. Bose-Einstein Condensation (Cambridge University Press, 1995).

[2] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell. *Observation of Bose-Einstein condensation in a dilute atomic vapor*. Science 269, 198 (1995).

theoretical study of condensates of atomic vapours has become an entire field of research in its own right.

The great attraction of the dilute atomic condensates is that they are probably the closest experiments can get to the realisation of an ideal quantum gas. The systems are very cold and dilute and therefore display features of quantum degeneracy in a clear and unobscured manner. Furthermore, the magnetic and electric dipole moments of the atoms of the system allow one to manipulate the condensate almost at will. One further aspect of these systems, their predictable deviations from the ideal behaviour, make the gaseous condensates particularly interesting. The systems are ideally suited to perform very precise measurements of properties, which depend on the detailed nature of the interactions in these many-body system.

Collective excitations were one of the first such features to be studied in the new condensates [3, 4, 5]. Measurements in fully and partially condensed systems found that excitation frequencies shift and get increasingly damped at higher temperatures. Explaining the observed excitation frequencies and lifetimes forms one of the rare opportunities to test predictions of finite temperature field theories against hard experimental data and presents one of the most stringent tests of our understanding of interactions in these cold quantum gases. The measurements of excitations in the new condensates immediately renewed interest in the long standing problem of a microscopic description of excitations in Bose gases. The dramatic effects of superfluidity and superconductivity in condensed systems are a direct consequence of the modification of the excitation spectrum due to the presence of the condensate [6]. The nature of excitations in a dilute Bose gases therefore had been studied extensively with regard to the possibility of describing the phenomenon of superfluidity in liquid Helium [7]. Unlike the case of Helium,

[3] D. S. Jin, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell. *Collective excitations of a Bose-Einstein condensate in a dilute gas*. Phys. Rev. Lett. 77, 420 (1996).

[4] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, *et al.*. *Collective excitations of a Bose-Einstein condensate in a magnetic trap*. Phys. Rev. Lett. 77, 988 (1996).

[5] D. S. Jin, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell. *Temperature-dependent damping and frequency shifts in collective excitations of a dilute Bose-Einstein condensate*. Phys. Rev. Lett. 78, 764 (1997).

[6] D. R. Tilley and J. Tilley. Superfluidity and Superconductivity (Adam Hilger, 1990).

[7] A. Griffin. *A brief history of our understanding of BEC: From Bose to Beliaev*. In Proceedings of the International School of Physics - Enrico Fermi (edited by M. Inguscio, S. Stringari, and C. E. Wieman), p. 1 (IOS Press, 1999).

the assumptions needed for perturbative field theories to be valid are well satisfied in the case of the new gaseous condensates.

In his seminal treatment of the dilute Bose gas Bogoliubov described the excitations of the system of interacting Bosons in terms of non-interacting quasiparticles and established that they resemble phonons in the long wavelength limit [8]. Beliaev extended this treatment and perturbatively included interactions between the Bogoliubov quasiparticles, which previously had been neglected [9]. The Bose gas at finite temperatures was first studied by Lee and Yang using a pseudo-potential method [10]. The properties of excitations at finite temperatures were first studied by Mohling and Sirlin [11] and Mohling and Morita [12]. The zero temperature Beliaev formalism was extended to the range of finite temperatures by Popov [13, 14]. The work of Beliaev and Popov has only recently been reexamined in detail by Shi [15].

Much of these treatments of the dilute Bose gas was originally limited to homogeneous systems, but recent work has focussed on extending them to describe the spatially confined gases of the experiments. Fedichev and Shlyapnikov employ the formalism of Beliaev and Popov [16], whereas Morgan uses an approach more akin to the work of Mohling *et al* [17]. In this thesis we will use a time-dependent mean-field scheme to describe the condensate and its excitations. It is based around

[8] N. Bogolubov. *On the theory of superfluidity*. J. Phys. USSR 11, 23 (1947).

[9] S. T. Beliaev. *Application of the methods of quantum field theory to a system of bosons*. Sov. Phys. JETP 34, 289 (1958).

[10] T. D. Lee and C. N. Yang. *Low-temperature behavior of a dilute Bose system of hard spheres*. Phys. Rev. 112, 1419 (1958).

[11] F. Mohling and A. Sirlin. *Low-lying excitations in a Bose gas of hard spheres*. Phys. Rev. 118, 370 (1960).

[12] F. Mohling and M. Morita. *Temperature dependence of the low-momentum excitations in a Bose gas of hard shperes*. Phys. Rev. 118, 681 (1960).

[13] N. V. Popov and L. Faddeev. *An approach to the theory of the low temperature Bose gas*. JETP 20, 890 (1965).

[14] N. V. Popov. *Greens functions and thermodynamic functions of a non-ideal Bose gas*. JETP 20, 1185 (1965).

[15] H. Shi. Finite Temperature Excitations in a dilute Bose-condensed gas. Ph.D. thesis, University of Toronto (1997).

[16] P. O. Fedichev and G. V. Shlyapnikov. *Finite-temperature perturbation theory for a spatially inhomogeneous Bose-condensed gas*. Phys. Rev. A 58, 3146 (1998).

[17] S. A. Morgan. A Gapless Theory of Bose-Einstein Condensation in Dilute Gases at Finite Temperature. Ph.D. thesis, University of Oxford (1999).

the Gross-Pitaevskii equation (GPE), which describes the condensate as one single macroscopic wavefunction, varying in space and time. During the research leading to this thesis the same approach has also been pursued by Minguzzi and Tosi [18] as well as Giorgini [19, 20].

Quantitative calculations based on the relatively simple theories of the GPE and the Bogoliubov excitations are remarkably successful in describing the properties of the trapped condensates of the recent experiments at zero temperatures. Finite temperature calculations of excitations, however, have been limited by various approximations. Calculations of temperature dependent excitation energies have neglected certain second order terms and thus were unable to describe the damping of excitations [21]. Calculations of damping in turn were based on approximations to the density of states of the system [22]. Recently Reidl *et al.* presented a unified treatment of shifts and lifetimes, which again was limited by approximations [23].

In the following we will derive and calculate a theory for excitations at finite temperatures, which improves on previous approximate treatments. The thesis is divided into three parts:

i. The first section spans Chapters 2 and 3 and forms an introduction to Bose Einstein condensation and its collective excitations.

ii. The second section derives and discusses finite temperature theories of the condensate and its excitations.

   Chapter 4 presents a finite-temperature mean-field scheme which describes the condensate and the surrounding thermal cloud in the linear regime. We

[18] A. Minguzzi and M. P. Tosi. *Linear density response in the random-phase approximation for confined Bose vapours at finite temperature.* J. Phys. Condens. Matter 9, 10211 (1997).

[19] S. Giorgini. *Damping in dilute Bose gases: A mean field approach.* Phys. Rev. A 57, 2949 (1998).

[20] S. Giorgini. *Collisionless dynamics of dilute Bose gases: Role of quantum and thermal fluctuations.* Phys. Rev. A 61, 063615 (2000).

[21] D. W. Hutchinson, R. J. Dodd, and K. Burnett. *Gapless finite-t theory of collective modes of a trapped gas.* Phys. Rev. Lett. 81, 2198 (1998).

[22] P. O. Fedichev, G. V. Shlyapnikov, and J. T. M. Walraven. *Damping of low-energy excitations of a trapped Bose-Einstein condensate at finite temperatures.* Phys. Rev. Lett. 80, 2269 (1998).

[23] J. Reidl, A. Csordás, R. Graham, and P. Szépfalusy. *Shifts and widths of collective excitations in trapped Bose gases by the dielectric effect.* Phys. Rev. A 61, 043606 (2000).

demonstrate that this gives a well defined theory for homogeneous gases and show how it can describe a trapped gas with static thermal component.

In Chapter 5 we formulate a theory for excitations in trapped systems. We again consider the time evolution of the mean-field at finite temperatures and treat the interactions between normal modes of the mean field in a systematic perturbation scheme. We derive an expression for the linear response of the mean-field to an external driver, which closely models the recent experimental measurements of excitations.

iii. The third and final section is concerned with quantitative calculations of finite temperature excitations.

The calculations avoid any major approximations and are the first of their kind to explicitly account for the discrete nature of excitations in trapped systems. We study the specific case of excitations in spherically symmetric traps and show that excitations couple strongly to a small number of modes, giving resonance structure in their frequency spectra. Where possible we calculate temperature dependent energy shifts and decay rates. For particular modes we show that the simple picture of a decay rate fails. We make detailed quantitative predictions which can be put to the test in suitable experiments.

Chapter 2

Bose-Einstein Condensation

This introductory chapter sets out to define the subject of the thesis, the Bose-Einstein Condensate. We start by revisiting the statistics of identical particles and discuss the condensation of an ideal gas of bosons, and then turn to the properties of condensates found in more physical systems. We find that spatial confinement and interactions fundamentally change nearly all of the properties of the ideal BEC. The most convenient way to deal with interacting many-body systems is to use the language of second quantisation. We present its key elements axiomatically and write the Hamiltonian in a second-quantised form. We then introduce the mean field approximation and derive from the Hamiltonian the Gross-Pitaevskii equation, the basis of most studies of BEC in trapped gases. The chapter closes by giving a general definition of Bose-Einstein Condensates in interacting systems.

2.1 Quantum Statistics, Bosons, and Condensation

Classical physics assumes every particle has a definite position and momentum at any given moment in time. Each particle can then be assigned a point in phase space, which follows a unique trajectory in time. Two otherwise identical particles always differ by their trajectories and thus can, in principle, be distinguished from another, irrespective of how feasible this may be in practice. Quantum mechanics, however, abandons the classical concept of definite trajectories and instead describes particles using wave functions. When the wave functions of two otherwise identical particles overlap it is impossible to keep track of them separately.

If we use quantum mechanics to describe a system of two or more identical particles we therefore must deal with them as *fundamentally* indistinguishable. We have to construct our wavefunctions such that physical observables are unaffected by the exchange of two identical particles. In other words, the two wavefunctions $|a_1, a_2, ...\rangle$ and $|a_2, a_1, ...\rangle$ can only differ by a phase factor. Since exchanging particles twice should leave us with the original wavefunction the phase factor can only take the values of $+1$ or -1. Wavefunctions are said to be symmetric under particle exchange, if the phase factor is $+1$, and antisymmetric if -1.

The symmetry of wavefunctions has far reaching implications. The Spin - Statistics theorem states that particles with integer spin can only exist in symmetric states, whereas particles with half-integer spin exist only in antisymmetric ones. The theorem follows as a consequence of requiring quantum theory to be consistent with special relativity and is backed by abundant experimental evidence. Particles with symmetric wavefunctions and integer spin are termed bosons. Fermions are particles with antisymmetric wavefunctions and half-integer spin. The Pauli exclusion principle states that at most one fermion can occupy a given quantum state. The population factor of a given state, n_i, can only take the values one or zero. Unlike fermions, bosons do not mind sharing the same quantum state, in fact they quite like to do so. We will show that under certain conditions all bosons of a system will crowd into a single state and form a so-called Bose-Einstein condensate. If we consider the collision of two bosonic particles the transition rate of the scattering process,

$$\Gamma_{(1,2)\to(3,4)} \quad \propto \quad n_1 n_2 (1 + n_3)(1 + n_4), \tag{2.1}$$

depends not only on the population of the initial but also of the final states. During a scattering process a boson is more likely to end up in a state if this state is already occupied. For classical particles the transition rate would only be proportional to $n_1 n_2$. The appearance of the $(1 + n_3)(1 + n_4)$ 'Bose enhancement' factors again is a consequence of the symmetry of the wavefunctions and is known to play a critical role in the formation process of a condensate [24]. Applying the principle of detailed balance to the above transition rate and using the conservation of energy

[24] H.-J. Miesner, D. M. Stamper-Kurn, M. R. Andrews, D. S. Durfee, *et al.*. *Bosonic stimulation in the formation of a Bose-Einstein condensate.* Science 279, 1005 (1998).

gives us the equilibrium occupation of a state of energy ϵ_i at temperature T

$$n_i(\epsilon_i, T) = \frac{1}{e^{(\epsilon_i-\mu)/k_B T} - 1}. \tag{2.2}$$

where k_B is Boltzmann's constant. This is the Bose-Einstein distribution function and describes the quantum statistics of bosonic particles. At high temperatures it goes over to the Boltzmann statistics for classical particles, $n_i = e^{-(\epsilon_i-\mu)/k_B T}$. The parameter μ in the above equations accounts for the fact that we require the total number of particles of the system to be fixed

$$N = \sum_{k=0}^{\infty} n_k. \tag{2.3}$$

Quantum statistics of identical particles apply not only to elementary particles, such as the fermionic constituents of matter or the bosonic carriers of the four principle forms of interaction. As long as the excitation energies of the internal degrees of freedom of composite particles are large in comparison to the interaction energies of the system, i.e. provided that the composite particles are indistinguishable, the spin-statistics relation is equally valid [25]. The dilute vapours of alkali atoms used in the experiments certainly satisfy this condition.

Since indistinguishability lies at the heart of quantum statistics, its effects become important whenever the inter-particle separation $d = (N/V)^{-1/3}$ is comparable to the spatial spread of the quantum mechanical wavefunction of the particles. The spread of the wavefunction depends on temperature and is given by its de Broglie wavelength $\lambda_{dB} = (2\pi\hbar^2/mk_BT)^{1/2}$, with m as the mass of the particle. This allows a rough estimate for the temperature at which the effects of quantum degeneracy set in for any fermionic or bosonic gas,

$$k_B T \approx \frac{\hbar^2}{m}\left(\frac{N}{V}\right)^{3/2}. \tag{2.4}$$

2.1.1 Condensation of an ideal gas of bosons

At sufficiently low temperatures quantum statistics force an ideal gas of bosons to condense. This phenomenon follows as a direct consequence of the Bose-Einstein distribution function, equation (2.2), and the constraint that the total number of

[25] P. Ehrenfest and J. R. Oppenheimer. *Note on the statistics of nuclei.* Phys. Rev. 37, 333 (1931).

particles must be be conserved, equation (2.3). For free particles in three dimensions we can replace the summation over states by an integral, $\sum_i \to (V/2\pi) \int d^3k$ and with $\epsilon = p^2/2m$ obtain an expression for the number density of the system

$$\frac{N}{V} = \frac{2\pi(2m)^{\frac{3}{2}}}{h^3}\left[\frac{n_0}{V} + \int \epsilon^{\frac{1}{2}}\left[e^{(\epsilon_i-\mu)/k_BT} - 1\right]^{-1} d\epsilon\right]. \tag{2.5}$$

Because the integrand gives zero weight to the $k = 0$ ground state we have explicitly retained the term $n_0 = [e^{-\mu/k_BT} - 1]^{-1}$. The chemical potential for bosons must always be smaller than zero, $\mu < 0$. Otherwise the population factors could take negative values. n_0 therefore is negligible for all but very small temperatures. If the system is to be kept at constant density, N/V, lowering the temperature has to be accompanied by a rise in the chemical potential. Near some temperature T_C when the chemical potential is locked close to zero, the ground state begins to become populated. The point where the ground state population just vanishes

$$\frac{N}{V} = \frac{2\pi(2m)^{\frac{3}{2}}}{h^3}\left[\int \epsilon^{\frac{1}{2}}\left[e^{\epsilon_k/k_BT_C} - 1\right]^{-1} d\epsilon\right], \tag{2.6}$$

defines the critical temperature,

$$T_C = \frac{h^2}{2\pi m k_B}\left(\frac{N}{V\zeta(3/2)}\right)^{\frac{2}{3}}, \tag{2.7}$$

with $\zeta(3/2) = 2.612$. If the system is cooled down below the critical temperature number conservation implies that all particles begin to crowd into the ground state. The macroscopically occupied energy ground state is the Bose-Einstein condensate. Rephrased above expression shows that condensation sets in when the de Broglie wavelength becomes comparable with the inter-particle spacing

$$\frac{N}{V}\lambda_{dB}^3 > 2.612. \tag{2.8}$$

The condensate fraction as a function of temperature is given by

$$\frac{n_0}{N} = 1 - \left(\frac{T}{T_C}\right)^{3/2}. \tag{2.9}$$

The condensation of an ideal gas is one of the few model systems for a phase transition whose properties such as compressibility, total energy, or specific heat can be calculated exactly. Like most exactly solvable systems the condensation of the ideal gas can be mapped on to the phase transition of the Ising model [26]. Implications of this analogy will be discussed in connection with the mean field approximation in section 2.3.

2.1.2 Dimensions and spatial confinement

A feature common to all phase transitions is that they are, strictly speaking, only well defined in the thermodynamic limit. All experimental systems have finite numbers and finite volumes which lead to a smoothing out of the critical temperature to a region where condensation begins to set in. In the recent experiments on condensates in atomic gases these finite size effects, however, are only of secondary importance [27, 28].

A far greater effect is that the confining potential can alter the nature of the phase transition altogether. If spatial confinement reduces the dimensions of a system, transitions may not occur at all. The spontaneous magnetisation of the Ising model, for instance, happens only in more than one dimension. The ideal Bose gas condenses only in dimensions $d > 2$, which can be shown using the following simple argument. In two dimensions the density of states of the system is constant $f(\epsilon)d\epsilon = (Am)/(2\pi\hbar^2)d\epsilon$. When lowering the temperature at constant density as in the 3-d gas, the zero energy state therefore does not get treated differently than the other states. It gradually becomes more and more populated, but there is no sudden onset of this process. Only in the limit that $T \rightarrow 0$ the ground state population becomes much larger than the population of the neighbouring states, $n_0 \gg n_i$ and a BEC phase transition therefore does not occur.

As an aside, it is worth noting that even though a two dimensional system does not Bose-condense, an interacting 2-d Bose gas does undergo a similar transition called Kosterlitz-Thouless transition. This is associated with the formation of bound pairs of vortices below a critical temperature [29]. The system forms a

[26] J.D.Gunton and M.J.Buckingham. *Condensation of the ideal Bose gas as a cooperative transition*. Phys. Rev. 166, 152 (1968).

[27] W. Ketterle and N. J. van Druten. *Bose-Einstein condensation of a finite number of particles trapped in one or three dimenstions*. Phys. Rev. A 54, 656 (1996).

[28] J. R. Ensher, D. S. Jin, M. R. Matthews, C. E. Wieman, and E. A. Cornell. *Bose-Einstein condensation in a dilute gas: Measurement of energy and ground-state occupation*. Phys. Rev. Lett. 77, 4984 (1996).

[29] J. M. Kosterlitz and D. J. Thouless. *Ordering, metastability, and phase transitions in two-dimensional systems*. J. Phys. C 7, 1181 (1973).

'quasi-condensate' built of small Bose-condensed units. Within each of these units the system is phase coherent, but the phases are not correlated with each other. In section 2.4. we will discuss that BEC implies that the phase is coherent over the entire system.

If a Bose gas is confined in a spatially varying potential the condensation process is fundamentally altered in comparison to condensation in an n-dimensional box. The volume available to the system becomes dependent on the mean energy of the system. With decreasing energy the effective volume of the system decreases as well. This leads to an increase in density which, in turn, raises the critical temperature [30]. For sufficiently confining potentials, condensation becomes possible in two or even one dimension. The experiments in dilute atomic gases are performed in harmonic trap geometries, $V_{trap}(\mathbf{r}) = m/2\sum_i \omega_i^2 r_i^2$. Depending on the experimental set up, the harmonic oscillator strengths ω_i are usually equal in the x-y plane and differ in the third dimension, yielding either pancake- or cigar-shaped atomic clouds. The density of states in such a trap is $f(\epsilon)d\epsilon = 1/2\hbar\omega(\epsilon/\hbar\omega)d\epsilon$, where $\omega = (\omega_1\omega_2\omega_3)^{1/3}$ is the geometric mean frequency. As a result of the trapping potential, the critical temperature becomes

$$T_C = \frac{\hbar\omega}{k_B}\left(\frac{N}{\zeta(3)}\right)^{1/3}, \tag{2.10}$$

where $\zeta(3) = 1.202$. Since the particle number is large in most cases of interest the critical temperature generally is much greater than the energy spacing of the trap levels. The condensate fraction as a function of temperature can be written as

$$\frac{n_0}{N} = 1 - \left(\frac{T}{T_C}\right)^3. \tag{2.11}$$

2.1.3 The role of interactions

Unlike in the model of the ideal gas, interactions are present in real physical systems and affect all aspects of their condensation. The first physical system BEC was found to play a role in was the superfluid phase of liquid helium. Due to its exceptionally weak inter-atomic interactions, bosonic ^{4}He remains liquid down to the very lowest temperatures where quantum degeneracy sets in and the system undergoes condensation. Due to the relatively high density of the system, approx.

[30] V. S. Bagnato, D. E. Pritchard, and D. Kleppner. *Bose-Einstein condensation in an external potential.* Phys. Rev. A 35, 4354 (1987).

$10^{20}\mathrm{cm}^{-3}$, the effect of the interactions still is sufficiently strong that only 10% of the atoms occupy the ground state of the system. This renders a perturbative treatment of the interactions useless and to a great extent masks the effects of quantum degeneracy.

The recent experiments on vapours of alkali atoms deal with much more dilute systems, and thus avoid most of the problems encountered in liquid helium. The effect of the interactions in these dilute gases is very weak. This is illustrated by the fact that the experimentally observed critical temperature is within a few percent of the ideal gas result according to equation (2.10). Further, they are found to have no appreciable depletion at low temperatures [28]. However, since the conditions for condensation of such systems lie in a regime which is thermodynamically forbidden, the experiments have to deal with metastable systems of spin-polarised alkali atoms.

The magnitude of the interactions in these dilute gases may be small, yet their effect is significant. For instance, condensates with attractive and repulsive interactions clearly differ in their properties. For smaller condensates the total energy of the system is made up of comparable contributions from the external trap potential and the pair interactions. For larger condensates the kinetic energy of the atoms becomes small in comparison to the interaction energy and if $n_0 a/d_{h.o.} \gg 1$, where $d_{h.o.} = (\hbar/m\omega_0)^{1/2}$ is the oscillator length, one often neglects the kinetic energy altogether (Thomas-Fermi approximation). Most importantly, the excitation energies of the condensate strongly depend on the nature of the inter-atomic interactions.

In fact, interactions are crucial to obtain the low temperatures required for condensation. Two-body collisions, proportional to the square of the density, ensure the system equilibrates thermally, which is necessary when evaporatively cooling the system to the transition temperature. Three-body collisions, proportional to the cube of the density, however, result in atoms being lost from the trap. They scatter particles into non-trapped states and in the process even heat up the remaining atoms. Only for relatively low densities of $10^{14}\mathrm{cm}^{-3}$ do the two-body rates dominate the three-body ones so that a metastable gas can find its thermal equilibrium long before it eventually disappears from the trap. For very dilute gases therefore extremely low temperatures of 10^{-5} to 10^{-8}K are required in order to get the de Broglie wavelengths to overlap and the system to condense.

[28] J. R. Ensher, D. S. Jin, M. R. Matthews, C. E. Wieman, and E. A. Cornell. *Bose-Einstein condensation in a dilute gas: Measurement of energy and ground-state occupation.* Phys. Rev. Lett. 77, 4984 (1996).

Because the gases in the experiments are very dilute the interactions can be modelled by a zero-range potential. At very low temperatures low-energy s-wave collisions dominate the interactions. We thus can approximate the binary collision in 3-d by a contact interaction

$$V(\mathbf{r}-\mathbf{r}') \approx U_0\delta(\mathbf{r}-\mathbf{r}'), \quad U_0 = \frac{4\pi\hbar^2 a}{m}. \tag{2.12}$$

The interactions thus are characterised by a single parameter, the s-wave triplet scattering length in vacuo, a. The contact interaction is, in fact, an approximation to an effective interaction, the two-body T-matrix, which is directly related to the inter-atomic potential $V(\mathbf{r})$. We will discuss aspects of this approximation in chapter 4.

For the condensed atomic gases of the recent experiments the important length scales compare as follows:

$$\lambda_{dB} > d_{mfp} \gg a. \tag{2.13}$$

The de Broglie wavelength λ_{dB} is greater than the inter particle spacing d_{mfp}, allowing the system to condense. The inter particle spacing, in turn, is much greater than the scattering length a, which indicates that the system is dilute.

2.2 The second-quantised Hamiltonian

The formalism of second quantisation is a generalisation of one-particle quantum mechanics which incorporates the indistinguishability of particles and is the most convenient notation to describe a many-particle system. Its key aspects are best introduced axiomatically [31]:

1. There is a vacuum state $|0\rangle$ with N=0 particles, where $\langle 0|0\rangle = 1$.

2. The single particle operators $\hat{a}_i$ and $\hat{a}_j^\dagger$ obey the commutation relations for bosons
$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_j^\dagger, \hat{a}_j^\dagger] = 0, \ \ [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{i,j}. \tag{2.14}$$

3. The single particle operator $\hat{a}_i^\dagger$ describes the addition of a particle of state i to the system, thus projecting onto the space of N+1 particles. The conjugate

[31] E. Merzbacher. Quantum Mechanics, 2nd ed. (Wiley, 1961).

operator $\hat{a}_i$ does the reverse.

$$\begin{aligned}
\hat{a}_i^\dagger \left|N, n_0, n_1, ..., n_i, ...\right\rangle &= \sqrt{n_i+1}\left|N+1, n_0, n_1, ..., n_i+1, ...\right\rangle, && (2.15)\\
\hat{a}_i \left|N, n_0, n_1, ..., n_i, ...\right\rangle &= \sqrt{n_i}\left|N-1, n_0, n_1, ..., n_i-1, ...\right\rangle, && (2.16)\\
\hat{a}_i|0\rangle = 0. &&& (2.17)
\end{aligned}$$

4. Fock space is spanned by the basis generated by repeated actions of the operators $\hat{a}_i^\dagger$ on $|0\rangle$. Its vectors are written as $|N, n_i\rangle$, where N,i, and n_i are integers with $\sum_i n_i = N$, and denote N-particle states symmetric under particle exchange. Their symmetry stems from the commutation relations of the operators. Fock space is formally equivalent to a system of uncoupled harmonic oscillators. It is the product of single-particle eigenspaces, each characterised by the orthonormal basis of single-particle states $\{\phi_i\}$.

5. Observables take the form of second-quantised operators. The single particle energy $H_{sp}(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\nabla_r^2 + V_{trap}(\mathbf{r})\right)$ takes the form of a single particle operator
$$\hat{H}_{sp} = \sum_{i,j}\langle i|H_{sp}|j\rangle a_i^\dagger a_j. \tag{2.18}$$
Binary collisions of the form $V(\mathbf{r}-\mathbf{r}')$ are described by
$$\hat{V}_{tp} = \frac{1}{2}\sum_{nijk}\langle ni|V|jk\rangle a_n^\dagger a_i^\dagger a_j a_k. \tag{2.19}$$
Here we have used the Dirac notation $\langle i|H_{sp}|j\rangle = \int d\mathbf{r}\ \phi_i^*(\mathbf{r})H_{sp}(\mathbf{r})\phi_j(\mathbf{r})$ and $\langle ni|V_{tp}|jk\rangle = \int\int d\mathbf{r}d\mathbf{r}'\ \phi_n^*(\mathbf{r})\phi_i^*(\mathbf{r}')V_{tp}(\mathbf{r}-\mathbf{r}')\phi_j(\mathbf{r}')\phi_k(\mathbf{r})$.

The many-body Hamiltonian for a system of structureless bosons with pairwise interactions thus can be written as

$$\hat{H} = \sum_{ij}\langle i|H_{sp}|j\rangle \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2}\sum_{nijk}\langle ni|V|jk\rangle \hat{a}_n^\dagger \hat{a}_i^\dagger \hat{a}_j \hat{a}_k. \tag{2.20}$$

The formalism has been defined such that if we change between representations $\{\phi_i\}$ and $\{\chi_i\}$ using a unitary transformation, the respective field operators transform analogously, $\hat{a}_i = \sum_j \hat{b}_j c_{ji}$, $c_{ji} = \langle\phi_j|\chi_i\rangle$. If we extend such a transformation to the continuous spectrum of the single-particle position eigenstates, we can write

$$\hat{\Psi}^\dagger(\mathbf{r}) = \sum_i \hat{a}_i^\dagger \phi_i^*(\mathbf{r}), \quad \hat{\Psi}(\mathbf{r}) = \sum_i \hat{a}_i \phi_i(\mathbf{r}). \tag{2.21}$$

$\hat{\Psi}^\dagger(\mathbf{r})$ is the Bose field operator and represents the creation of a single particle ϕ_i at position $\mathbf{r}$. The field operators obey the same commutation relations as the single particle operators. In terms of the Bose field operator the many-body Hamiltonian becomes

$$\begin{aligned} \hat{H} = & \int d\mathbf{r}\ \hat{\Psi}^\dagger(\mathbf{r},t) H_{sp}(\mathbf{r}) \hat{\Psi}(\mathbf{r},t) \\ + & \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}'\ \hat{\Psi}^\dagger(\mathbf{r},t)\hat{\Psi}^\dagger(\mathbf{r}',t) V(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r}',t). \end{aligned} \tag{2.22}$$

2.3 The mean field approximation and the Gross-Pitaevskii equation

When dealing with Bose condensed systems it is useful to describe the Bose field in terms of a mean field $\Phi(\mathbf{r},t)$ and fluctuations $\hat{\delta}(\mathbf{r},t)$,

$$\hat{\Psi}(\mathbf{r},t) = \Phi(\mathbf{r},t) + \hat{\delta}(\mathbf{r},t). \tag{2.23}$$

The thermal average of the fluctuations around the mean value vanishes

$$\langle \hat{\Psi}(\mathbf{r},t) \rangle = \Phi(\mathbf{r},t), \quad \langle \hat{\delta}(\mathbf{r},t) \rangle = 0, \tag{2.24}$$

where $\langle \hat{\Psi} \rangle = \mathrm{tr}[\hat{\rho}\hat{\Psi}]$ and $\hat{\rho}$ is the density matrix of the system at thermal equilibrium. The above prescription is, to start with, merely a definition. The mean field approximation assumes that the condensate is characterised by the mean field and that the fluctuations give only small corrections, which can be dealt with perturbatively. Whether the fluctuations are small in comparison to a non-vanishing mean value depends on the density and the temperature of the system.

Experiments show that the mean field picture is valid for a fully condensed dilute gas. As noted earlier, the interactions in the dilute atomic gases are sufficiently weak that at low temperatures they give rise to only a negligible depletion of the ground state. We thus are justified in taking the mean field to be the condensate wavefunction itself and neglecting the fluctuations altogether. We can derive an equation of motion for the wave function of the mean field by commuting the field operator with the Hamiltonian and taking the average

$$i\hbar\frac{\partial}{\partial t}\Phi(\mathbf{r},t) = H_{sp}(\mathbf{r})\Phi(\mathbf{r},t) + NU_0|\Phi(\mathbf{r},t)|^2\Phi(\mathbf{r},t). \tag{2.25}$$

This is the nonlinear Schrödinger equation (NLSE) or Gross-Pitaevskii equation (GPE) [32, 33]. The nonlinearity stems from the interaction term of the Hamiltonian. Because of the nonlinearity the normalisation of $\Phi(\mathbf{r})$ is no longer independent of its equation of motion, but is directly linked to the number of particles. Here we have chosen the normalisation $\int d\mathbf{r}\ |\Phi(\mathbf{r})|^2 = 1$, with N as the total number of particles entering the GPE itself.

Provided the number of non-condensed atoms is negligible, the GPE gives a very good description of a wide range of the condensate's ground state properties, such as shapes and density profiles [34]. A series of recent experiments showing signatures of superfluidity in trapped condensates can be modelled by the GPE as well. At JILA vortices were generated using a phase imprinting method in a two-species condensate [35], following a proposal by Williams and Holland which was based on the GPE [36]. The MIT experiment found evidence of a critical velocity when stirring a condensate [37], a behaviour which could be modelled by the GPE as shown by Jackson *et al.* [38]. At Oxford, observation of the scissors mode was evidence of superfluidity in trapped BECs [39], as predicted by Guéry-Odelin and Stringari [40]. The ENS experiment observed vortex formation when

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[35] M. R. Matthews, B. P. Anderson, P. C. Haljan, D. S. Hall, *et al.*. *Vortices in a Bose-Einstein condensate.* Phys. Rev. Lett. 83, 2498 (1999).

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[40] D. Guéry-Odelin and S. Stringari. *Scissors mode and superfluidity of a trapped Bose-Einstein*

rotating condensate [41], the measured critical frequencies of which again could be described using the GPE [42].

In chapter 3 we will use the GPE to study the condensate's excitations. Even calculations of finite temperature excitations will be based on the GPE. We will, however, have to account for the presence of the thermal cloud. The fluctuations, $\hat{\delta}(\mathbf{r}, t)$, describe not only the zero temperature depletion of the ground state. They also account for the thermal excitations of atoms out of the condensate. At higher temperatures they therefore can no longer be neglected. Provided the fluctuations are included perturbatively, the mean field picture still gives a good description of the system for a wide range of temperatures. At sufficiently high temperatures, however, the perturbation scheme will fail, leading to a break down of mean field theory. In the course of this thesis we will see that the validity of mean-field theory at finite temperatures is directly related to theories for the mean-field's excitations. We will return to this point in the final chapter of this thesis.

2.3.1 The mean field and broken symmetry

If we interpret $\langle\hat{\Psi}(\mathbf{r}, t)\rangle$ as the condensate wavefunction, the existence of the mean value of the field operator becomes the defining characteristic of the condensate. This view is consistent with the general theory of critical phenomena. In the thermodynamic limit the condensation process of a three dimensional ideal Bose gas can be mapped on to the cooperative transition of a two dimensional lattice of interacting spins [26]. At the critical point of the phase transition the individual spins of the Ising model align and give rise to a net magnetisation. The magnetic moment of the system takes the role of the order parameter and its non-zero value implies that a symmetry of the system, the invariance under spatial rotations, has been broken. This process is known as 'spontaneous symmetry breaking' and is linked to zero energy Goldstone excitations [43]. In the Bose gas the order parameter of the cooperative transition is the mean value of the field operator.

condensed gas. Phys. Rev. Lett. 83, 4452 (1999).

[41] K. W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard. *Vortex formation in a stirred Bose-Einstein condensate*. Phys. Rev. Lett. 84, 806 (2000).

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[43] J. Goldstone. *Field theories with 'superconductor' solutions*. Nuovo Cimento 19, 154 (1961).

The broken symmetry is related to the phase of the mean value of the field. If the order parameter is non-zero the system has a well-defined phase, $\langle \hat{\Psi} \rangle = \Phi = |\Phi| e^{\imath\theta}$ even though the Hamiltonian is invariant under phase rotation $\hat{\Psi} \rightarrow \hat{\Psi} e^{\imath\theta}$.

When applying these results of the thermodynamic limit to systems of finite volume and number, conceptual difficulties arise. All finite systems have, in principle, a definite number of particles. Atoms are not created or destroyed and this rules out the existence of nonvanishing mean fields. Particle number and phase are conjugate variables and it is not possible to have a definite number of atoms in the condensate and simultaneously a definite condensate phase. The mean field scheme and its broken symmetry therefore cannot be rigorously exact.

Approaches to the theory of the Bose gas, which explicitly conserve the particle number of the system, however, lead to descriptions of the condensed system very similar to the results obtained using the mean field picture. In the limit of a large ground state population the two are the same (see the discussions of [44, 45, 17]). For example, GPE can be derived without the mean field by using the Schrödinger equation for a N-particle system. If we write the N-particle wavefunction as a product of N single particle wavefunctions, integrate over all but one particle index and assume $N \approx (N-1)$ we obtain the same equation as above. The nonlinearity again appears as an effect of condensate-condensate interactions. The mean field approximation thus is nothing more than a symmetry-breaking approximation or a 'convenient fiction' [46], which ultimately is justified by the fact that rigorous number-conserving approaches yield the same results. The key aspect both have in common is that they assume that the ground state of the system, the condensate, is macroscopically occupied, which leads to the following definition.

[44] C. W. Gardiner. *Particle-number-conserving Bogoliubov method which demonstrates the validity of the time-dependent Gross-Pitaevskii equation for a highly condensed Bose gas.* Phys. Rev. A 56, 1414 (1997).

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2.4 General definition of BEC

We define Bose-Einstein Condensation as a *macroscopic occupation of a single quantum state*. In condensates of dilute gases this corresponds directly to the now famous pictures taken by the initial experiments, which show the atoms gather in the ground state of the system spatially located in the minimum of the confining trap potential. In strongly interacting systems like superfluid helium the definition of BEC in terms of a macroscopically occupied state is still valid. Atoms condense in momentum space, leading to a population of the zero-momentum state which far exceeds the populations of any other single state. For strongly interacting systems, however, often a different definition of BEC is used. It focuses on the long-range phase coherence within the condensate.

The link between BEC and phase coherence was first emphasised in the work of Penrose and Onsager [47]. They consider the single-particle density matrix $\rho(\mathbf{r}, \mathbf{r}')$, which describes the first order correlation of particles at points $\mathbf{r}'$ and $\mathbf{r}$. If a single quantum state is macroscopically occupied $\rho(\mathbf{r}, \mathbf{r}')$ is non-zero for large spatial separations

$$\rho(\mathbf{r}, \mathbf{r}') = \langle \hat{\psi}(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \rangle \xrightarrow{|r-r'| \to \infty} \phi(\mathbf{r}) \phi^\dagger(\mathbf{r}'), \tag{2.26}$$

which implies that the phase must be correlated over the entire system. The function $\phi(\mathbf{r})$ can be identified as the eigenfunction of the density matrix which has a macroscopic eigenvalue. Equation (2.26) is often referred to as a criterion for 'off-diagonal long-range order' (ODLRO), in contrast to diagonal long-range order, which implies the system has some form of spatial ordering, e.g. the spatial periodicity of a crystal lattice. For the homogeneous Bose gas, ODLRO implies a form of order in momentum space, the macroscopic occupations of a single state. It is important to note that ODLRO does not necessarily imply a broken symmetry. In the thermodynamic limit, spontaneous symmetry breaking and the emergence of a mean value for the field operator of the condensate wavefunction are criteria for Bose condensation. The long-range phase-coherence then immediately follows from the existence of the well-defined phase of the mean field. As noted before, finite systems do not display a broken symmetry and thus do not have a fixed global phase. They do have long-range phase coherence, though, in the sense that

[47] O. Penrose and L. Onsager. *Bose-Einstein condensation and liquid helium*. Phys. Rev. 104, 576 (1956).

the relative phase between two points within the condensate is well defined.

If a condensate does not have a fixed global phase it may seem perplexing that two overlapping condensates of the same species form an interference pattern, as observed at MIT [48]. The observed interference pattern, however, can be explained without assuming any particular phase properties of the two clouds of atoms. The fringes appear as a result of the measurement of the position of the particles in the region where the two condensates overlap. One cannot distinguish from which of the two condensates the measured particle comes. The measurement thus in effect entangles the two condensates, giving rise to a relative phase between the two [49]. The value of the relative phase is undetermined before the actual measurement, but once it has been established it is robust. The relative phase also is 'transitive'. A measurement of the relative phase between one condensate and two others fixes the relative phase between the two other condensates [50]. Further evidence for the phase coherence of BEC in atomic vapours was found in an experiment performed at Munich [51]. It measured the relative phase between two spatially separated regions of the same system. At positions $\mathbf{r}$ and $\mathbf{r}'$ atoms were transferred out of the trap. Falling under gravity the two beams of output-coupled atoms overlapped. For a condensed system an interference pattern was measured in the region of overlap, which was taken as evidence of a phase relation between $\mathbf{r}$ and $\mathbf{r}'$ in the condensate. The resolution of the interference pattern was found to decrease with a rise in temperature and disappeared altogether at $T > T_C$.

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[50] J. A. Dunningham and K. Burnett. *Phase standard for Bose-Einstein condensates.* Phys. Rev. Lett. 82, 3729 (1999).

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Chapter 3

Excitations at Zero Temperature

In the following we study excitations of interacting Bose condensates at zero temperature. By 'zero temperature' we mean that we assume the temperatures are sufficiently low that the excited states are sparsely populated and non-condensed atoms can be neglected altogether.

If we consider a non-interacting gas, excitations of the condensate are single particles with an energy larger than that of the macroscopically occupied ground state. For the homogeneous gas the excitations thus are simply plane waves and for trapped systems they are given by the eigenmodes of the trapping potential. In interacting systems, however, a single atom travelling through the system interacts with its immediate surrounding, pushing and pulling its neighbouring atoms as it goes along. The combined system of 'bare' atom plus 'cloud', by which we mean the effect of the single atom on its surrounding, can be viewed as a new fictitious body called 'quasiparticle'. Properties of the quasiparticles like mass, energy, and lifetime strongly depend on the nature of the interactions and generally differ from the properties of the bare particle. Quasiparticles represent excited energy levels of the interacting many body system and thus are also referred to as 'elementary' excitations. A generally very different form of excitations of interacting many-body systems are called 'collective' excitations. They describe density fluctuations of the system and involve collective wave-like motion of all the particles in the system simultaneously. The collective modes disappear if there are no interactions, while elementary excitations still exist in a non-interacting gas.

In the absence of any thermal component collective dynamics of the condensate are simply described by the GPE. The linear response of the time-dependent GPE to an external perturbation yields the energies and wavefunctions of the collective excitations as eigenmodes of the system [52, 53]. In a second approach we study the quasiparticle excitations of the condensate. We diagonalise a quadratic approximation of the full Hamiltonian and thus obtain the energies of the elementary excitations of the system [8]. We find that the two approaches yield the same results.

That the elementary and collective excitations coincide for a condensed system at zero temperature is not surprising. Since all particles are described by a single eigenstate of the interacting many-body system, exciting particles from this state immediately implies collective behaviour. The equivalence of the two forms of excitations can be shown more formally by considering the two-particle propagator or density response function

$$\chi(\mathbf{r},\mathbf{r}') = \langle \hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}^{\dagger}(\mathbf{r}')\hat{\Psi}(\mathbf{r}')\rangle, \tag{3.1}$$

and the single-particle propagator

$$\rho_1(\mathbf{r},\mathbf{r}') = \langle \hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r}')\rangle, \tag{3.2}$$

where the energies of the two forms of excitations are given by the poles of the respective propagators. If we neglect the presence of non-condensed atoms the equivalence of collective and elementary excitations indeed is trivial. Inserting the mean field decomposition and neglecting all terms involving $\langle\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle$ immediately proves that the poles of the two propagators coincide. Gavoret and Noziéres [54] show that that a full treatment of the Bose gas gives the same result. They deal with the interactions perturbatively, thus including the zero-temperature condensate depletion due to collisions between condensed particles, but they still assume that no thermally excited particles are present. They find that to arbitrary order

[52] P. A. Ruprecht, M. Edwards, K. Burnett, and C. W. Clark. *Probing the linear and nonlinear excitations of Bose-condensed neutral atoms in a trap*. Phys. Rev. A 54, 4178 (1996).

[53] M. Edwards, P. A. Ruprecht, K. Burnett, R. J. Dodd, and C. W. Clark. *Collective excitations of atomic Bose-Einstein condensates*. Phys. Rev. Lett. 77, 1671 (1996).

[8] N. Bogolubov. *On the theory of superfluidity*. J. Phys. USSR 11, 23 (1947).

[54] J. Gavoret and P. Noziéres. *Structure of the perturbation expansion for the Bose liquid at zero temperature*. Ann. Phys. (NY) 28, 349 (1964).

in the perturbation expansion the energies of collective and elementary excitations are the same in the long-wavelength regime. The two forms of excitations generally also coincide at finite temperatures, but we will reserve a more detailed discussion for the concluding chapter of this thesis.

3.1 Linear response of the mean field

In the experiment excitations are observed as the response of the system to a weak external perturbation, e.g. of a sinusoidal modulation of the confining trap potential. We follow the treatment of Ruprecht *et al.* [52] and include the perturbation into the time dependent GPE like

$$i\hbar\frac{\partial}{\partial t}\Phi(\mathbf{r},t) = \left[H_{sp}(\mathbf{r}) + NU_0|\Phi(\mathbf{r},t)|^2 + f_+(\mathbf{r})e^{-\imath\Omega t} + f_-(\mathbf{r})e^{\imath\Omega t}\right]\Phi(\mathbf{r},t). \tag{3.3}$$

Here Ω is the frequency of the perturbation and $f_\pm(\mathbf{r})$ are the respective perturbation amplitudes.

The perturbation forces a shape modulation onto the Bose gas. To find the response of the condensate to the driving field we assume that it takes the form of a sum of the unperturbed ground state and a general response oscillating at the frequency of the driver

$$\Phi(\mathbf{r},t) = e^{-\imath\mu t/\hbar}[\Phi_0(\mathbf{r}) + u(\mathbf{r})e^{-\imath\Omega t} + v(\mathbf{r})e^{\imath\Omega t}]. \tag{3.4}$$

In our linear response treatment μ enters as the ground state energy of the condensate. By writing the perturbation and its response in the above form we consider sound like density fluctuations. We insert the above into the into equation (3.3), retain terms of up to linear order in $u(\mathbf{r})$ and $v(\mathbf{r})$, and obtain three equations. The first is the time independent Gross-Pitaevskii equation for the condensate ground state

$$\left[H_{sp}(\mathbf{r}) + NU_0|\Phi_0(\mathbf{r})|^2\right]\Phi(\mathbf{r}) = \mu\Phi_0(\mathbf{r}) \tag{3.5}$$

where $\int|\Phi_0(\mathbf{r})|^2 d\mathbf{r} = 1$. For the excitations we get the coupled equations

$$\begin{aligned} \left[\mathcal{L}(\mathbf{r}) - \hbar\Omega\right]u(\mathbf{r}) + \mathcal{M}(\mathbf{r})v(\mathbf{r}) &= f_+(\mathbf{r})\,\Phi_0(\mathbf{r}), && (3.6)\\ \mathcal{M}^*(\mathbf{r})u(\mathbf{r}) + \left[\mathcal{L}(\mathbf{r}) + \hbar\Omega\right]v(\mathbf{r}) &= f_-(\mathbf{r})\,\Phi_0(\mathbf{r}). && (3.7)\end{aligned}$$

[52] P. A. Ruprecht, M. Edwards, K. Burnett, and C. W. Clark. *Probing the linear and nonlinear excitations of Bose-condensed neutral atoms in a trap.* Phys. Rev. A 54, 4178 (1996).

Here we have defined

$$\mathcal{L}(\mathbf{r}) = H_{sp}(\mathbf{r}) - \mu + 2NU_0\Phi_0(\mathbf{r})^2, \tag{3.8}$$

which is the energy of an excited particle in presence of the condensate's mean field. It comprises the single-particle energy and the energy due to collision of the excitation with the condensate. The term $2U_0\Phi_0(\mathbf{r})^2$ contains the contribution of the direct (Hartree) and the exchange (Fock) interactions. The term

$$\mathcal{M}(\mathbf{r}) = NU_0[\Phi_0(\mathbf{r})]^2 \tag{3.9}$$

accounts for the formation of a pair of excitations due to collisions of two condensate atoms. This Bogoliubov process couples the two excitation amplitudes of opposite frequency, u and v, and is responsible for the condensate depletion.

We can write the above equation in a more condensed matrix form as

$$(H - \sigma_3\hbar\Omega)\Phi_{ex}(\mathbf{r}) = -\sigma_3 f(\mathbf{r}). \tag{3.10}$$

Where

$$H = \begin{pmatrix} \mathcal{L} & \mathcal{M} \\ \mathcal{M}^* & \mathcal{L} \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad f(\mathbf{r}) = \begin{pmatrix} f_+(\mathbf{r}) \\ f_-(\mathbf{r}) \end{pmatrix}. \tag{3.11}$$

The solutions to the homogeneous matrix problem $(H - \sigma_3\Omega_p)\Phi_i(\mathbf{r}) = 0$ are given by the Bogoliubov-deGennes equations and define the normal modes of the excitations $\Phi_i = (u_i, v_i)$ with eigenvalues Ω_i

$$\mathcal{L}(\mathbf{r})u_i(\mathbf{r}) + \mathcal{M}(\mathbf{r})v_i(\mathbf{r}) = \hbar\Omega_i u_i(\mathbf{r}), \tag{3.12}$$

$$\mathcal{L}(\mathbf{r})v_i(\mathbf{r}) + \mathcal{M}^*(\mathbf{r})u_i(\mathbf{r}) = -\hbar\Omega_i v_i(\mathbf{r}). \tag{3.13}$$

The eigenvalues Ω_i indeed give the resonances in the linear response, which becomes obvious if we expand the excitation and the perturbation in the normal modes

$$\Phi_{ex}(\mathbf{r}) = \sum_i c_i\phi_i(\mathbf{r}), \quad f(\mathbf{r}) = \sum_i f_i\phi_i(\mathbf{r}), \tag{3.14}$$

and insert them into equation (3.10),

$$\Phi_{ex}(\mathbf{r}) = -\sum_i \frac{f_i}{\hbar(\Omega_i - \Omega)}\phi_i(\mathbf{r}). \tag{3.15}$$

The response of the system is maximal if the perturbation matches one of the eigenfrequencies of the system.

3.2 Diagonalising the quadratic Hamiltonian

A second approach towards describing collective excitations of the Bose gas focuses on the Hamiltonian and aims to find stationary states of the system. The general Hamiltonian of an interacting many-body system, as in equation(2.22), contains products of operators of higher than quadratic order and thus cannot be diagonalised exactly. Bogoliubov showed in 1947 in his seminal treatment of the dilute Bose gas that a system with large ground state population N_0 can be approximately described by a Hamiltonian which is only quadratic in field operators. This approximate Hamiltonian then can be brought into diagonal form [8].

We shall follow Bogoliubov's original treatment use the mean field description. It is important to note that this is by no means necessary. A number conserving approach leads to the same results [44]. Since assuming a mean field does not conserve particle number, we use the grand canonical Hamiltonian $\hat{H} - \mu\hat{N}$ rather than simply $\hat{H}$, the chemical potential μ being chosen (as a function of temperature) so that the mean number of particles is constant.

If we insert the mean field decomposition, equation (2.23), into the many-body Hamiltonian and use the contact potential approximation we can group terms of the Hamiltonian according to the number of fluctuation operators

$$\hat{H} = E_0 + \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4. \tag{3.16}$$

The first of these terms is the energy functional of $\Phi(\mathbf{r})$ which, when minimised, immediately leads to the GPE for the condensate wavefunctions

$$E_0 = N\int d\mathbf{r}\;\Phi(\mathbf{r})^*\left[H_{sp}(\mathbf{r}) - \mu + \frac{1}{2}NU_0|\Phi(\mathbf{r})|^2\right]\Phi(\mathbf{r}). \tag{3.17}$$

The contribution linear in the fluctuating operator vanishes when $\Phi(\mathbf{r})$ satisfies the

[8] N. Bogolubov. *On the theory of superfluidity*. J. Phys. USSR 11, 23 (1947).

[44] C. W. Gardiner. *Particle-number-conserving Bogoliubov method which demonstrates the validity of the time-dependent Gross-Pitaevskii equation for a highly condensed Bose gas*. Phys. Rev. A 56, 1414 (1997).

Gross-Pitaevskii equation,

$$\hat{H}_1 = \sqrt{N}\int d\mathbf{r}\ \Phi^*(\mathbf{r})\left[H_{sp}(\mathbf{r}) - \mu + NU_0|\Phi(\mathbf{r})|^2\right]\hat{\delta}(\mathbf{r}) + h.c. \tag{3.18}$$

The remaining terms, quadratic, cubic and quartic in fluctuation operators are

$$\begin{aligned}\hat{H}_2 &= \int d\mathbf{r}\ \hat{\delta}^\dagger(\mathbf{r})\left[H_{sp}(\mathbf{r}) - \mu + 2NU_0|\Phi(\mathbf{r})|^2\right]\hat{\delta}(\mathbf{r}) \\ &+ \int d\mathbf{r}\ \hat{\delta}^\dagger(\mathbf{r})\left[\frac{NU_0}{2}\Phi(\mathbf{r})\Phi(\mathbf{r})\right]\hat{\delta}^\dagger(\mathbf{r}) + h.c. \end{aligned}\tag{3.19}$$

$$\hat{H}_3 = \int d\mathbf{r}\sqrt{N}U_0\Phi^*(\mathbf{r})\hat{\delta}^\dagger(\mathbf{r})\hat{\delta}(\mathbf{r})\hat{\delta}(\mathbf{r}) + h.c. \tag{3.20}$$

$$\hat{H}_4 = \int d\mathbf{r}\ \frac{U_0}{2}\hat{\delta}^\dagger(\mathbf{r})\hat{\delta}^\dagger(\mathbf{r})\hat{\delta}(\mathbf{r})\hat{\delta}(\mathbf{r}). \tag{3.21}$$

If we neglect the cubic and quartic terms, $\hat{H}_3$ and $\hat{H}_4$, and have $\Phi(\mathbf{r})$ satisfy the GPE, the remaining Hamiltonian is a sum of a constant and a quadratic form and can be diagonalised by the Bogoliubov transformation

$$\hat{\delta}(\mathbf{r}) = \sum_i [u_i(\mathbf{r})\hat{\beta}_i - v_i^*(\mathbf{r})\hat{\beta}_i^\dagger]. \tag{3.22}$$

It defines a basis of coherent linear superpositions of creation and annihilation operators which, for the transformation to be canonical, must obey the commutation relations for Bosons, $[\hat{\beta}_i, \hat{\beta}_j^\dagger] = \hat{\delta}_{i,j}$, $[\hat{\beta}_i, \hat{\beta}_j] = [\hat{\beta}_i^\dagger, \hat{\beta}_j^\dagger] = 0$. These imply that the transformation coefficients must satisfy the following orthogonality and symmetry relations

$$\int d\mathbf{r}\,[u_i^*(\mathbf{r})u_j(\mathbf{r}) - v_i^*(\mathbf{r})v_j(\mathbf{r})] = \delta_{ij}, \tag{3.23}$$

$$\int d\mathbf{r}\,[u_i^*(\mathbf{r})v_j(\mathbf{r}) - v_i^*(\mathbf{r})u_j(\mathbf{r})] = 0. \tag{3.24}$$

If the wavefunctions $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$ satisfy the Bogoliubov-de Gennes equations (3.13), the Bogoliubov transformation then recasts the quadratic Hamiltonian in a basis of non-interacting quasiparticles,

$$H = E_0 + \sum_i \epsilon_i \hat{\beta}_i{}^\dagger \hat{\beta}_i \tag{3.25}$$

where $\epsilon_i = \hbar\Omega_i$ is the energy of a quasiparticle in level i.

3.2.1 Orthogonality of excitations to the condensate

It is important to note that the broken symmetry approach of sections 3.1 and 3.2 does not require explicitly the wavefunctions of excitations, $u_i(\mathbf{r})$ and $v_j(\mathbf{r})$, to be orthogonal to the condensate groundstate $\phi_0(\mathbf{r})$

$$u_i^{ortho}(\mathbf{r}) = u_i(\mathbf{r}) - a_i\phi_0(\mathbf{r}), \quad a_i = \int d\mathbf{r}\phi_0^*(\mathbf{r})u_i(\mathbf{r}). \tag{3.26}$$

Both $u_i^{ortho}(\mathbf{r})$ and $u_i(\mathbf{r})$ satisfy the BdG equations. This is in contrast to number conserving treatments of the quadratic Hamiltonian, where orthogonality to the condensate is a necessary requirement for the linear term of the Hamiltonian, H_1, to be equal to zero [17]. The excitation energies, however, remain the same, whether the excitations are orthogonal to the condensate or not. Since the energies of the excitations are measured relative to the energy of the condensate ground state. Mixing in a zero energy component will not change the excitation energies themselves.

In homogeneous systems the issue of orthogonality does not arise at all. There the excitations are described by plane waves, or alternatively delta functions in their momentum representation, which do not overlap with the zero momentum ground state. In trapped systems, however, all wavefunctions are spatially dependent and an overlap of excitations with the ground state can occur. Problems arise when we use the quasiparticle transformation to calculate expectation values of pairs of fluctuation operators, which we will be necessary for finite temperature treatments.

$$\rho(\mathbf{r},t) = \langle\hat{\delta}^\dagger(\mathbf{r},t)\hat{\delta}(\mathbf{r},t)\rangle = \sum_i(|u_i(\mathbf{r})|^2 + |v_i(\mathbf{r})|^2)n_i + |v_i(\mathbf{r})|^2 \tag{3.27}$$

will describe the excited state population density and

$$\kappa(\mathbf{r},t) = \langle\hat{\delta}(\mathbf{r},t)\hat{\delta}(\mathbf{r},t)\rangle = \sum_i u_i(\mathbf{r})v_i^*(\mathbf{r})(1+2n_i), \tag{3.28}$$

the pair anomalous average, will be linked to collision induced correlations between particles. Here we have used $n_i = \langle\hat{\beta}_i^\dagger\hat{\beta}_i\rangle$ for the population of the respective quasiparticle level. These quantities only describe the populations of, and correlations

[17] S. A. Morgan. A Gapless Theory of Bose-Einstein Condensation in Dilute Gases at Finite Temperature. Ph.D. thesis, University of Oxford (1999).

within, the thermal cloud correctly if the excitations do not contain a condensate contribution. For the course of this thesis we therefore chose to define our excitation wavefunctions $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$ as solutions of the BdG equations in the sub-space orthogonal to the condensate. By restricting ourselves to this sub-space we also bypass the 'problem of the missing eigenvector', which is known to arise when diagonalising the quadratic Hamiltonian of a bosonic system in a basis including the ground state [55, 45].

3.2.2 The homogeneous Bose gas

Since the next chapter will largely focus on finite temperature excitations in homogeneous systems it is worth considering the homogeneous case at zero temperatures in more detail. In absence of a confining potential the spatial dependence of all quantities disappears and momentum conservation ensures that the quasiparticles become linear superpositions of particles and holes of opposite momenta,

$$\hat{\delta}_k = u_k \hat{\beta}_k - v_k \hat{\beta}^\dagger_{-k}. \tag{3.29}$$

The coefficients u_k and v_k become simple numbers, which we chose to be real, and the BdG equations can be solved analytically. Bogoliubov derived the now famous dispersion relation for the weakly interacting homogeneous Bose gas to be

$$\begin{aligned} \epsilon_k &= \sqrt{2nU_0\epsilon_k^{sp} + (\epsilon_k^{sp})^2} \\ &\approx \begin{cases} \sqrt{U_0 n/m}\ \hbar k, & \text{for } k \to 0, \\ (\hbar k)^2/2m, & \text{for } k \to \infty. \end{cases} \end{aligned} \tag{3.30}$$

Here $n = N/V$ is the number density, and $\epsilon_k^{sp} = (\hbar k)^2/2m$ is the free particle energy. High energy excitations of the Bose gas resemble free particles. For low-lying excitations the presence of the condensate changes the dispersion relation to be linear in k, which is characteristic for phonon-type excitations. The linear scaling of the energy for small k means that the gradient of the dispersion relation has a lower bound. The gas requires a minimum amount of energy to form an excitation, which implies the system will exhibit superfluid behaviour.

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[55] J. P. Blaizot and G.Ripka. Quantum theory of finite systems, pp. 58–68 (MIT Press).

[45] Y. Castin and R. Dum. *Low-temperature Bose-Einstein condensates in time-dependent traps: Beyond the u(1) symmetry-breaking approach.* Phys. Rev. A 57, 3008 (1998).

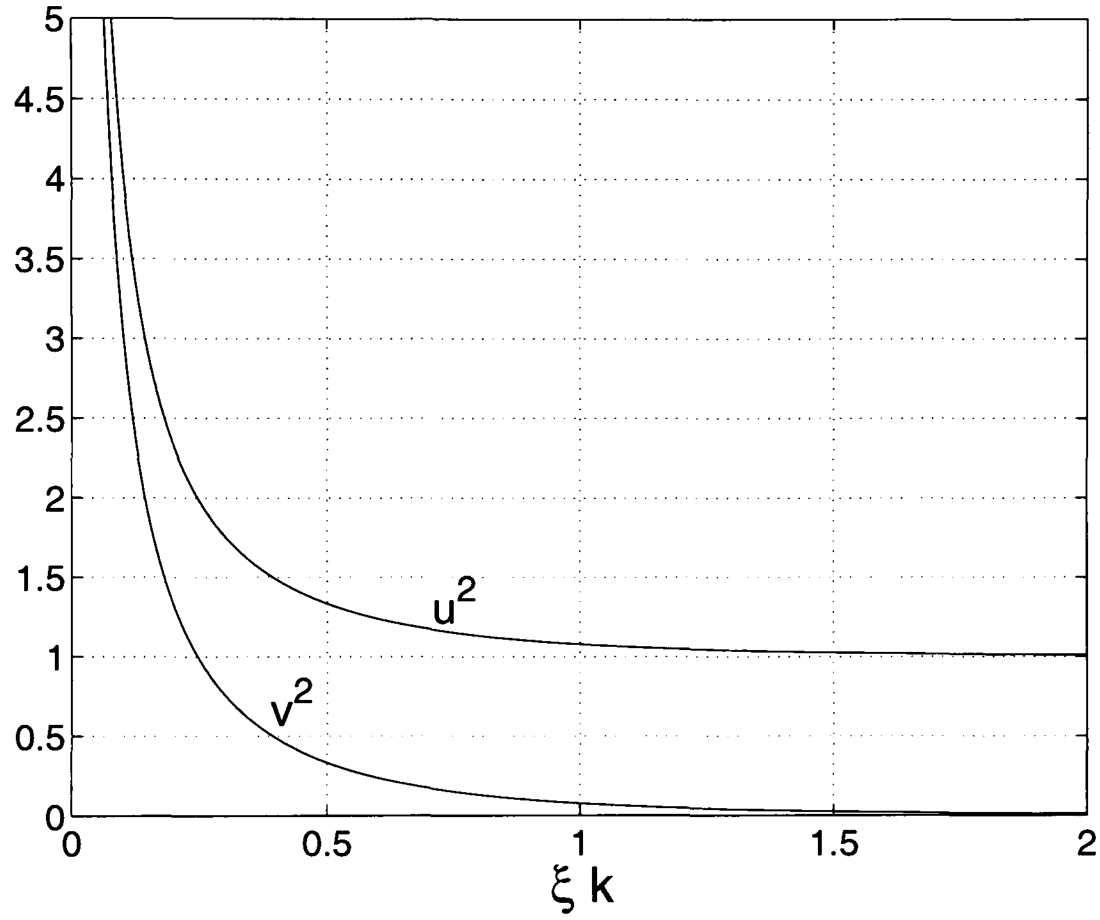

Figure 3.1: The square of the quasiparticle coefficients, u^2 and v^2 as a function of momentum. For momenta $\xi k > 1$ the coefficient v becomes small and $\hat{\delta}_k \simeq \hat{\beta}_k$. For momenta $\xi k < 1$ the phonon-type excitations are a proper superposition of particle with momentum k and a hole with $-k$.

The characteristic length scale of the system $\xi = (\sqrt{8\pi n a})^{-1}$ is called the healing length. If we rewrite the dispersion relation in terms of ξ,

$$\epsilon_k = nU_0\, \xi k\, \sqrt{2 + \xi^2 k^2}, \tag{3.31}$$

it becomes clear that the phonon branch of the spectrum goes over to the quadratic one when $\xi k \approx 1$ ($\xi \approx 0.1\mu m$ for ^{87}Rb experiments). The coefficients u_k and v_k are given by the following equation

$$v_k^2 = u_k^2 - 1 = \frac{1}{2}\left(\frac{\epsilon_k^{sp} + nU_0}{\epsilon_k} - 1\right) = \frac{1}{2}\left(\frac{(\xi k)^2 + 1}{\xi k\sqrt{2 + (\xi k)^2}} - 1\right), \tag{3.32}$$

which, we note, is divergent for $k \to 0$.

3.3 First finite temperature extensions of T=0 theory

Our zero temperature theory was based on the assumption that we can neglect the presence of any thermal component of the system and assume all particles to be in the condensed phase. The remainder of this thesis will turn to the problem of describing the dynamics of a condensate when the effects of non-condensed atoms can no longer be neglected.

When heating up a system from zero to some finite temperature, the primary effect is that the condensate itself gets depleted as condensed atoms are thermally excited into the surrounding non-condensed cloud. The simplest approximate finite temperature theory accounts for the depletion by adjusting the number of condensed particles in the GPE to its now temperature dependent value, but otherwise ignores the thermal component. The GPE and its linear response then describe excitations very well for temperatures up to $0.5\,T_C$ [56].

Further finite temperature effects, which are more difficult to deal with, have to do with the fact that interactions are no longer simply collisions between condensed particles, as given by the non-linearity in the GPE. We have to include collision processes involving thermal atoms and account for the effect their presence has on all other forms of collisions. An excitation of the condensate no longer interacts

[56] R. J. Dodd, M. Edwards, C. W. Clark, and K. Burnett. *Collective excitations of Bose-Einstein-condensed gases at finite temperatures*. Phys. Rev. A 57, R32 (1998).

only with the mean field but also with the thermal cloud, leading to damping of the excitation. The disagreement of the GPE and experimental data on excitation energies for $T > 0.5T_C$ suggests, that the effects of thermal atoms on collisions become important at higher temperatures.

In our equations all effects of non-condensed atoms are described by the fluctuation operator $\hat{\delta}(\mathbf{r}, t)$. To include fluctuations into the description of a finite temperature system, we keep terms which involve pairs of the fluctuation operators $\hat{\delta}(\mathbf{r}, t)$ when deriving the equation for the mean field. This gives the generalised GPE

$$i\hbar\frac{d}{dt}\Phi(\mathbf{r},t) = \Big[H_{sp}(\mathbf{r}) + N_0U_0|\Phi(\mathbf{r},t)|^2 + 2U_0\rho(\mathbf{r},t)\Big]\Phi(\mathbf{r},\mathbf{t}) + U_0\kappa(\mathbf{r},t)\Phi^*(\mathbf{r},t). \tag{3.33}$$

We can study the excitations of a finite temperature system using a linear response analysis analogous to section 3.1. The standard approach assumes the averages ρ and κ to be time independent [57]. We will find that this assumption leads to an inconsistent description of our system. Following the standard linear response treatment we obtain for the static condensate and its excitations

$$\mu\Phi(\mathbf{r}) = \Big[H_{sp}(\mathbf{r}) + N_0U_0|\Phi(\mathbf{r})|^2 + 2U_0\rho(\mathbf{r})\Big]\Phi(\mathbf{r},\mathbf{t}) + U_0\kappa(\mathbf{r})\Phi^*(\mathbf{r}), \tag{3.34}$$

$$\begin{aligned} \mathcal{L}(\mathbf{r})u_j(\mathbf{r}) + \mathcal{M}(\mathbf{r})v_j(\mathbf{r}) &= \epsilon_j u_j(\mathbf{r}), \\ \mathcal{L}(\mathbf{r})v_j(\mathbf{r}) + \mathcal{M}^*(\mathbf{r})u_j(\mathbf{r}) &= -\epsilon_j v_j(\mathbf{r}). \end{aligned} \tag{3.35}$$

These equations are commonly referred to as the generalised GPE and the Hartree-Fock-Bogoliubov (HFB) equations, where $\mathcal{L}(\mathbf{r})$ and $\mathcal{M}(\mathbf{r})$ take the form

$$\begin{aligned} \mathcal{L}(\mathbf{r}) &= H_{sp}(\mathbf{r}) - \mu + 2N_0U_0|\Phi_0(\mathbf{r})|^2 + 2U_0\rho(\mathbf{r}), \\ \mathcal{M}(\mathbf{r}) &= U_0\Phi_0(\mathbf{r})^2\kappa(\mathbf{r}). \end{aligned} \tag{3.36}$$

and reduce to the ordinary GPE and BdG equations if we set $\rho(\mathbf{r})$ and $\kappa(\mathbf{r})$ to zero.

The same set of equations can be derived using a diagonalisation approach similar to the one of section 3.2. The conventional treatment uses a factorisation approximation which reduces the the cubic and quartic terms of the Hamiltonian,

[57] R. J. Dodd. Bose-Einstein condensation in atomic alkali gases. Ph.D. thesis, University of Maryland (College Park) (1997).

equations (5.5,5.6), to linear and quadratic forms respectively [58],

$$
\begin{aligned}
\hat{\delta}^{\dagger}\hat{\delta}\hat{\delta} &\approx 2\rho\hat{\delta} + \kappa\hat{\delta}^{\dagger}, &(3.37)\\
\hat{\delta}^{\dagger}\hat{\delta}^{\dagger}\hat{\delta}\hat{\delta} &\approx 4\rho\hat{\delta}^{\dagger}\hat{\delta} + \kappa^{*}\hat{\delta}\hat{\delta} + \kappa\hat{\delta}^{\dagger}\hat{\delta}^{\dagger}. &(3.38)
\end{aligned}
$$

The factorisation approximation on the triplets is, in fact, not justified [17] and gives rise to non-physical features in our equations which we will discuss below. If we do employ above approximations, however, we obtain a Hamiltonian linear and quadratic in the fluctuation operators which can then be diagonalised by the Bogoluibov transformation. The resulting equations are again the generalised GPE and the HFB equations, equations (3.34,3.35-5.36).

The HFB equations are not a suitable theory to describe low-lying excitations of finite temperature systems. The problems of HFB manifest themselves in ultra-violet and infra-red divergences of contributions involving the anomalous average, $\kappa(\mathbf{r})$ [59]. We will discuss these issues in more detail in the following chapter. An additional serious problem of HFB is that it fails to predict a gapless energy spectrum for the homogeneous gas [58]. For systems, where the range of excitation energies are not limited by external trapping potentials, one expects to find a zero energy excitation of the system, which corresponds to a phase rotation of the condensate.

That a system of Bosons must display a gapless spectrum of excitation energies was first shown by Hugenholtz and Pines [60]. Using a field theoretical formalism akin to the one of Beliaev, they calculated the energy of a long wavelength excitation as a pole of the one-particle Greens function. They thus were able to show that, to all orders in the interaction potential, the excitation energy is equal to zero for zero momentum. Inserting

$$\epsilon_0 = 0,\ u_0(\mathbf{r}) = \phi(\mathbf{r}),\ v_0(\mathbf{r}) = -\phi^{*}(\mathbf{r}), \tag{3.39}$$

[58] A. Griffin. *Conserving and gapless approximations for an inhomogeneous Bose gas at finite temperatures*. Phys. Rev. B 53, 9341 (1996).

[17] S. A. Morgan. A Gapless Theory of Bose-Einstein Condensation in Dilute Gases at Finite Temperature. Ph.D. thesis, University of Oxford (1999).

[59] D. A. W. Hutchinson, K. Burnett, R. J. Dodd, S. A. Morgan, *et al.*. *Gapless mean-filed theory of Bose-Einstein condensates*. J. Phys. B 33, 3825 (2000).

[60] N. M. Hugenholtz and D. Pines. *Ground-state energy and excitation spectrum of a system of interacting bosons*. Phys. Rev. 116, 489 (1959).

into the BdG, equation (3.13), shows that the GPE satisfies the BdG equation for such a solution. The HFB equations, however, do not do so, unless one assumes the anomalous fluctuations to be zero. Setting $\kappa(\mathbf{r}) = 0$ not only renders the equations gapless but also avoids any of the IR and UV divergences.

If we neglect the the anomalous fluctuations within the HFB equations we obtain what is referred to as the HFB-Popov approximation. It gives a spectrum which at T=0 coincides with the Bogoliubov theory and goes over to the finite-temperature HFB spectrum at high temperatures. HFB-Popov neglects the detailed effects of thermal collisions and ignores all dynamical aspects of the thermal cloud altogether. It is equivalent to the Bogoliubov theory when assuming that the only effect of the thermal component is to change the static external potential

$$V(\mathbf{r}) \to V(\mathbf{r}) + 2U_0\rho(\mathbf{r}), \tag{3.40}$$

which, despite being fairly involved computationally, does not improve significantly on calculations using the GPE with a temperature adjusted N_0 [56].

Our first attempt of including $\kappa(\mathbf{r})$ into our formalism failed because key assumptions were not justified. In the linear response treatment we assumed the fluctuations to be static. In the diagonalisation approach we used the factorisation approximation on the triplets. In the next chapter we will show that including time dependent fluctuations of $\rho(\mathbf{r}, t)$ and $\kappa(\mathbf{r}, t)$ into a linear response treatment not only consistently includes correlations into our formalism but also describes lifetimes of the excitations.

[56] R. J. Dodd, M. Edwards, C. W. Clark, and K. Burnett. *Collective excitations of Bose-Einstein-condensed gases at finite temperatures*. Phys. Rev. A 57, R32 (1998).

Chapter 4

Time dependent Mean Fields at Finite Temperatures

In this chapter we study the linear response of a Bose condensed gas to an external perturbation at finite temperatures. More specifically, we study the coupled dynamics of both the condensate and the surrounding thermal cloud in the linear regime. We include the effects the time dependent mean field of the condensate has on the population of non-condensed particles and how they in turn act back onto the condensate. This description presents a simple way to understand the interaction between condensate and non-condensed atoms and enables us to include the effect the condensate has on collision dynamics. We do not use the Popov approximation, which involves neglecting the anomalous correlations. Instead we include all time dependent correlations - normal and anomalous - consistently to second order in the inter-atomic interaction potential V. This enables us to formulate a theory which deals with all forms of interactions in a systematic fashion and includes damping.

It is worth commenting on the distinction frequently made between 'collisionless' and 'collisional' or 'hydrodynamic' regimes. The collisional regime refers to a scenario of relatively high densities where the the mean free path of the particles is much smaller than the wavelength of the excitation, $d_{mfp} \ll \lambda_{ex}$. In such a collision dominated regime one can approximate the thermal component of the system to be in local thermodynamic equilibrium (LTE), which then enables a description of the system in terms of two-fluid hydrodynamics (see e.g. [61]). The term collisionless

[61] E. Zaremba, A. Griffin, and T. Nikuni. *Two-fluid hydrodynamics for a trapped weakly-*

regime refers to lower densities, and corresponds to the conditions found in most of the recent experiments. If the mean free path is comparable to the wavelength of the low-lying excitations we no longer can assume the thermal component to be in LTE. The treatments of this thesis are free of such approximations and thus fall into the category of 'collisionless' theories.

Any formalism put forward to describe an inhomogeneous Bose gas can be usefully analysed by examining its implications in the corresponding homogeneous case. In section 4.2 we apply our general formalism to the specific case of a homogeneous system and present an explicit V^2 treatment of the weakly interacting gas. It then is straightforward to relate our approach to effective interactions, two- and many-body T-matrices, as expounded by Stoof *et al.* [62] and Shi and Griffin [63]. The formalism shows from first principles that the damping of excitations in homogeneous systems is given by Fermi's Golden Rule for Landau and Beliaev processes, which allows us to link the formalism to well known results from the Bose gas theory. It also includes kinetics due to non-condensed atom collisions as well. By treating the static and dynamic aspects of the pair and triplet averages in a consistent fashion we show that the equations for the excitations do not exhibit an energy gap for the weakly interacting gas.

In section 4.3 we discuss how our effective interactions can be replaced by contact potentials. We find that the usual procedure of replacing the inter-atomic potential V by $U_0\delta(\mathbf{r})$ is inadequate and renders our theory ultra-violet divergent. A suitable renormalisation, however, can rectify this problem. Renormalised a U_0^2 treatment is equivalent to our V^2 analysis.

In section 4.4 we show how our general formalism can be used to go beyond V^2 and give self-consistent descriptions of finite temperature condensates with a static thermal component. We explicitly write out gapless equations for a condensate with static thermal cloud and give a criterion for their validity for trapped systems. The chapter concludes with a discussion of infra-red divergences in theories for homogeneous and trapped systems.

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interacting Bose gas. Phys. Rev. A 57, 4695 (1998).

[62] H. T. C. Stoof, M. Bijlsma, and M. Houbiers. *Theory of interacting quantum gases*. J. Res. Natl. Inst. Stand. Tech. 101, 443 (1996).

[63] H. Shi and A. Griffin. *Finite-temperature excitations in a dilute Bose-condensed gas*. Phys. Rep. 304, 1 (1998).

4.1 Linearisation the Mean Field at finite temperatures

In the following we choose to write the Bose field operators in the basis of single particle states which allows us to take the single particle energy to be diagonal $\langle i|H_{sp}|j\rangle = \omega_i \delta_{ij}$ ($\hbar = 1$ henceforth). This gives us for the Hamiltonian

$$\hat{H} = \sum_i \omega_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \sum_{nijk} \langle ni|V|jk\rangle \hat{a}_n^\dagger \hat{a}_i^\dagger \hat{a}_j \hat{a}_k. \tag{4.1}$$

The matrix element of the interaction terms has been conveniently symmetrised to be

$$\langle ni|V|jk\rangle = \frac{1}{2}[(ni|V|jk) + (ni|V|kj)]. \tag{4.2}$$

Following the mean field approach of chapter 2 we decompose the single particle field operator $\hat{a}$ as

$$\hat{a}_i(t) = z_i(t) + \hat{c}_i(t)\,,\; \langle \hat{a}_i(t)\rangle = z_i(t). \tag{4.3}$$

The mean value $z_i(t)$ is the expansion coefficient of the coherent part of the condensate, $\Phi(\mathbf{r},t) = \sum_i \phi_i(\mathbf{r}) z_i(t)$. $\hat{c}_i(t)$ gives the coefficient of the quantum and thermal fluctuations about the mean value of the field and has a vanishing average value. For simplicity we will from now on drop the explicit 'hat' notation in the operators.

In order to obtain the finite temperature equation of motion for the condensate, we need to calculate the rate of change of the mean field $z_n(t)$. In analogy to the $T = 0$ linear response treatment of chapter 3 we use the Heisenberg equation of motion for operator $\hat{a}_n(t)$ and take the expectation value to get

$$\begin{aligned} i\frac{d}{dt} z_n(t) &= \omega_n z_n(t) + \sum_{ijk} \langle ni|V|jk\rangle \Big\{ z_i^*(t) z_j(t) z_k(t) \\ &\quad + 2\rho_{ji}(t) z_k(t) + \kappa_{jk} z_i^*(t) + \lambda_{ijk}(t) \Big\}. \end{aligned} \tag{4.4}$$

Here we have introduced in basis state notation of the one-body density matrix or normal pair average

$$\rho_{ij}(t) \equiv \langle c_j^\dagger(t) c_i(t)\rangle, \tag{4.5}$$

the anomalous pair average

$$\kappa_{ij}(t) \equiv \langle c_j(t) c_i(t)\rangle, \tag{4.6}$$

and the triplet anomalous average

$$\lambda_{ijk}(t) \equiv \langle c_i^\dagger(t) c_j(t) c_i(t) \rangle. \tag{4.7}$$

At this point our equation of motion (4.4) is exact. The problem is that we cannot in general obtain closed expressions for the correlations $\rho_{ij}(t)$, $\kappa_{ij}(t)$, and $\lambda_{ijk}(t)$. We can, however, find approximate expressions by considering the linear response to an external perturbation. To do this we assume the system is initially in equilibrium, with the condensed part $z_n(t)$ at rest, and the non-condensed particles having a thermal distribution. The anomalous average κ_{ij}, as well as the other correlation functions, will have some static value. We then suppose that we disturb the system by applying a small periodic perturbation, e.g. to the trap potential. The coherent part of the condensate begins to oscillate at a frequency $\tilde{\omega}$ with a small amplitude δz_n. Since the perturbation is taken to be weak we assume the system responds linearly to it. The oscillation of the condensate will affect the thermal particles and leads to changes in the quantities $\rho_{ij}(t)$, $\kappa_{ij}(t)$, and $\lambda_{ijk}(t)$. The changes in $\rho_{ij}(t)$, $\kappa_{ij}(t)$, and $\lambda_{ijk}(t)$ will then appear in the equation of motion for $z_n(t)$, equation (4.4), and thus act back on the oscillating condensate. For a self-consistent description of the system this back-action loop has to be handled in an iterative manner, which we turn to in section 4.4. To describe the scenario analytically, we linearise the equation of motion, equation (4.4),

$$\begin{aligned} z_n(t) &= e^{-\imath\mu t}\,[\,z_n^0 + \delta z_n(t)\,], && (4.8)\\ \rho_{ji}(t) &= \rho_{ji}^0 + \delta\rho_{ji}(t), && (4.9)\\ \kappa_{ji}(t) &= e^{-2\imath\mu t}\,[\kappa_{ji}^0 + \delta\kappa_{ji}(t)], && (4.10)\\ \lambda_{ijk}(t) &= e^{-\imath\mu t}\,[\,\lambda_{ijk}^0 + \delta\lambda_{ijk}(t)\,], && (4.11) \end{aligned}$$

and neglect terms quadratic in the fluctuations, equation (4.4). This gives us the following equation for the ground state

$$\mu z_n^0 \;=\; \omega_n z_n^0 + \sum_{ijk}\langle ni|V|jk\rangle\left\{\, z_j^0 z_k^0 z_i^{0\,*} + \kappa_{jk}^0 z_i^{0\,*} + 2\rho_{ji}^0 z_k^0 + \lambda_{ijk}^0 \right\}, \tag{4.12}$$

and for the excitations we obtain

$$\imath\frac{d}{dt}\delta z_n(t) \;=\; (\omega_n - \mu)\,\delta z_n$$

$$
\begin{aligned}
&+\sum_{ijk}\langle ni|V|jk\rangle \ \left\{z_j^0\, z_k^0\, \delta z_i^* + \kappa_{jk}^0\, \delta z_i^*\right\} \\
&+\sum_{ijk}\langle ni|V|jk\rangle \ \left\{2z_i^{0\,*}\, z_j^0\, \delta z_k \ + \ z_i^{0\,*}\, \delta\kappa_{jk}\right\} \\
&+\sum_{ijk}\langle ni|V|jk\rangle \ \left\{2\rho_{ji}^0\delta z_k \ + \ \delta\lambda_{ijk}\right\} \\
&+\sum_{ijk}\langle ni|V|jk\rangle \ \ 2\delta\rho_{ji} z_k^0.
\end{aligned}
\qquad (4.13)
$$

As before, μ enters above equations as the ground state energy of the condensate. Note that we have not replaced the inter-atomic potential V by the contact interaction U_0. By including the triplet anomalous average λ we are going beyond the conventional mean field theory. The triplet average is needed to properly account for collisions involving non-condensed atoms and hence to get a consistent finite temperature mean field description of the system. We also keep the pair anomalous average, neglected in the Popov approximation.

The equation for the excitations, equation (4.13), is very similar to the HFB equations of section 3.3. If we use the ansatz $\delta z_j(t) = u_{nj}e^{-\imath\Omega_n t} + v_{nj}e^{\imath\Omega_n t}$ and set the fluctuations to be static, $\delta\rho = \delta\kappa = \delta\lambda = 0$, we immediately obtain from equation (4.13) the HFB equations in number state notation, describing the quasiparticle amplitudes and energies. It thus is clear that the quasiparticle excitations of the total system can be thought of as the first approximation to the more accurate description of excitations which we seek here. When ignoring the fluctuations of the correlation functions the excitations of the system are just the quasiparticles. In this treatment, however, we go beyond the description of excitations in terms of quasiparticles and include the time dependence of the correlation functions. We thus include the effect the dynamics of the mean field has on the thermal cloud and the back action of the thermal could on the condensate.

To obtain a closed equation describing the interplay between the condensed and non-condensed part of the system we have to express the pair and triplet averages in terms of the perturbation δz_i, and this is what we turn to do next. For this we use their definition in terms of the fluctuation operators $c_i(t)$. The time dependent perturbation of the mean field affects the time evolution of the fluctuation operator $c_i(t)$. The dynamics of this quantity can be found analogously to above treatment of the quantity $z_i(t)$. Such a full analysis, however, would lead to a very complex set of equations. The equations take a much simpler form if we move from the number state basis, $\{c_i\}$, to the quasiparticle basis, $\{b_i\}$, using the Bogoliubov transformation

$$c_i = \sum_j \left\{ u_{ij} b_j + v_{ij}^* b_j^\dagger \right\}. \tag{4.14}$$

We recall from section 3.2 that the Hamiltonian of the unperturbed system can be diagonalised if we approximate it by a form which is quadratic in the field operators. The Bogoliubov transformation (4.14) then gives the quadratic Hamiltonian in the quasiparticle basis

$$\hat{H} = E_0 + \sum_i \Omega_i b_i^\dagger b_i. \tag{4.15}$$

In absence of any perturbation, $\delta z(t)$, the quasiparticles thus have the trivial time evolution

$$b_i(t) = b_i(t')\, e^{-\imath \Omega_i (t-t')}. \tag{4.16}$$

Under the influence of the perturbation δz_i the time evolution of the quasiparticle operators varies only slowly from the above form. This allows us to integrate to first order the equation of motion for the quasiparticle operators when the perturbation is present. Having obtained the expression for $b_i(t)$ we will be able to construct expressions for $\rho_{ij}(t)$ and $\kappa_{ij}(t)$. In effect we are treating the dynamics of the system using perturbation theory in the quasiparticle basis.

In order to proceed we have to be more specific how the perturbation δz_i changes the Hamiltonian. In its quadratic form the Hamiltonian can be written as [64]

$$\hat{H} = \frac{1}{2} \sum_{pq} \left\{ h_{pq} c_p^\dagger c_q + h_{pq} c_q c_p^\dagger + \Delta_{pq} c_p^\dagger c_q^\dagger + \Delta_{pq}^* c_q c_p \right\}, \tag{4.17}$$

where h_{pq} and Δ_{pq} are defined as

$$h_{ij} \equiv \langle i|\hat{\mathbf{h}}|j\rangle \equiv \langle i|\hat{H}_0 - \mu|j\rangle + 2\sum_{kl} \langle ik|V|lj\rangle \left[z_k^* z_l + \rho_{lk} \right], \tag{4.18}$$

$$\Delta_{ij} \equiv \langle ij|\hat{\mathbf{\Delta}}\rangle \equiv \sum_{kl} \langle ij|V|kl\rangle \left[\kappa_{kl} + z_k z_l \right]. \tag{4.19}$$

They are the generalisation of the terms $\mathcal{L}(\mathbf{r})$ and $\mathcal{M}(\mathbf{r})$ of Chapter 2, which in basis state notation read

$$\mathcal{L}_{ij} = \langle i|\hat{H}_0 - \mu|j\rangle + 2\sum_{kl} \langle ik|V|lj\rangle \left[z_k^* z_l \right], \tag{4.20}$$

[64] J. P. Blaizot and G.Ripka. Quantum theory of finite systems (MIT Press, 1986).

$$\mathcal{M}_{ij} = \sum_{kl} \langle ij|V|kl\rangle \, [z_k z_l] \, . \tag{4.21}$$

Substituting $z_i(t) \to z_i^0 + \delta z_i(t)$ into the Hamiltonian (4.17) allows us to write the perturbation as a linearisation around the equilibrium Hamiltonian,

$$\hat{H}(t) \to \hat{H}^{Equ} + \delta \hat{H}(t) \iff h_{pq} \to h_{pq}^0 + \delta h_{pq}(t), \; \Delta_{pq} \to \Delta_{pq}^0 + \delta\Delta h_{pq}(t). \tag{4.22}$$

The perturbations $\delta h_{pq}(t)$ and $\delta\Delta_{pq}(t)$ then have the form

$$\delta h_{pq}(t) = \delta\langle p|\hat{H}^0|q\rangle + 2\sum_{kl} \langle pk|V|lq\rangle \left\{ \delta z_k^*(t) z_l^0 + z_k^{0*} \delta z_l(t) + \delta\rho_{lk}(t) \right\} \tag{4.23}$$

$$\delta\Delta_{pq}(t) = \sum_{kl} \langle pq|V|kl\rangle \left\{ \delta z_k(t) z_l^0 + z_k^0 \delta z_l(t) + \delta\kappa_{kl}(t) \right\}, \tag{4.24}$$

where we have neglected terms with $(\delta z)^2$. The time evolution of the quasiparticle operators under influence of the external perturbation is now given by the Heisenberg equation of motion

$$\imath \frac{db_i}{dt} = [b_i, \hat{H}] = \Omega_i b_i + [b_i, \delta\hat{H}(t)]. \tag{4.25}$$

4.2 Homogeneous condensates at finite temperatures

For the purposes of exposition, we now limit our discussion to the case of homogeneous systems. This simplifies the equations and allows us to explain the physical content of the equations more easily.

In the following we also are going to limit ourselves to second order in the two-particle interaction potential V. We can, therefore, neglect the $\delta\rho(t)$ and $\delta\kappa(t)$ contributions to the matrix elements of the perturbed quadratic Hamiltonian equations (4.23)-(4.24). In the absence of a confining potential the single particle operators create and annihilate free particles. Thus the labelling of the operator $a_p = z_p + c_p$ will refer to the momentum p of the free particle rather than the energy eigenstate of the trap. The condensate is, of course, in the zero momentum state so we write

$$z_p^0 = z_0^0 \, \delta_{p,0} \simeq \sqrt{n_0} \, \delta_{p,0}, \tag{4.26}$$

n_0 being the number of particles in the zero momentum state. Since we are dealing with the homogeneous case we can use equation (4.26) as well as momentum conservation to simplify equation (4.13)

$$
\begin{aligned}
\imath\frac{d}{dt}\delta z_p = \quad & (\omega_p - \mu)\,\delta z_p \\
+ \quad & \langle p, -p|V|00\rangle\; n_0 \delta z^*_{-p} + \sum_{ijk}\langle pi|V|jk\rangle\; \kappa^0_{jk}\delta z^*_i && (4.27)\\
+ \quad & \langle p0|V|0p\rangle\; 2n_0\;\delta z_p\; + \sum_{jk}\langle p0|V|jk\rangle\; \sqrt{n_0}\,\delta\kappa_{jk} && (4.28)\\
+ \quad & \sum_{ijk}\langle pi|V|jk\rangle\; 2\rho^0_{ji}\delta z_p\; + \sum_{ijk}\langle ni|V|jk\rangle\;\delta\lambda_{ijk} && (4.29)\\
+ \quad & \sum_{ij}\langle pi|V|j0\rangle\; 2\sqrt{n_0}\,\delta\rho_{ji}. && (4.30)
\end{aligned}
$$

We recall that in the homogeneous case the quasiparticle transformation also simplifies to

$$
\begin{aligned}
c_p &= u_p b_p + v_p b^\dagger_{-p}\,, \quad c^\dagger_p = u_p b^\dagger_p + v_p b_{-p},\\
b_p &= u_p c_p - v_p c^\dagger_{-p}\,, \quad b^\dagger_p = u_p c^\dagger_p - v_p c_{-p}.
\end{aligned} \tag{4.31}
$$

Assuming the system is perturbed with the frequency $\tilde{\omega}$ we can write

$$
\delta z_k(t) = \delta z_{k+}\, e^{\imath\tilde{\omega}t} + \delta z_{k-}\, e^{-\imath\tilde{\omega}t} = \delta z_{k\pm}\, e^{\pm\imath\tilde{\omega}t}, \tag{4.32}
$$

and the equations (4.23) and (4.24) for the homogeneous case become

$$
\begin{aligned}
\delta h_{pq}(t) = \quad & 2\sum_l \langle pl|V|0q\rangle\sqrt{n_0}\,\delta z^*_{l\mp}\; e^{\pm\imath\tilde{\omega}t} + 2\sum_l\langle p0|V|lq\rangle\sqrt{n_0}\,\delta z_{l\pm}\; e^{\pm\imath\tilde{\omega}t}\\
\equiv \quad & \delta h_{pq\pm}\; e^{\pm\imath\tilde{\omega}t},
\end{aligned} \tag{4.33}
$$

$$
\begin{aligned}
\delta\Delta_{pq}(t) \;&=\; 2\sum_l\langle pq|V|l0\rangle\sqrt{n_0}\,\delta z_{l\pm}\; e^{\pm\imath\tilde{\omega}t}\\
&\equiv\; \delta\Delta_{pq\pm}\; e^{\pm\imath\tilde{\omega}t}.
\end{aligned} \tag{4.34}
$$

We recall, the time evolution of the quasiparticle operators is given by the Heisenberg equation of motion

$$
\imath\frac{db_i}{dt} = [b_i,\,\hat{H}] \;= \Omega_i b_i + [b_i,\,\delta\hat{H}(t)]. \tag{4.35}
$$

Using the quasiparticle transformation equation (4.31) to calculate the commutator and then integrating the equation of motion to first order, we obtain an expression for the time evolution of the quasiparticle operators in presence of the perturbation δz

$$b_i(t) = b_i^0 \, e^{-\imath\Omega_i t} + \sum_p e^{-\imath\Omega_i t} \, [\, b_p^0 D_{ip}^1(t) + b_p^{0\,\dagger} D_{ip}^2(t) + b_{-p}^0 D_{ip}^3(t) + b_{-p}^{0\,\dagger} D_{ip}^4(t)]. \quad (4.36)$$

Here we have used the notation

$$D_{ip}^1(t) = u_i u_p \; \delta h_{ip} \pm \int_0^t \frac{dt'}{i} e^{-\imath(\Omega_p - \Omega_i \mp \tilde{\omega})t'} + v_i u_p \; \delta\Delta^*_{p,-i} \pm \int_0^t \frac{dt'}{i} e^{-\imath(\Omega_p - \Omega_i \pm \tilde{\omega})t'}, \quad (4.37)$$

$$D_{ip}^2(t) = v_i u_p \; \delta h_{p,-i} \pm \int_0^t \frac{dt'}{i} e^{\imath(\Omega_p + \Omega_i \pm \tilde{\omega})t'} + u_i u_p \; \delta\Delta_{p,i} \pm \int_0^t \frac{dt'}{i} e^{\imath(\Omega_p + \Omega_i \pm \tilde{\omega})t'}, \quad (4.38)$$

$$D_{ip}^3(t) = v_i v_p \; \delta h_{p,-i} \pm \int_0^t \frac{dt'}{i} e^{-\imath(\Omega_p - \Omega_i \mp \tilde{\omega})t'} + u_i v_p \; \delta\Delta_{p,i} \pm \int_0^t \frac{dt'}{i} e^{-\imath(\Omega_p - \Omega_i \mp \tilde{\omega})t'}, \quad (4.39)$$

$$D_{ip}^4(t) = u_i v_p \; \delta h_{ip} \pm \int_0^t \frac{dt'}{i} e^{\imath(\Omega_p + \Omega_i \pm \tilde{\omega})t'} + v_i v_p \; \delta\Delta^*_{p,-i} \pm \int_0^t \frac{dt'}{i} e^{\imath(\Omega_p + \Omega_i \mp \tilde{\omega})t'}. \quad (4.40)$$

These equations when used in full include all the terms of the full second order theory of Beliaev [9, 65].

4.2.1 V^2 treatment and the weak coupling regime

With an equation for $b_i(t)$ at hand we can move on and construct $\rho_{ji}(t)$ and $\kappa_{ji}(t)$ as functions of δz. Using the Bogoliubov transform the pair anomalous average becomes

$$\begin{aligned} \kappa_{ji}(t) = \langle c_i(t) c_j(t) \rangle &= u_i u_j \langle b_i(t) b_j(t) \rangle + v_i u_j \langle b^\dagger_{-i}(t) b_j(t) \rangle \\ &+ u_i v_j \langle b_i(t) b^\dagger_{-j}(t) \rangle + v_i v_j \langle b^\dagger_{-i}(t) b^\dagger_{-j}(t) \rangle. \end{aligned} \quad (4.41)$$

The quasiparticle coefficients, u_p and v_p, are given by the steady state solution

[9] S. T. Beliaev. *Application of the methods of quantum field theory to a system of bosons.* Sov. Phys. JETP 34, 289 (1958).

[65] S. T. Beliaev. *Energy-spectrum of a non-ideal Bose gas.* Sov. Phys. JETP 7, 299 (1958).

of equation (4.13) without any perturbation present. The equation for v_p reads

$$v_p = \sum_{jk} \frac{\langle p, -p|V|jk\rangle}{-\Omega_p - (\omega_p - \mu)} [z_j^0 z_k^0 + \kappa_{jk}^0]. \tag{4.42}$$

To simplify matters we from now on limit our equations to second order in the inter-atomic potential V. The expressions for the normal and anomalous averages will be used in context of equation (4.27-4.27), where they appear linearly in V. We thus can neglect contributions which are quadratic in the quasiparticle coefficient v_p. From $u_i^2 - v_i^2 = 1$ it then immediately follows that $u_i \simeq 1$ and we get

$$\begin{aligned} \rho_{ji}(t) &= \langle c_i(t)^\dagger c_j(t)\rangle = \langle b_i(t)^\dagger b_j(t)\rangle + v_i\langle b_{-i}(t)b_j(t)\rangle + v_j\langle b_i^\dagger(t)b_{-j}^\dagger(t),\rangle \\ \kappa_{ji}(t) &= \langle c_i(t)c_j(t)\rangle = \langle b_i(t)b_j(t)\rangle + v_i\langle b_{-i}^\dagger(t)b_j(t)\rangle + v_j\langle b_i(t)b_{-j}^\dagger(t)\rangle. \end{aligned} \tag{4.43}$$

We only require v_p to first order in V and therefore neglect the κ_{jk}^0 term in equation (4.42). The term is kept in self-consistent formulations of the theory, which include select terms to all orders in V. The single particle energies ω_p, give the kinetic energy and potential energy of an excitation and are measured with respect to the ground state of the trap. However, they do not include the dressing due to interactions. The quasiparticle energies Ω_p, of course, include these effects and are measured with respect to the chemical potential μ. In a non-interacting system we have $\omega_p = \Omega_p + \mu$, which allows us to rewrite v_p in the limit of weak interactions as

$$v_p = \frac{\langle p, -p|V|00\rangle}{-2\Omega_p} n_0. \tag{4.44}$$

Consistently including only terms to first order in V we further neglect contributions quadratic in the perturbation terms D_{ip}, when calculating the products of quasiparticle operators. The normal average of two quasiparticle operators at equilibrium we take to be diagonal, $\langle b_i^{0\,\dagger} b_j^0\rangle = n_i\delta_{i,j}$, where $n_i = [e^{\Omega_i/kT} - 1]^{-1}$ is the thermal population. Anomalous averages of quasiparticles at equilibrium are zero, $\langle b_i^0 b_j^0\rangle = 0$. We therefore derive to first order in V

$$\rho_{ji}^0 = n_i\delta_{i,j}, \qquad \kappa_{ji}^0 = \delta_{-ij}\,(1+2n_j)\,\frac{\langle i, -i|V|00\rangle}{-2\Omega_i}\, n_0, \tag{4.45}$$

$$\delta\rho_{ji}(t) = (n_i - n_j)\,\delta h_{ji}(t)\int_0^t \frac{dt'}{i}\, e^{-\imath(\Omega_i - \Omega_j \mp \bar{\omega})(t-t')}, \tag{4.46}$$

$$\delta\kappa_{ji}(t) = (1 + n_i + n_j)\, \delta\Delta_{ij}(t) \int_0^t \frac{dt'}{i}\, e^{-\imath(\Omega_i+\Omega_j\pm\tilde{\omega}-2\mu)(t-t')}. \tag{4.47}$$

An expression for $\lambda_{ijk}(t)$ can be obtained more easily than the ones for $\rho_{ji}(t)$ and $\kappa_{ji}(t)$. It can straightforwardly be written as a function of δz_i using its own equation of motion, which is given in Appendix B. Using the linearisations from equation (4.7) we get following expressions for λ_{ijk} and $\delta\lambda_{ijk}$ to first order in V

$$\lambda^0_{ijk} = \sum_s \langle jk|V|is\rangle\ 2\left(n_i[1+n_k+n_j] - n_j n_k\right) z^0_s \int_0^t \frac{dt'}{i}\ e^{-\imath(\omega_j+\omega_k-\omega_i-\mu)(t-t')}, \tag{4.48}$$

$$\delta\lambda_{ijk} = \sum_s \langle jk|V|is\rangle\ 2\left(n_i[1+n_k+n_j] - n_j n_k\right) \delta z_s(t) \int_0^t \frac{dt'}{i}\ e^{-\imath(\omega_j+\omega_k-\omega_i\pm\tilde{\omega}-\mu)(t-t')}. \tag{4.49}$$

To ensure that the integrals in above expressions for $\delta\rho$, $\delta\kappa$, and λ are well behaved we introduce an infinitesimal convergence factor ϵ into the exponential of the integrand. This notation explicitly includes the imaginary part of the contour integral, which we can rewrite as

$$\int_0^t \frac{dt'}{i} e^{-\imath(\Delta\omega-\imath\epsilon)(t-t')} = -P\left(\frac{1}{\Delta\omega}\right) - \imath\pi\delta(\Delta\omega). \tag{4.50}$$

The approximation implicitly made in taking the upper limit of the integral to infinity is equivalent to saying the pair and triplet averages obtain a steady state value from $t = -\infty \to 0$ with the interaction adiabatically being switched on.

In this chapter we have found the V^2 treatment is equivalent to assuming the quasiparticle coefficient v_k to be small. This is the same as saying that the interactions between the particles are sufficiently weak so that we do not have to include the full dressing of an excitation by the mean field when describing the change in time evolution of a quasiparticle due to the interactions of the dynamic condensate with the dynamic thermal component. In other words, if we view a quasiparticle as a mixture between a propagating particle and a counter-propagating particle-hole, $b^\dagger_p = u^\dagger_p c_p + v_p c_{-p}$, we predominantly consider the effect of the thermal cloud on the 'particle' part of an excitation $u^\dagger_p c_p$. We term the range where this approximation holds the weak coupling regime. Assuming v_k to be small will only be valid for sufficiently high momenta $\xi k > 1$, as can be seen from Fig. 3.1. Thus the weak coupling approximation implies a low momentum cut-off, limiting the range of validity of the V^2 treatment of the homogeneous Bose gas. For a trapped systems, where the healing length becomes comparable to the size of the system, the low momentum cut-off due to the trapping potential means that assuming weak coupling is generally valid. We shall discuss further implications of the weak coupling approximation in section 4.5.

4.2.2 Effective interactions, $\hat{T}_{2B}$ and $\hat{T}_{MB}$

In the following we use the fact that the terms containing the anomalous averages κ^0, $\delta\kappa$ and $\delta\lambda$ modify the interaction potential V in the terms, which in equation (4.27-4.30) are written to their left, to effective interactions or T-matrices [66]. The pair anomalous averages account for repeated collision processes between condensed atoms. The triplet anomalous average describes collisions between condensed and thermal atoms in an analogous fashion but also describe collisions between non-condensed particles.

In weakly interacting systems the dominant contributions from the pair anomalous averages can be interpreted as correlations between two condensate atoms while repeatedly interacting with each other during a complete binary collision. Processes of this form are generally described by an effective interaction, the T-matrix for two-body collisions [67]

$$\begin{aligned} \hat{T}_{2B}(z) &= V + V\frac{1}{z-\hat{H}}\hat{T}_{2B}(z) \\ &= V + \sum_{j,k} V|jk\rangle \frac{1}{z-(\omega_j+\omega_k)}\langle kj|\hat{T}_{2B}(z). \end{aligned} \tag{4.51}$$

Here z is the energy of the collision and ω_k is the energy of the free particle. The two body T-matrix sums over all possible two-body scattering processes (ladder diagrams), without taking into account that the surrounding medium has an effect of these collisions.

Since we are dealing with binary collisions not in vacuum but within a condensate, the two colliding particles actually do experience the presence of the other particles of the system. These effects are included in the so called many-body T-matrix, $\hat{T}_{MB}$. Firstly, one has to allow for Bose-enhancement of scattering in and out of the intermediate states which are now populated. $\hat{T}_{MB}$ thus contains the characteristic $(1 + n + n)$ population terms. Secondly, one has to account for the fact that the colliding particles do not propagate freely during the repeated

[66] N. P. Proukakis, K. Burnett, and H. T. C. Stoof. *Microscopic treatment of biary interactions in the nonequilibrium dynamics of partially Bose-condensed trapped gases*. Phys. Rev. A 57, 1230 (1998).

[67] R. Taylor. Scattering theory (Wiley, 1972).

collision, but experience the effect of the mean field leading to a change in their frequencies and wave functions. In our treatment we ignore the change in their wave functions, but account for their frequency shift using quasiparticle energies Ω_i in the energy denominator,

$$\hat{T}_{MB}(z) = V + \sum_{ij} V|ij\rangle \frac{[1+n_j+n_k]}{z-(\Omega_i+\Omega_j)} \langle ij|\hat{T}_{MB}(z). \tag{4.52}$$

Combining the two definitions allows to re-express $\hat{T}_{MB}$ in terms of $\hat{T}_{2B}$

$$\begin{aligned} \hat{T}_{MB}(z) &= \hat{T}_{2B}(z') + \sum_{ij} \hat{T}_{2B}(z')|ij\rangle \frac{1+n_j+n_k}{z-(\Omega_i+\Omega_j)} \langle ij|\hat{T}_{MB}(z) \\ &\quad - \sum_{j,k} \hat{T}_{2B}(z')|jk\rangle \frac{1}{z'-(\omega_j+\omega_k)} \langle kj|\hat{T}_{MB}(z). \end{aligned} \tag{4.53}$$

When we insert the expression for κ^0_{ji} (4.47) into the equations for the excitation, equation (4.30), we obtain

$$\begin{aligned} &\langle p,-p|V|00\rangle\, n_0 \delta z^*_{-p} + \sum_{ijk} \langle pi|V|jk\rangle\, \kappa^0_{jk} \delta z^*_i \\ &= \langle p,-p \left| V + \sum_k V|k,-k\rangle \frac{[1+2n_k]}{-2\Omega_k} \langle k,-k|V \right| 00\rangle\, n_0 \delta z^*_{-p}. \end{aligned} \tag{4.54}$$

By definition the operators b_i and c_i do not include the condensate ground state and summations over n_i always exclude the zero momentum state. Above equation shows that we can replace V by an effective interaction, i.e. the $\hat{T}_{MB}$-matrix, defined according to the Lippmann-Schwinger relation to second order in the interaction potential

$$\langle p,-p|\hat{T}_{MB}(0)|00\rangle = \langle p,-p \left| V + \sum_k V|-k,k\rangle \frac{[1+2n_k]}{-2\Omega_k} \langle -k,k|V \right| 00\rangle. \tag{4.55}$$

It is important to bear in mind that our effective interaction is only equivalent to the second order expression for the many-body T-matrix within the weak coupling approximation, on which the derivation of the pair averages has been based. We further note that our definition of the effective interaction $\hat{T}_{MB}$ uses the exact second order expression for the anomalous average and thus does not diverge in the limit of high momenta. When we substitute the value for $\delta\kappa_{ji}(t)$ into the equation for the excitations, equation (4.28), we get

$$\begin{aligned}
&\langle p0|V|0p\rangle\, 2n_0\,\delta z_p \;+\sum_{jk}\langle p0|V|jk\rangle\,\sqrt{n_0}\,\delta\kappa_{jk}\\
=\;& 2\,n_0\delta z_n\,\langle p0\left|V+\sum_{jk} V|jk\rangle\frac{[1+n_j+n_k]}{-(\Omega_k+\Omega_j\pm\tilde{\omega})}\langle jk|V\right|0p\rangle\\
&-\imath\pi 2\,n_0\delta z_n\sum_{jk}[1+n_j+n_k]\,|\langle jk|V|0p\rangle|^2\,\delta(\Omega_k+\Omega_j\pm\tilde{\omega}).
\end{aligned}\tag{4.56}$$

We then can define an effective interaction for (4.29) in a similar fashion,

$$\langle p0|\hat{T}_{MB}(\pm\tilde{\omega})|0p\rangle \;=\; \langle p0\left|V+\sum_{jk} V|jk\rangle\frac{[1+n_j+n_k]}{-(\Omega_k+\Omega_j\pm\tilde{\omega})}\langle jk|V\right|0p\rangle.\tag{4.57}$$

Unlike the equilibrium quantity κ^0, $\delta\kappa$ contributes an imaginary part, which represents damping of the excitation. We shall discuss this issue below.

The anomalous average $\delta\lambda$ represents correlations during collisions of the coherent excitation with non-condensed particles. For (4.29) we can introduce an effective interaction, $\hat{T}_{MB}(\omega_i-\mu\pm\tilde{\omega})$, in a similar way as before,

$$\begin{aligned}
&\sum_{ijk}\langle pi|V|jk\rangle\,2\rho^0_{ji}\delta z_p\;+\;\sum_{ijk}\langle pi|V|jk\rangle\;\delta\lambda_{ijk}\\
=\;&\sum_i\,2\,n_i\delta z_p\langle pi\left|V+\sum_{jk}V|jk\rangle\frac{[1+n_j+n_k]}{-(\omega_j+\omega_k-\omega_i\pm\tilde{\omega}-\mu)}\langle jk|V\right|ip\rangle\\
&-\,\imath\pi\sum_i\,2\,n_i\delta z_p\sum_{jk}[1+n_j+n_k]\,|\langle jk|V|ip\rangle|^2\;\delta(\omega_j+\omega_k-\omega_i\pm\tilde{\omega}-\mu)\\
&+\text{ collisional terms.}
\end{aligned}\tag{4.58}$$

As in the case of $\delta\kappa$, $\delta\lambda$ contributes imaginary terms. Since $\delta\lambda$ also describes the collisions between two thermal particles and their effect on the coherent excitations, it additionally gives a collisional term which goes linearly with the product populations of the thermal levels involved

$$\lim_{\epsilon\to 0}\,2\delta z_p\sum_{ijk} n_j n_k\,\frac{|\langle pi|V|jk\rangle|^2}{(\omega_j+\omega_k-\omega_i\pm\tilde{\omega}-\mu-\imath\epsilon)}.\tag{4.59}$$

4.2.3 Discussion of self-energies, shifts and widths

Before discussing the the physical interpretation of the contributions from the correlations, we write out the full V^2 expression for the coherent excitation in matrix form, in which all values for the correlations have been substituted

$$i\frac{d}{dt}\begin{pmatrix}\delta z_p\\ \delta z^*_{-p}\end{pmatrix} = \begin{pmatrix}\mathcal{L}' & \mathcal{M}'\\ -\mathcal{M}'^* & -\mathcal{L}'^*\end{pmatrix}\begin{pmatrix}\delta z_p\\ \delta z^*_{-p}\end{pmatrix}, \tag{4.60}$$

where the matrix elements now have real and and imaginary components

$$\mathcal{L}' = L - i2\pi\Gamma_L, \quad \mathcal{M}' = M - i2\pi\Gamma_M. \tag{4.61}$$

An alternative notation expresses the equation for the excitations in terms of self-energies

$$\Sigma^{11}_{ij} = \mathcal{L}' - \langle i|H_{sp}|j\rangle + \mu\delta_{ij}, \quad \Sigma^{12}_{ij} = \mathcal{M}', \tag{4.62}$$

which are the contributions of the fully interacting system minus the single particle energies. Above we have used the following notation:

$$\begin{aligned}
L \;=\;& (\omega_p - \mu) + 2n_0\langle p0|\hat{T}_{MB}(\pm\tilde{\omega})|0p\rangle \\
&+2\sum_i n_i\langle pi|\hat{T}_{MB}(\omega_i - \mu \pm \tilde{\omega})|ip\rangle \\
&-4n_0\sum_{ij}\frac{[n_i - n_j]}{(\Omega_i - \Omega_j \pm \tilde{\omega})}\,|\langle j0|V|pi\rangle|^2 \\
&-2\sum_{ijk}\frac{n_j n_k}{(\omega_j + \omega_k - \omega_i \pm \tilde{\omega} - \mu)}\,|\langle pi|V|jk\rangle|^2, \qquad (4.63)\\
M \;=\;& n_0\langle p,-p|\hat{T}_{MB}(\pm\tilde{\omega})|00\rangle \\
&-4n_0\sum_{ij}\frac{[n_i - n_j]}{(\Omega_i - \Omega_j \pm \tilde{\omega})}\langle pi|V|j0\rangle\langle -p,j|V|0i\rangle, \qquad (4.64)\\
\Gamma_L \;=\;& 2n_0\sum_{ij}[n_i - n_j]\;|\langle j0|V|pi\rangle|^2\;\delta(\Omega_i - \Omega_j \pm \tilde{\omega}) \\
&+ n_0\sum_{jk}[1 + n_j + n_k]\;|\langle jk|V|0p\rangle|^2\;\delta(\Omega_k + \Omega_j \pm \tilde{\omega}) \\
&+\sum_i n_i\sum_{jk}[1 + n_j + n_k]\;|\langle jk|V|ip\rangle|^2\;\delta(\omega_j + \omega_k - \omega_i \pm \tilde{\omega} - \mu) \\
&+\sum_{ijk} n_j n_k\;|\langle pi|V|jk\rangle|^2\;\delta(\omega_j + \omega_k - \omega_i \pm \tilde{\omega} - \mu), \qquad (4.65)\\
\Gamma_M \;=\;& 2n_0\sum_{ij}[n_i - n_j]\;\langle pi|V|j0\rangle\langle -p,j|V|0i\rangle\;\delta(\Omega_i - \Omega_j \pm \tilde{\omega}). \qquad (4.66)
\end{aligned}$$

The matrix notation of equation (4.60) accounts for the characteristic coupling of states with opposite momenta caused by the translationally invariant condensate. Matrix element M, equation (4.63), contains the energy of the excitation $(\omega_p - \mu)$ and energy terms due to collisions between condensed particles as known from the standard HFB equations. However, unlike in the HFB equations, the two particle interaction term V has been replaced by an approximate many body T-matrix, which contains additional energy shifts. The second and third line in equation (4.63) are further frequency shifts arising from collisions of thermal particles with a collective excitation, stemming from the $\delta\rho$ term, and collisions between excited states, given by $\delta\lambda$. Matrix L, equation (4.64), contains terms which represent coupling between excitations of opposite momenta. The first term again describes collisions within the condensate and its T-matrix incorporates the energy shift from κ^0 equation (4.54). The second term accounts for the extra coupling due to collisions with thermal particles. We note that the momentum dependences of the matrix elements of $\hat{T}_{MB}$ in M and L are the same as in Beliaev's treatment of the homogeneous Bose gas. As long as the wavelength of the excitation is large in comparison with the size of the interaction region the momentum dependence of the matrices is negligible, $\langle 00|\hat{T}_{MB}|p,-p\rangle \simeq \langle 00|\hat{T}_{MB}|00\rangle$ [65]. This will certainly hold for the dilute alkali condensates.

The first term in Γ_L, equation (4.65), is the imaginary part of the contribution of $\delta\rho$ and gives the the decay of the coherent excitation δz_p due to Landau Damping and comes from the $\delta\rho$ term. The energy of the excitation p is absorbed and is used to excite a quasiparticle from the level i to the level j with $\Omega_i \pm \tilde{\omega} = \Omega_j$. The decay rate expectedly goes linear with the difference in populations between the quasiparticle levels i and j

$$\frac{d}{dt}\delta z_p = \ldots - \pi\, 4n_0\delta z_p \sum_{ij} [n_i - n_j] \left|\langle j0|V|pi\rangle\right|^2 \delta(\Omega_i - \Omega_j \pm \tilde{\omega}). \tag{4.67}$$

The second term in equation (4.65) describes Beliaev damping of the excitation δz_p and comes from the imaginary part of the $\delta\kappa$ contribution equation (4.56). We note that unlike $\delta\kappa$, κ_0 does not give contributions to lifetimes, but only to the energy shift (see equation (4.64)). Beliaev damping involves the breaking up of the excitation with momentum p, while interacting with the condensate, to create two lower lying excitations with momenta i and j and contains population factors for

[65] S. T. Beliaev. *Energy-spectrum of a non-ideal Bose gas*. Sov. Phys. JETP 7, 299 (1958).

Bose enhanced scattering into populated excited states

$$\frac{d}{dt}\delta z_p = \ldots \quad - \quad \pi\, 2n_0 \delta z_p \sum_{jk} [1 + n_j + n_k] \left| \langle jk|V|0p\rangle \right|^2 \delta(\Omega_i + \Omega_j \pm \tilde{\omega}). \quad (4.68)$$

The imaginary part given by $\delta\lambda$, the third term in equation (4.65) describes the decay of the excitation δz_p due to interactions with excited particles. At very low temperatures, where the population of the level n_i is almost negligible in comparison to n_0, this process will be far less important than the Landau and Beliaev damping mechanisms. The final damping term in equation (4.65) is given by the imaginary part of the term representing collisions between two excited states, equation (4.59). For sufficiently dilute gases at low temperatures the product $n_j n_k$ will be small, but it is the contribution which gives the collisional line width and phase diffusion of a condensate viewed as a coherent matter wave source, i.e. an atom laser. The fact that the collision terms involving only excited states contain undressed single particle frequencies rather than the correct quasiparticle frequencies is due to the fact that we are limiting ourselves to second order in V. The off-diagonal damping term Γ_M, equation (4.66), comes from the imaginary part of the $\delta\rho$ contribution. It gives the overlap of Landau damping type transitions of the excitations p and $-p$ with the same intermediate levels involved.

We have shown that our linear response analysis gives us the decay rates due to Landau and Beliaev damping in terms of Fermi's Golden Rule (FGR) for the relevant transitions involved. Giorgini re-derived the damping rates for homogeneous systems using a formalism akin to the one presented here [19]. Pitaevskii and Stringari have done the same using FGR as a starting point [68] and obtained the well known results of T^4 dependence for Landau damping in homogeneous Bose systems for low temperatures ($k_B T < \mu$) (see also [69])

$$\Gamma_{Landau} \propto \frac{\Omega_k}{\hbar} \left(\frac{k_B T}{n_0 U_0} \right)^4 (n_0 a^3)^{1/2}. \quad (4.69)$$

[19] S. Giorgini. *Damping in dilute Bose gases: A mean field approach.* Phys. Rev. A 57, 2949 (1998).

[68] L. P. Pitaevskii and S. Stringari. *Landau damping in dilute Bose gases.* Phys. Lett. A 235, 398 (1997).

[69] P. C. Hohenberg and P. C. Martin. *Microscopic theory of superfluid helium.* Ann. Phys. 34, 291 (1965).

For ($k_BT > \mu$) they obtain (see also [70, 15])

$$\Gamma_{Landau} \propto \frac{\Omega_k}{\hbar} \frac{k_BT}{n_0 U_0} (n_0 a^3)^{1/2}. \tag{4.70}$$

At zero temperatures only the Beliaev term gives rise to damping. Its momentum dependence has been found to be for $k\xi < 1$ [65]

$$\Gamma_{Beliaev} \propto \frac{1}{\hbar^3 m n_0} k^5. \tag{4.71}$$

In the limit of high momenta, $k\xi > 1$, it is known to scale linearly with momentum as

$$\Gamma_{Beliaev} \propto \frac{a^2 n_0}{m} \hbar k. \tag{4.72}$$

4.2.4 Gaplessness

We recall that a theory is gapless if the excitation energies can take all values down to zero, i.e. if the equations for the excitations with zero frequency are the same as the equation for the ground state. We show that our linear response formalism is gapless by considering the equations for the static condensate equation (4.12) and for the time varying part equation (4.13). Without loss of generality we shall neglect collisions between thermal particles, equation (4.59). The equation for the static condensate can be upgraded in an analogous fashion as the one for the excitations of the condensate. Substituting the expressions for the equilibrium values for ρ^0, κ^0, and λ^0, equations (4.45,4.48), into the equation for the static ground state, equation (4.12) gives, after replacing the V's by T-matrices as before:

$$0 = \left(-\mu + 2\sum_i \langle pi|\hat{T}_{MB}(\omega_i - \mu)|ip\rangle \, n_i \right) z_p^0 + \langle p, -p|\hat{T}_{MB}(0)|00\rangle \, n_0 \, z_{-p}^{0\,*}. \tag{4.73}$$

The equilibrium quantity κ^0 gives corrections to the effective interaction leading to $\hat{T}_{MB}$, but does not contribute imaginary parts to the equations. The same applies to the contribution of the triplet anomalous average λ^0. Even though the integral

[70] S. H. Payne and A. Griffin. *Goldstone phonons in a Bose-condensed gas at finite temperature: One-loop approximation*. Phys. Rev. B 32, 7199 (1985).

[15] H. Shi. Finite Temperature Excitations in a dilute Bose-condensed gas. Ph.D. thesis, University of Toronto (1997).

[65] S. T. Beliaev. *Energy-spectrum of a non-ideal Bose gas*. Sov. Phys. JETP 7, 299 (1958).

in equation (4.48) in principle does contain an imaginary part there are, however, no energy conserving loss processes possible.

Substituting $\delta z_p(t) = \delta z_{p+}e^{+\imath\tilde{\omega}t} + \delta z_{p-}e^{-\imath\tilde{\omega}t}$ into the equation for the time varying part of the condensate equation (4.59) our formalism gives equations for δz_{p+} and δz^*_{p-}. The excitation with zero energy and zero momentum, $\tilde{\omega} = 0$ and $p = 0$, is $(\delta z_{0+}, \delta z^*_{0-}) = (z^0, -z^0)$ and then both become

$$\begin{aligned} 0 = \quad & \Big(-\mu + 2\sum_i \langle 0i|\hat{T}_{MB}(\omega_i - \mu)|i0\rangle n_i \Big) z^0 \\ & - \langle 00|\hat{T}_{MB}(0)|00\rangle n_0 \, z^0 + 2\langle 00|\hat{T}_{MB}(0)|00\rangle n_0 \, z^0. \end{aligned} \tag{4.74}$$

which is equivalent to the equation of the condensate ground state with $p = 0$. As discussed earlier, HFB-treatments of Bose condensates display an energy gap in the excitation spectrum of the homogeneous gas. The reason for this is that HFB does not deal with all forms of two particle collisions in a consistent manner. More specifically, the HFB treatment assumes the operators to be static (or equivalently makes use of factorisation approximations), which amount to the neglect of terms which introduce T-matrices into the equations for the excitations. This then gives equations inconsistent in order of V, which results in a gap in the excitation spectrum.

The HFB-Popov approximation, however, does give a gapless description of the condensates' excitations by neglecting all anomalous averages κ, $\delta\kappa$, λ, and $\delta\lambda$. From equations (4.45-4.49) we can see that neglecting these terms amounts to a first order theory in V. The equations thus again support a zero frequency mode.

In our linear response formalism we have shown that the pair and triplet anomalous averages give contributions which allow to regroup the bare inter-atomic interaction terms to effective interactions. The condensate-condensate interactions involve κ^0 and $\delta\kappa$ terms. The modification of condensate-excited state interactions is given by the λ terms. The two types of interaction terms are not necessarily the same. By consistently including these effects to second order in V we obtained a gapless theory.

4.3 Contact potentials and ultra-violet divergences

So far we have not used the prescription of section 2.1.3 to replace the inter-atomic potential by a contact potential, $V(\mathbf{r} - \mathbf{r}') \simeq U_0\delta(\mathbf{r} - \mathbf{r}')$. Instead we have kept all interaction terms in their exact form and systematically introduced effective interactions for the various forms of collisions. Our resulting equations are well defined and do not exhibit any ultra-violet divergences.

For numerical calculations it is, of course, unfeasible to calculate excitation energies using the full inter-atomic potential. Scattering theory shows that the collisional properties of cold atoms in dilute systems are characterised by a single parameter, the s-wave scattering length a. This quantity can be measured experimentally in terms of scattering cross sections or using photo-association or -dissociation techniques [71, 72]. The low momentum limit ($\omega_k < \hbar^2/2ma$) of the two-body T-matrix in three dimensions is a constant, proportional to the s-wave scattering length,

$$\langle 00|\hat{T}_{2B}(0)|00\rangle = U_0 = \frac{4\pi\hbar^2 a}{m}. \tag{4.75}$$

This then gives a contact potential $\hat{T}_{2B}(\mathbf{r},0) = U_0\delta(\mathbf{r}-\mathbf{r}')$ in its spatial representation [67, 62].

Since it really is $\hat{T}_{2B}(0)$ which can be replaced by a contact potential one has to be careful if one approximates V by a contact potential instead. One is essentially preempting the upgrading of interaction terms from V to $T_{2B}(z)$ and thus has to ensure that one does not double-count the terms which actually introduce $\hat{T}_{2B}(z)$. Further, one has to account for the fact that the two-body T-matrix generally is momentum dependent and tends towards zero in the high momentum limit, $\hat{T}_{2B}(z) \to 0$ for $z \to \infty$. If one replaces all momentum dependent effective interaction terms by a zero momentum approximation one has to make sure that this does not render the equations ultra-violet divergent. That ultra-violet divergences only enter as artifacts of inadequate approximations to the effective interactions

[71] J. Dalibard. *Collisional dynamics of ultra-cold atomic gases*. In Proceedings of the International School of Physics - Enrico Fermi (edited by M. Inguscio, S. Stringari, and C. E. Wieman), p. 321 (IOS Press, 1999).

[72] D. J. Heinzen. *Ultracold atomic interactions*. In Proceedings of the International School of Physics - Enrico Fermi (edited by M. Inguscio, S. Stringari, and C. E. Wieman), p. 351 (IOS Press, 1999).

[67] R. Taylor. Scattering theory (Wiley, 1972).

[62] H. T. C. Stoof, M. Bijlsma, and M. Houbiers. *Theory of interacting quantum gases*. J. Res. Natl. Inst. Stand. Tech. 101, 443 (1996).

can be seen when considering the V^2 expression for the many-body T-matrix

$$\begin{aligned}\langle p,-p|\hat{T}_{MB}(0)|00\rangle &= \langle p,-p|V|00\rangle + \sum_k \langle p,-p|V|k,-k\rangle \frac{[1+2n_k]}{-2\Omega_k}\langle k,-k|V|00\rangle \\ &\rightarrow U_0 + U_0^2 \sum_k [1+2n_k]\frac{1}{-2\Omega_k} \\ &= U_0 - U_0^2 4\pi \int_{k_0}^{\infty} \frac{k^2 dk}{2\Omega_k}[1+2n_k] \\ &= -\infty. \end{aligned} \tag{4.76}$$

For high momenta the energies of the excitations go over to their free particle limit, $\Omega_k \rightarrow \omega_k = k^2/2m$, and it is clear that entire theory has become UV divergent.

Neither the double counting, nor the the ultra-violet divergences occur when one properly expresses $\hat{T}_{MB}$ in terms of $\hat{T}_{2B}$, as given by equation (4.53), and then replaces $\hat{T}_{2B}$ by a contact potential. This procedure is equivalent to replacing V by $U_0\delta(\mathbf{r})$ straight away and then subtracting the perturbative higher order terms of $\hat{T}_{2B}$ to avoid double counting the vacuum contributions of the anomalous averages. In our V^2 theory the correction terms are simply

$$\hat{T}_{2B} - U_0 = U_0^2 \sum_k \frac{1}{-2\omega_k}. \tag{4.77}$$

Since $n_k = [e^{\Omega_k/k_BT} - 1]^{-1} \rightarrow 0$ for $k \rightarrow \infty$, it is clear that this 'renormalisation' also removes the UV divergence of our expression for $\hat{T}_{MB}$. The exact renormalisation procedure can be approximated by dropping the '1' in the $[1 + n_k + n_j]$ terms of the anomalous correlations. The approximation lies in the neglecting the difference between the quasiparticle energy $1/2\Omega_k$ and the single particle energy $1/2\omega_k$ in the energy denominator, i.e. many-body effects at zero temperature.

Provided that the equations are properly UV-renormalised, a U_0^2 treatment of the homogeneous Bose gas is equivalent to the V^2 treatments presented in this chapter.

4.4 Trapped condensates at finite temperatures

Many quantitative calculations of excitations in trapped condensates at finite temperature so far have been based on theories which assume the thermal component of the system to be static [21, 73]. These theories can be easily derived when considering the linear response of the mean field. It provides an ideal framework to discuss how the presence of other atoms modifies the collisions between two particles and how these effects in turn modify the dynamics of the condensed system.

We recall the equations for the mean field and its linear response read

$$\mu z_n^0 = \omega_n z_n^0 + \sum_{ijk} \langle ni|V|jk\rangle \left\{ z_j^0 z_k^0 z_i^{0\,*} + \kappa_{jk}^0 z_i^{0\,*} + 2\rho_{ji}^0 z_k^0 + \lambda_{ijk}^0 \right\}, \tag{4.78}$$

$$\begin{aligned} \imath\frac{d}{dt}\delta z_n(t) &= (\omega_n - \mu)\,\delta z_n \\ &+ \sum_{ijk} \langle ni|V|jk\rangle \left\{ z_j^0\, z_k^0\, \delta z_i^* + \kappa_{jk}^0\, \delta z_i^* \right\} \\ &+ \sum_{ijk} \langle ni|V|jk\rangle \left\{ 2 z_i^{0\,*}\, z_j^0\, \delta z_k + z_i^{0\,*}\, \delta\kappa_{jk} \right\} \\ &+ \sum_{ijk} \langle ni|V|jk\rangle \left\{ 2\rho_{ji}^0 \delta z_k + \delta\lambda_{ijk} \right\} \\ &+ \sum_{ijk} \langle ni|V|jk\rangle\ 2\delta\rho_{ji} z_k^0. \end{aligned} \tag{4.79}$$

The standard HFB equations follow from above equations straightforwardly if we assume the population of thermal particles to be static $\delta\rho = 0$. We further neglect the fluctuations in the anomalous average $\delta\kappa = 0$ and the triplet correlations altogether.

$$\mu z_n^0 = \omega_n z_n^0 + \sum_{ijk} \langle ni|V|jk\rangle \left\{ z_j^0 z_k^0 z_i^{0\,*} + \kappa_{jk}^0 z_i^{0\,*} + 2\rho_{ji}^0 z_k^0 \right\}, \tag{4.80}$$

$$\begin{aligned} \imath\frac{d}{dt}\delta z_n(t) &= (\omega_n - \mu)\,\delta z_n + \sum_{ijk} \langle ni|V|jk\rangle \left\{ z_j^0\, z_k^0\, \delta z_i^* + 2 z_i^{0\,*}\, z_j^0\, \delta z_k \right\} \\ &+ \sum_{ijk} \langle ni|V|jk\rangle \left\{ \kappa_{jk}^0\, \delta z_i^* + 2\rho_{ji}^0 \delta z_k \right\}. \end{aligned} \tag{4.81}$$

[21] D. W. Hutchinson, R. J. Dodd, and K. Burnett. *Gapless finite-t theory of collective modes of a trapped gas*. Phys. Rev. Lett. 81, 2198 (1998).

[73] D. W. Hutchinson, E. Zaremba, and A. Griffin. *Finite temperature excitations of a trapped Bose gas*. Phys. Rev. Lett. 78, 1842 (1997).

We further follow the standard procedure and replace the bare inter-atomic potential $V(\mathbf{r}, \mathbf{r}')$ with an effective contact potential $U_0\delta(\mathbf{r} - \mathbf{r}')$. If we then specify our perturbation by writing $\delta z_j(t) = u_{nj}e^{-i\Omega_n t} + v_{nj}e^{i\Omega_n t}$ we arrive at the basis state notation of equation (3.35). The HFB-Popov equations then follow by additionally neglecting κ^0.

4.4.1 Gapless HFB

We now derive a theory for trapped gases with static thermal component, which avoids problems of an energy gap as well as ultra-violet divergences. Since we assume the populations of thermal particles to be static, $\delta\rho_{ji} = 0$, the treatment consequently will not account for the full damping effects of the previous sections.

Again, we include the anomalous averages and their fluctuations to define effective interactions. We can derive equations for κ^0_{jk} and $\delta\kappa_{jk}$ by linearising the equation of motion for κ_{jk}, as given in Appendix A.

$$\kappa^0_{jk} \simeq \frac{(1+n_j+n_k)}{2\mu - \omega_j - \omega_k}\sum_{lm}\langle jk|\hat{V}|lm\rangle[z^0_l z^0_m + \kappa^0_{lm}], \tag{4.82}$$

$$\delta\kappa_{jk} \simeq \frac{(1+n_j+n_k)}{2\mu - \omega_j - \omega_k}\sum_{lm}\langle jk|\hat{V}|lm\rangle[2\delta z_l z_m + \delta\kappa_{lm}]. \tag{4.83}$$

Inserting κ_{jk} into equations (4.78, 4.79) allows us to define effective interactions as in the homogeneous case

$$\sum_{ijk}\langle ni|\hat{V}|jk\rangle\; z^{0\,*}_i(z^0_j z^0_k + \kappa^0_{jk}) = \sum_{ijk}\langle ni|\hat{T}_{MB}|jk\rangle\; z^{0\,*}_j z^0_i z^0_j, \tag{4.84}$$

where we again have defined an effective interaction

$$\hat{T}_{MB} \simeq \hat{V} + \sum_{jk}\hat{V}|jk\rangle\frac{(1+n_j+n_k)}{2\mu - \omega_j - \omega_k}\langle jk|\hat{T}_{MB}, \tag{4.85}$$

which is an approximation to the full many-body T-matrix. Unlike in our treatment of the homogeneous gas, this time we have retained the κ^0_{lm} term in equation (4.82). We thus do no longer limit ourselves to a certain order in V but instead obtain the recursive Lippmann-Schwinger equation, defining an effective interaction non-perturbatively to all orders in V. Expressed in terms of interaction diagrams, we include ladder diagrams to all orders but neglect terms involving more complicated processes.

The effective interaction is only an approximation to the full many-body T-matrix because it contains single particle energies in the energy denominator, $(2\mu - \omega_j - \omega_k)$. The proper definition of $\hat{T}_{MB}$ has the corresponding quasiparticle energies in their place, $(-\Omega_j - \Omega_k)$, which accounts for the effect of the mean field on the propagation of the particles during a collision process. Our treatment of the homogeneous gas of the previous sections included this effect, albeit only in the weak coupling limit. In above treatment of the trapped gas we neglect this effect.

The λ and $\delta\lambda$ terms can be grouped to effective interactions in a similar fashion for condensate-excited state collisions. If we insert effective interactions in all terms we obtain the Gapless-HFB (GHFB) equations

$$0 = (\omega_n - \mu)\, z_n^0 + \sum_{ijk} \langle ni|\hat{T}_{MB}|jk\rangle \; z_j^0 z_k^0 z_i^{0\,*} + \sum_{ik} 2n_i \, \langle ni|\hat{T}_{MB}|ik\rangle z_k^0, \tag{4.86}$$

$$\begin{aligned} \imath\frac{d}{dt}\delta z_n(t) \;&=\; (\omega_n - \mu)\,\delta z_n(t) + \sum_{ijk} \langle ni|\hat{T}_{MB}|jk\rangle \;\; z_j^0\, z_k^0\, \delta z_i^*(t) \\ &\quad + \sum_{ijk} 2\, \langle ni|\hat{T}_{MB}|jk\rangle \;\; 2z_i^{0\,*}\, z_j^0\, \delta z_k(t) \\ &\quad + \sum_{ik} 2n_i\, \langle ni|\hat{T}_{MB}|ik\rangle \;\; \delta z_k(t). \end{aligned} \tag{4.87}$$

By including both κ_{ij} and $\delta\kappa_{ij}$, we have introduced the same form of effective interactions for all terms involving condensate-condensate collisions and which is necessary to obtain a gapless theory. If we insert $[u_0(\mathbf{r}), v_0(\mathbf{r})] = [\psi_0(\mathbf{r}), -\psi_0^*(\mathbf{r})]$ we immediately see that above set of equations supports a zero-frequency mode.

Having assumed the thermal component of the system to be static means our equations are, strictly speaking, not self-consistent. Changes in excited state populations from the anomalous averages would in principle still be included. To retain a consistent picture we neglect imaginary contributions from κ and λ and the damping associated with it.

For calculations it is convenient to express $\langle \hat{T}_{MB} \rangle$ in terms of contact interactions. We shall use $\tilde{U}_{\text{con}}$ for condensate-condensate collisions and $\tilde{U}_{\text{exc}}$ for the terms describing collisions between condensed and excited particles. In general the two effective interactions are momentum dependent and they need not necessarily be the same. We should expect the interaction between condensed and excited atoms to be similar to that between two condensate atoms, as long as the change in relative momenta of the colliding particles between the two cases is not too great.

However, in the limit of high relative momenta the condensate-excited state interactions are best described by the two-body T-matrix since many-body effects die out in this regime [62].

If we assume $\langle \hat{T}_{MB} \rangle$ to be approximately momentum independent we can use $\langle 00|\hat{T}_{2B}|00\rangle = U_0\delta(\mathbf{r}-\mathbf{r}')$, where $U_0 = 4\pi\hbar^2 a/m$ is the usual dilute Bose gas effective interaction strength, to write

$$
\begin{aligned}
\langle \hat{T}_{MB} \rangle \simeq \langle 00|\hat{T}_{MB}|00\rangle &= \left\langle 00 \left| \hat{T}_{2B} + \sum_{ij} \hat{T}_{2B}|ij\rangle \frac{[1+n_j+n_k]}{2\mu - \omega_i - \omega_j}\langle ij|\hat{T}_{MB} \right| 00 \right\rangle \\
&= \langle 00|\hat{T}_{2B}|00\rangle + \sum_{jk}\langle 00|\hat{T}_{2B}|jk\rangle \frac{\kappa_{jk}}{z_j z_k} \\
&\rightarrow U_0\left[1 + \frac{\tilde{m}(\mathbf{r})}{\psi^2(\mathbf{r})}\right].
\end{aligned} \tag{4.88}
$$

At sufficiently high temperatures we expect the modification of the two-body effective interaction U_0 due to many-body effects to affect the excitation energies. If we set $\tilde{U}_{\text{con}}(\mathbf{r}) = \tilde{U}_{\text{exc}}(\mathbf{r}) = U_0$ GHFB reduces to the HFB-Popov theory. This, of course, corresponds to assuming that the presence of the other atoms in the trap has no influence on the nature of the collisions within the condensate.

This derivation of a gapless theory for finite temperature excitations forms the basis of recent tests of these theories against HFB-Popov and experimental data [21] (Figure 4.1). In the case of the three dimensional isotropic trap the differences between HFB-Popov and gapless self-consistent calculations still are negligible. More noticeable are the differences between the two approaches for anisotropic trap configurations as realized at JILA. Calculations of the temperature dependence of low lying modes show that gapless self-consistent equations give frequencies which are shifted downwards relative to HFB-Popov results. For the lower $m = 2$ mode this is in agreement with the experiments, but it does not explain the reported upward shift of the higher $m = 0$ mode observed of the experiment [5]. The remaining disagreement between theory and experiment suggests that neglecting

[62] H. T. C. Stoof, M. Bijlsma, and M. Houbiers. *Theory of interacting quantum gases*. J. Res. Natl. Inst. Stand. Tech. 101, 443 (1996).

[21] D. W. Hutchinson, R. J. Dodd, and K. Burnett. *Gapless finite-t theory of collective modes of a trapped gas*. Phys. Rev. Lett. 81, 2198 (1998).

[5] D. S. Jin, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell. *Temperature-dependent damping and frequency shifts in collective excitations of a dilute Bose-Einstein condensate*. Phys. Rev. Lett. 78, 764 (1997).

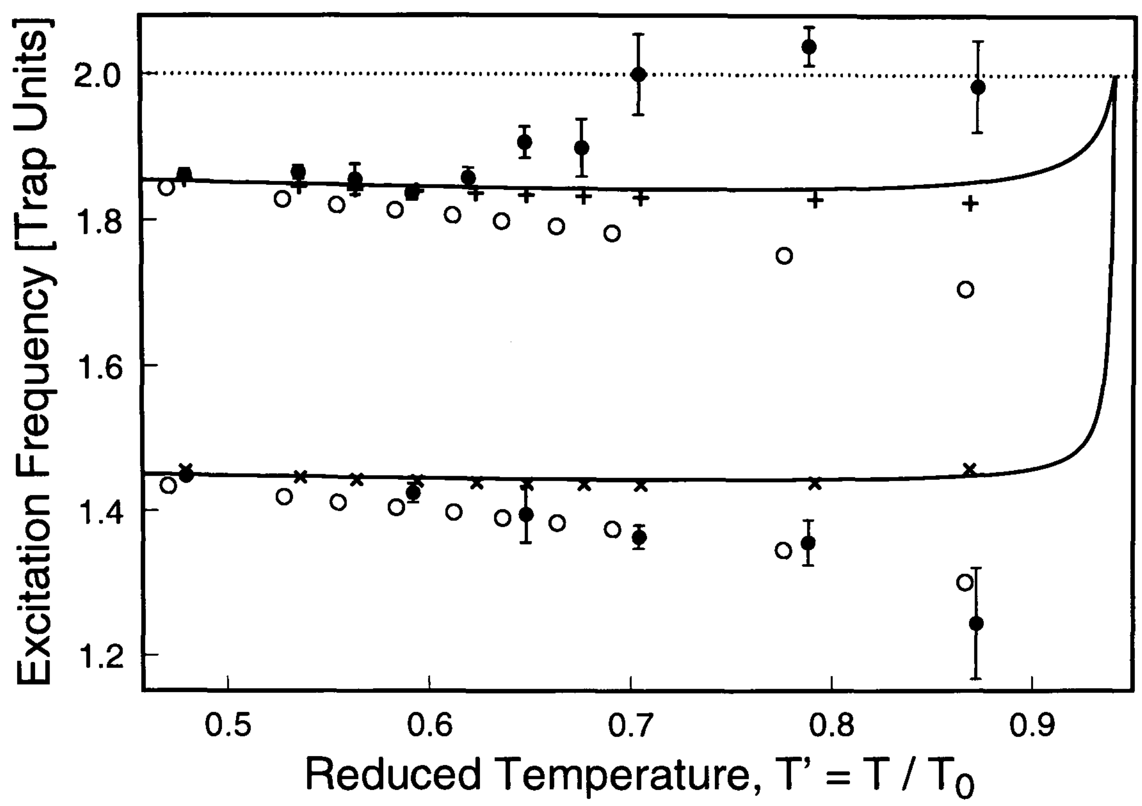

Figure 4.1: Experiment and theory of finite temperature excitations in anisotropic harmonic traps: Full circles with error bars represent measured frequencies for the low-lying —m—=2 and the higher m=0 excitations, taken from D.S. Jin *et al.* Phys. Rev. Lett. **78**, 764 (1998). Theoretical calculations based on the GPE are given by the solid lines, HFB-Popov calculations are labelled by 'x', and GHFB by 'o', taken from D.A.W.Hutchinson *et al*, J. Phys. B **33**, 1 (2000)).

the dynamics of the thermal component of the system is a severe limitation of the theory.

4.5 Infra-red divergences

Treatments of the dilute Bose gas which venture beyond the simple Bogoliubov theory of non-interacting quasiparticles are known to be troubled by infra-red divergences. These singularities occur in various contexts and one can distinguish between two scenarios in which one encounters infra-red divergent terms. The first scenario involves divergent terms in the contributions from the self-energies which cancel out exactly in the expression for physical quantities. These singularities thus are a feature of the formalism and have no physical interpretation. We will discuss how this problem affects our linear response analysis below.

A second form of infra-red problem occurs at high temperatures. Low momentum contributions to the higher order terms of the T-matrix expansion of effective interactions become comparable to the leading order term. The temperature dependent shifts become of the same magnitude of the quasiparticle energies themselves.

To phrase it in the terminology of the liquid Helium literature, long-wavelength fluctuations of the order parameter signal the break down of mean field theory [74]. We will return to this point in the concluding chapter of this thesis.

The work of Beliaev showed that a perturbative treatment of the T=0 Bose gas yields expressions for the self-energies which contain infra-red singularities [65]. Gavoret and Noziéres [54], however, showed that these divergent terms cancel out exactly in the final expressions for physical quantities, such as the quasiparticle energy. Recently this has been shown explicitly within the Beliaev Green's function formalism by Shi [15]. Popov and Fadeev [13] and Popov [14] extended of the T=0 Beliaev theory to finite temperatures. Just as in the T=0 temperature case, the formalism exhibits infra-red divergent terms. Shi was able to show that in the long wavelength limit they also cancel out in the calculation of physical quantities [15].

Our finite temperature for the homogeneous gas, equations (4.30-4.40), is based on a perturbative treatment in the quasiparticle basis. For the same reason as Beliaev's treatment it thus also contains terms which are divergent in the long wavelength limit. As shown in chapter 2 the quasiparticle coefficients from Bogoliubov theory diverge for $k\xi \ll 1$ (see Fig. 3.1). Therefore equations (4.36-4.40) diverge as well. It is only due to the identity $\int d\mathbf{r}[u^2(\mathbf{r}) - v^2(\mathbf{r})] = 1$ that expressions like the dispersion relation are finite. In analogy to Beliaev's work these singularities should cancel within out linear response treatment in calculations of physical quantities.

By subsequently limiting ourselves to V^2 we have restricted the our linear response treatment to the weak coupling regime. In this limit the average kinetic energy of colliding particles is much greater than the average interaction energy, $nU_0 \ll \hbar^2/2ma^2$, which allows us to assume the quasiparticle transformation coefficient v_k to be small and put $u_k = 1$. Thus the weak coupling assumption amounts to a low momentum cut off and avoids infra-red divergences present in the full expressions for the homogeneous gas.

[74] A. Griffin. Excitations in a Bose-Condensed Liquid, p. 145 (Cambridge University Press).

[65] S. T. Beliaev. *Energy-spectrum of a non-ideal Bose gas*. Sov. Phys. JETP 7, 299 (1958).

[54] J. Gavoret and P. Noziéres. *Structure of the perturbation expansion for the Bose liquid at zero temperature*. Ann. Phys. (NY) 28, 349 (1964).

[15] H. Shi. Finite Temperature Excitations in a dilute Bose-condensed gas. Ph.D. thesis, University of Toronto (1997).

[13] N. V. Popov and L. Faddeev. *An approach to the theory of the low temperature Bose gas*. JETP 20, 890 (1965).

[14] N. V. Popov. *Greens functions and thermodynamic functions of a non-ideal Bose gas*. JETP 20, 1185 (1965).

Our treatment of trapped condensates at finite temperatures, section 4.4, we have not used a quasiparticle transformation to find the equation of motion for the anomalous average $\kappa(t)$ and neglected the effect of the mean field during a collision process. We therefore avoid any of the infra-red problems associated with the use of the quasiparticle basis.

Chapter 5

Second Order Theories

The quantitative calculations of the final chapters of this thesis will be based on a formalism which, in the context of homogeneous systems, is often referred to as 'Beliaev approximation' or 'second order' theory. The latter term can be misleading in the sense that it treats all finite temperature effects to second order in a perturbative expansion. Instead, second order treatments consistently include all corrections to the energies of Bogoliubov excitations to *first* order in some small parameter and, as such, comprise a select number of second order terms of a perturbation series. For homogeneous systems the small parameters of such theories are (na^3) for $(T = 0)$ and $(k_B T/n_0 U_0).(n_0 a^3)^{1/2}$ for $(T \neq 0)$, and reflect two central features of the system: the diluteness of the gas and the weakness of the interparticle interactions. Both are well satisfied in the atomic gases of recent experiments and second order theories therefore form an adequate framework for their description.

The first treatment of this type was developed for homogeneous systems by Beliaev [9], and later work by Mohling *et al.*, Popov, and others followed along similar lines. Second order theories for trapped gases have recently been derived using various approaches. Fedichev and Shlyapnikov follow Beliaev's work in a treatment using a Green's functions formalism [16].

In a systematic perturbation treatment Morgan extends the approach of di-

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[9] S. T. Beliaev. *Application of the methods of quantum field theory to a system of bosons.* Sov. Phys. JETP 34, 289 (1958).

[16] P. O. Fedichev and G. V. Shlyapnikov. *Finite-temperature perturbation theory for a spatially inhomogeneous Bose-condensed gas.* Phys. Rev. A 58, 3146 (1998).

agonalising the quadratic Hamiltonian of section 3.2 to finite temperatures [17]. His treatment avoids the factorisation approximations of equations (3.37,3.38), but instead includes all terms linear in the small parameter of second order theories. Since Morgan's treatment demonstrates the derivation of a second order theory and the approximations involved in a clear and systematic fashion, we briefly summarise its main features in section 5.1. In section 5.2 we then compare and contrast it to the V^2 linear response treatment of the previous chapter.

Giorgini showed recently that a time dependent mean-field formalism, as presented in chapter 4, can be used to formulate a second order theory of the Bose gas [20]. In section 5.3 we use a similar approach and derive a second order expression for the density response of the mean field to an external perturbation. This quantity directly relates to experimental measurements of frequencies and lifetimes and will form the basis of the calculations of the remainder of this thesis.

5.1 Second order theory for trapped condensates; a perturbation scheme

The perturbative treatment of the Bose gas, as presented by Morgan, does not use a mean field prescription, but instead chooses a formalism which explicitly preserves the total number of particles. In this brief summary we will not emphasise this particular aspect of the formalism, since it will only play a secondary role in the structure of the final results. Just as in section 3.2, we write the grand canonical Hamiltonian as

$$\hat{H} = E_0 + \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4, \tag{5.1}$$

where we recall the individual terms were

$$E_0 = N_0 \int d\mathbf{r}\, \Phi(\mathbf{r})^* \left[H_{sp}(\mathbf{r}) - \mu + \frac{1}{2} N_0 U_0 |\Phi(\mathbf{r})|^2 \right] \Phi(\mathbf{r}), \tag{5.2}$$

$$\hat{H}_1 = \sqrt{N_0} \int d\mathbf{r}\, \Phi^*(\mathbf{r}) \left[H_{sp}(\mathbf{r}) - \mu + N_0 U_0 |\Phi(\mathbf{r})|^2 \right] \hat{\delta}(\mathbf{r}) + h.c. \tag{5.3}$$

[17] S. A. Morgan. A Gapless Theory of Bose-Einstein Condensation in Dilute Gases at Finite Temperature. Ph.D. thesis, University of Oxford (1999).

[20] S. Giorgini. *Collisionless dynamics of dilute Bose gases: Role of quantum and thermal fluctuations*. Phys. Rev. A 61, 063615 (2000).

$$\hat{H}_2 = \int d\mathbf{r}\, \hat{\delta}^\dagger(\mathbf{r})\Big[H_{sp}(\mathbf{r}) - \mu + 2N_0U_0|\Phi(\mathbf{r})|^2\Big]\hat{\delta}(\mathbf{r}) + \int d\mathbf{r}\, \hat{\delta}^\dagger(\mathbf{r})\left[\frac{N_0U_0}{2}\Phi(\mathbf{r})\Phi(\mathbf{r})\right]\hat{\delta}^\dagger(\mathbf{r}) + h.c. \tag{5.4}$$

$$\hat{H}_3 = \int d\mathbf{r}\sqrt{N_0}U_0\Phi^*(\mathbf{r})\hat{\delta}^\dagger(\mathbf{r})\hat{\delta}(\mathbf{r})\hat{\delta}(\mathbf{r}) + h.c. \tag{5.5}$$

$$\hat{H}_4 = \int d\mathbf{r}\, \frac{U_0}{2}\hat{\delta}^\dagger(\mathbf{r})\hat{\delta}^\dagger(\mathbf{r})\hat{\delta}(\mathbf{r})\hat{\delta}(\mathbf{r}). \tag{5.6}$$

In section 3.2 we showed for a condensate without thermal component, that the terms $\hat{H}_Q = E_0 + \hat{H}_1 + \hat{H}_2$ can be diagonalised using the Bogoliubov transformation. In the following we again use the (T=0) transformation to diagonalise the leading order contributions of the full Hamiltonian. The remaining terms $\hat{H}_3$, $\hat{H}_4$, and finite temperature terms of $\hat{H}_Q$ which are not included in the diagonalisation, we will deal with perturbatively. We thus base our second order theory of finite temperature excitations on non-interacting zero-temperature quasiparticles, based on a N_0 corresponding to the ground state population of a given temperature. Interactions between the quasiparticles and effects of the thermal cloud we then include in form of perturbative correction terms which give rise to temperature dependent energy shifts and lifetimes.

At (T=0) we found the equation for the ground state by minimising the functional $H_0[\Phi_0]$. At finite temperatures, however, it is necessary to consider the effect of the thermal component on the condensate. The finite temperature condensate ground state can be found by minimising the energy functional $(E_0+E_2)[\Phi_0]$, where $E_2 = \langle\hat{H}_2\rangle$, which gives the generalised GPE

$$\Big(H_{sp} + N_0U_0|\tilde{\Phi}(\mathbf{r})|^2 + 2U_0\rho(\mathbf{r})\Big)\tilde{\Phi}(\mathbf{r}) + U_0\kappa(\mathbf{r})\tilde{\Phi}^*(\mathbf{r}) = \tilde{\mu}\tilde{\Phi}(\mathbf{r}). \tag{5.7}$$

We denote the energy and the wavefunction of the generalised GPE ($T\neq0$) by $\tilde{\mu}$ and $\tilde{\Phi}_0$. If the condensate satisfies the generalised GPE, the linear Hamiltonian $\hat{H}_1$ no longer vanishes, but leaves the remainder

$$\Delta\hat{H}_1 = -\sqrt{N_0}\int d\mathbf{r}\,\Big\{[2U_0\rho(\mathbf{r})\Phi_0(\mathbf{r}) + U_0\kappa(\mathbf{r})\Phi_0^*(\mathbf{r})]\hat{\delta}^\dagger + h.c.\Big\}. \tag{5.8}$$

In general, it is necessary to distinguish carefully between energies and wavefunctions based on the ordinary GPE (T=0), μ, Φ_0, ϵ_p, $u_p(\mathbf{r})$, and $v_p(\mathbf{r})$, and the corresponding quantities of the finite temperature scenario involving the generalised GPE, which we denote with the tilde superscript. Only in self-consistent calculations of the second order theory is this explicit distinction unnecessary. The self-consistent procedure starts from quadratic energies and wavefunctions, corresponding to a given ground state population, to calculate temperature dependent corrections to excitation energies and wavefunctions. It then uses these results in the following iteration as input, recalculates the finite temperature corrections to energies and wavefunctions and obtains a new thermal distribution. Of the three parameters N, N_0 and T, which are related to each other by $N = N_0 + N_{ex}(T)$, the one which is not taken to be fixed is re-adjusted and the procedure is repeated until convergence is reached. Self-consistent calculations therefore implicitly account for the difference between zero and finite temperature energies and wavefunctions. In the following we will derive the theory for a purely perturbative calculation. We therefore have to account explicitly for the difference between the energies and wavefunctions with or without the presence of the thermal component and include additional energy shifts. From the quadratic term $\hat{H}_2$ we get the shift

$$\Delta\hat{H}_2 = \hat{H}_2[\tilde{\Phi}_0(\mathbf{r})] - \hat{H}_2[\Phi_0(\mathbf{r})]. \tag{5.9}$$

It can be associated with the change in condensate ground state energy and condensate shape when including the effect of the thermal cloud on the condensate, and we denote the corresponding energy shifts accordingly, $\langle\Delta\hat{H}_2\rangle = E_\mu + E_{shape}$. A further, more subtle, effect of the change in condensate ground state arises from the fact that the zero temperature excitation amplitudes $u(\mathbf{r})$ and $v(\mathbf{r})$ are no longer orthogonal to the new finite temperature ground state wavefunction $\tilde{\Phi}_0$. Due to selection rules this gives rise to an additional energy shift only for the excitations with zero angular momentum $l = 0$, which we also group into the term E_{shape}.

The zero temperature diagonalisation procedure therefore leaves the following terms unaccounted for,

$$\hat{H}_{pert} = \hat{H}_4 + \Delta\hat{H}_2 + \hat{H}_3 + \Delta\hat{H}_1, \tag{5.10}$$

which we will deal with perturbatively. To first order in perturbation theory only the terms with an even number of operators contribute and give

$$\begin{aligned} E^{(1)}(s) &= \langle s|\hat{H}_{pert}|s\rangle = \langle s|\hat{H}_4|s\rangle + \langle s|\Delta\hat{H}_2|s\rangle \\ &= E_4(s) + E_\mu(s) + E_{shape}(s), \end{aligned} \tag{5.11}$$

where $|s\rangle = |n_1, n_2, n_3, ...\rangle$ shall denote a quasiparticle number state of the many-body system. The first non-vanishing contribution of $\hat{H}_3 + \Delta\hat{H}_1$ comes in to second order in perturbation theory

$$E_3^{(2)}(s) = \sum_{i \neq s} \frac{|\langle i|\hat{H}_3 + \Delta\hat{H}_1|s\rangle|^2}{E_i - E_s}, \tag{5.12}$$

where the E_s are energies of the many-body system given by $E_s = \sum_j n_j \epsilon_j$. The perturbative energy shifts $E^{(1)}$ and $E_3^{(2)}$ thus give perturbative corrections to the total energy of the system. Since we are interested in the energy of one quasiparticle, i.e. the energy required to create it, we have to consider

$$\Delta E(p) = E(n_1, n_2, ...n_p + 1, ..) - E(n_1, n_2, ...n_p, ..). \tag{5.13}$$

The detailed calculations of Morgan give the following expressions for the perturbative shifts to the quasiparticle energies (using the contact potential approximation)

$$\Delta E_\mu(p) = [\mu - \tilde{\mu}] \int d\mathbf{r} \Delta\rho_p, \tag{5.14}$$

$$\Delta E_4(p) = U_0 \int d^3\mathbf{r}\, [2\rho(\mathbf{r})\Delta\rho_p(\mathbf{r}) + \kappa(\mathbf{r})\Delta\kappa_p(\mathbf{r})], \tag{5.15}$$

$$\begin{aligned}\Delta E_{shape}(p) = & -N_0 U_0 \Big\{ \int d\mathbf{r}[2\Delta\rho_p(\mathbf{r}) + \Delta\kappa_p(\mathbf{r})][\phi_0^2(\mathbf{r}) - \tilde{\phi}_0^2(\mathbf{r})] \\ & + \int d\mathbf{r}\phi_0^3(\mathbf{r})[u_p(\mathbf{r}) + v_p(\mathbf{r})] \int d\mathbf{r}[\phi_0(\mathbf{r}) - \tilde{\phi}_0(\mathbf{r})][u_p(\mathbf{r}) + v_p(\mathbf{r})] \Big\}.\end{aligned} \tag{5.16}$$

Above we have used the notation $\Delta\rho_p(\mathbf{r}) = (|u_p(\mathbf{r})|^2 + |v_p(\mathbf{r})|^2)$ and $\Delta\kappa_p(\mathbf{r}) = 2u_p(\mathbf{r})v_p^*(\mathbf{r})$. We further have used the fact that both $\kappa(\mathbf{r})$ and $\phi_0(\mathbf{r})$ can be chosen to be real. Evaluating $\Delta E_3(p)$ gives

$$\Delta E_3(p) = -\sum_{ij \neq 0} \frac{|A_{pij}^P|^2}{2(\epsilon_p + \epsilon_i + \epsilon_j)} [1 + n_i + n_j] \tag{5.17}$$

$$+\sum_{ij \neq 0} \frac{|B_{pij} + B_{pji}|^2}{2(\epsilon_p - \epsilon_i - \epsilon_j)} [1 + n_i + n_j] \tag{5.18}$$

$$+\sum_{ij \neq 0} \frac{|B_{ijp} + B_{ipj}|^2}{\epsilon_p - \epsilon_i + \epsilon_j} [n_j - n_i]. \tag{5.19}$$

where n_i is the population of the respective quasi-particle level. The matrix elements have been defined to be

$$
\begin{aligned}
A_{ijk} = & \sqrt{N_0}U_0 \int d\mathbf{r}\ \phi_0(\mathbf{r})[v_i(\mathbf{r})u_j(\mathbf{r})u_k(\mathbf{r}) + u_i(\mathbf{r})v_j(\mathbf{r})v_k(\mathbf{r})], \\
B_{ijk} = & \sqrt{N_0}U_0 \int d\mathbf{r} \left\{ \phi_0^*(\mathbf{r})[u_i^*(\mathbf{r})u_j(\mathbf{r})u_k(\mathbf{r}) + v_i^*(\mathbf{r})v_j(\mathbf{r})u_k(\mathbf{r}) + v_i^*(\mathbf{r})u_j(\mathbf{r})v_k(\mathbf{r})] \right. \\
& \left. + \phi_0(\mathbf{r})[u_i(\mathbf{r})u_j(\mathbf{r})v_k(\mathbf{r}) + u_i^*(\mathbf{r})v_j(\mathbf{r})u_k(\mathbf{r}) + v_i^*(\mathbf{r})v_j(\mathbf{r})v_k(\mathbf{r})] \right\},
\end{aligned} \tag{5.20}
$$

and A^P_{ijk} denotes a sum over all permutations of indices.

We find that the second order perturbative term, $\Delta E_3(p)$, is of the same order of magnitude as the first order terms $\Delta E_4(p) + \Delta E_\mu(p) + \Delta E_{shape}(p)$. Rather than taking all terms to the same order in perturbation theory, we include all terms of the same size. This, in fact, is the central feature of the second order treatment. It gives a valid prescription for the quasiparticle spectrum, provided the perturbative shifts are small compared to the quadratic theory energies. For homogeneous systems at zero temperature this is the case if

$$na^3 \ll 1, \tag{5.21}$$

where $n = N_0/\Omega$ is the particle number density. At finite temperatures ($k_BT/n_0U_0 \gg 1$) the perturbative expansion is valid if

$$(k_BT/n_0U_0).(n_0a^3)^{1/2} \ll 1. \tag{5.22}$$

Due to the spatial dependence of quantities, it is more difficult to give similar criteria for trapped systems. The calculations of the following chapters, however, will show, that the perturbative contributions are indeed small for temperatures all the way up to T_C.

The structure of $\Delta E_3(p)$ complicates the calculation of the perturbative corrections. It contains energy differences in the denominator, which can become small or even vanish. If the denominator is off-resonance the contribution of $\Delta E_3(p)$ corresponds to virtual transitions, which contribute energy shifts to the energy of a quasiparticle. If, however, the energies of the denominator match, these virtual transitions are energetically allowed and become real transitions, changing the populations of the excited states. For homogeneous systems the spectrum of excitations is continuous. Therefore every quasiparticle energy ϵ_p has an unlimited number of energy matches, representing channels it can couple to. The summation over states of $\Delta E_3(p)$ becomes an integral and the integral can be solved to give a real and an imaginary part [17]. The real part gives the energy shift of the second order perturbation term, whereas the imaginary part is the damping rate of the excitation.

$$E(p) = \epsilon_p + \Delta E_4(p) + \Delta E_{shape}(p) + \Delta E_\mu(p) + Re(\Delta E_3(p)), \tag{5.23}$$

$$\Gamma(p) = -2Im(\Delta E_3(p))/\hbar. \tag{5.24}$$

This is the equivalent to the situation found in chapter 4, equation (4.50), where the result of similar energy matches was to introduce an imaginary component into the equation of motion for the excitation. In trapped systems the situation is more complicated. The spectrum of quasiparticle states is discrete and the summation in $\Delta E_3(p)$ can generally no longer be re-expressed analytically. For particular quasiparticle energies ϵ_p there may be no exact energy matches, but the energy denominator may still get very small in an interval around ϵ_p. Taken as a function of a scanning energy z, $\Delta E_3(p, z)$ may well be rapidly varying in z,

$$\begin{aligned}
\Delta E_3(p,z) &= -\sum_{ij\neq 0} \frac{|A^P_{pij}|^2}{2\,(z+\epsilon_i+\epsilon_j)}\,[1+n_i+n_j] && (5.25)\\
&\quad + \sum_{ij\neq 0} \frac{|B_{pij}+B_{pji}|^2}{2\,(z-\epsilon_i-\epsilon_j)}\,[1+n_i+n_j] && (5.26)\\
&\quad + \sum_{ij\neq 0} \frac{|B_{ijp}+B_{ipj}|^2}{z-\epsilon_i+\epsilon_j}\,[n_j-n_i]\,. && (5.27)
\end{aligned}$$

How resonance structure in $\Delta E_3(p, z)$ affects the time evolution of an excitation emerges naturally in the context of a second order theory of time dependent mean fields, which we turn to in section 5.3.

5.2 Comparison of second order and V^2 theory

The perturbative second order treatment of section 5.1, and the V^2 linear response treatment of chapter 4 both improve on the Bogoliubov theory of quasiparticles by including effects of the thermal cloud on the ground state and its excitations

[17] S. A. Morgan. A Gapless Theory of Bose-Einstein Condensation in Dilute Gases at Finite Temperature. Ph.D. thesis, University of Oxford (1999).

using perturbation theory in a quasiparticle basis. They therefore share many of the central features of the description of excitation energy shifts and lifetimes.

The two approaches differ formally in the way they describe the system. The linear response treatment considers the equation of motion of the mean field. The diagonalisation approach instead considers expectation values of the Hamiltonian. Population changing processes, for instance, are described by Landau and Beliaev processes and involve the creation and destruction of a total of three quasiparticles in the presence of the condensate. Within the second order theory they are thus described by the $\hat{\delta}^\dagger\hat{\delta}\hat{\delta}$ and $\hat{\delta}^\dagger\hat{\delta}^\dagger\hat{\delta}$ terms of the cubic Hamiltonian H_3. Within the linear response treatment the commutators of the equation of motion reduce cubic terms to be taken quadratic. The mean field aspect of the approach requires that their average, and as a result the Landau and Beliaev processes are described by the time dependent quantities $\delta\rho_{ji}(t) = \delta\langle\hat{c}_j^\dagger\hat{c}_i\rangle$ and $\delta\kappa_{ij}(t) = \delta\langle\hat{c}_i\hat{c}_j\rangle$.

The structure of $\Delta E_3(p)$ closely resembles the expressions we obtained within the linear response treatment of the previous chapter. Equation (5.26) describes Beliaev processes in which a single quasiparticle spontaneously decomposes into two others. It has the same population factors and resonance conditions for the energies as the contribution from $\delta\kappa_{ij}$ within the linear response treatment . The third term, equation (5.27) corresponds to Landau processes in which two quasiparticles collide and coalesce to form a single quasiparticle and its structure is again similar to its conterpart of the time-dependent mean field, $\delta\rho_{ji}$. Within the linear response treatment the term $\delta\kappa$ not only accounts for population changing terms, but introduces effective interactions for the condensate–non-condensate collision terms. In the second order treatment $\Delta E_3(p)$ does exactly the same. Indeed, Morgan shows in detail that $\Delta E_3(p)$ is required to remove infra-red divergences in the theory. Both approaches include the static anomalous average, $\kappa(\mathbf{r})$ or κ_{ij}^0. In the linear response treatment we have shown explicitly that the interpretation of this correction is that it upgrades the condensate-condensate interactions which appear in the leading order contribution to $\mathcal{M}_{ij}$ so that these are described by a many-body T-matrix. Including this term proved crucial to render the theory gapless. Even though we have not expanded on this aspect of the second order theory above, Morgan shows that this is also the case for the second order theory.

The central difference of the two treatments is, of course, that our linear response analysis was limited to V^2, or equivalently U_0^2, whereas the perturbative treatment is an expansion to first order in the small parameter of equations (5.21) and (5.22). For example, the V^2 treatment does not include the spontaneous decay of three excitations, as given by the second order theory in equation (5.25). Since A_{ijk} is at least linear in the quasiparticle coefficient $v(\mathbf{r})$, $|A_{ijk}|^2$ immediately implies higher order than V^2. Further, the second order theory is not limited to the regime of weak coupling and thus can describe excitations in the long wavelength limit. In turn the second order theory does not include all second order perturbation theory terms, such as collisions between non-condensed atoms. Such processes certainly contribute to V^2 but do not enter the second order theory as they do not directly involve condensate atoms and thus contribute in higher than linear order in $(n_0 a^3)^{1/2}$. A perturbative treatment of the Hamiltonian to V^2 requires second order perturbation theory on $\hat{H}_4$ and would give the same results as the V^2 treatment [75].

5.3 Second order theory of time dependent mean fields

The equivalent of Morgan's second order theory can also be formulated within the framework of time dependent mean fields, as recently demonstrated by Giorgini [20]. Giorgini uses the same linear response ansatz as chapter 3 and includes the effect of the time dependent averages of fluctuation terms, $\delta\rho_{ji}(t)$ and $\delta\kappa_{ij}(t)$, into the equation of motion of the mean field. Despite stating that he is performing a treatment to second order in U_0^2, he does not do so consistently throughout. Instead he ignores some U_0^2 terms, like the collisions amongst thermal particles, but instead includes all terms contributing to first order in the small parameter of second order theories equations (5.21,5.22), and thus implicitly pursues an approach akin to Morgan.

In the following we will use a linear response formulation of the second order theory which we extend to explicitly include a time dependent external perturbation $P(t)$. The perturbation will correspond to the external driver, which in the experiments imparts the excitation onto the static system. We then derive an expression for the frequency response of the condensate to such an external perturbation, which directly relates to how experiments actually measure collective excitations of condensed systems. The inclusion of the external perturbation

[75] S. A. Morgan. (private communication) .

[20] S. Giorgini. *Collisionless dynamics of dilute Bose gases: Role of quantum and thermal fluctuations*. Phys. Rev. A 61, 063615 (2000).

modifies the Hamiltonian to become

$$\hat{H} \to \hat{H} + \int d\mathbf{r}\hat{\Psi}^\dagger(\mathbf{r},t)P(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t). \tag{5.28}$$

We then obtain as the generalised linearised GPE for the mean field

$$i\hbar\frac{\partial}{\partial t}\delta\Phi(\mathbf{r},t) = \mathcal{L}(\mathbf{r})\delta\Phi(\mathbf{r},t) + \mathcal{M}(\mathbf{r})\delta\Phi^*(\mathbf{r},t) + P(t)\Phi(\mathbf{r},t), \tag{5.29}$$

where we have defined the usual BdG matrix elements as

$$\begin{aligned}
\mathcal{L}(\mathbf{r}) &= H_{sp}(\mathbf{r}) - \mu + 2N_0U_0|\Phi_0(\mathbf{r})|^2 + 2U_0\rho(\mathbf{r}),\\
\mathcal{M}(\mathbf{r}) &= U_0\Phi_0(\mathbf{r})^2 + U_0\kappa(\mathbf{r}).
\end{aligned} \tag{5.30}$$

If we linearise with respect to the quantities $\delta\Phi(\mathbf{r},t)$, $\delta\rho(\mathbf{r},t)$, $\delta\kappa(\mathbf{r},t)$, and $P(\mathbf{r},t)$ we arrive at the following for the excitations of the mean field

$$\begin{aligned}
i\hbar\frac{d}{dt}\begin{pmatrix}\delta\Phi(\mathbf{r},t)\\ -\delta\Phi(\mathbf{r},t)^*\end{pmatrix} &= \begin{pmatrix}\mathcal{L} & \mathcal{M}\\ \mathcal{M}^* & \mathcal{L}\end{pmatrix}\begin{pmatrix}\delta\Phi(\mathbf{r},t)\\ \delta\Phi(\mathbf{r},t)^*\end{pmatrix} + \begin{pmatrix}P(t)\Phi_0(\mathbf{r})\\ P^*(t)\Phi_0^*(\mathbf{r})\end{pmatrix}\\
&+U_0\Phi_0\begin{pmatrix}2\delta\rho(\mathbf{r},t)+\delta\kappa(\mathbf{r},t)\\ 2\delta\rho^*(\mathbf{r},t)+\delta\kappa^*(\mathbf{r},t)\end{pmatrix}.
\end{aligned} \tag{5.31}$$

We now use the Fourier transform $\delta\Phi(\mathbf{r},t) = \int_{-\infty}^{\infty} d\omega\ \delta\Phi(\mathbf{r},\omega)e^{-i\omega t}$ to recast the generalised BdG equations in frequency space. With $\Phi(\mathbf{r},t) \to \Phi(\mathbf{r},\omega)$ and $\Phi(\mathbf{r},t)^* \to \Phi^*(\mathbf{r},-\omega)$ we obtain

$$\begin{aligned}
\hbar\omega\begin{pmatrix}\delta\Phi(\mathbf{r},\omega)\\ -\delta\Phi^*(\mathbf{r},-\omega)\end{pmatrix} &= \begin{pmatrix}\mathcal{L} & \mathcal{M}\\ \mathcal{M}^* & \mathcal{L}\end{pmatrix}\begin{pmatrix}\delta\Phi(\mathbf{r},\omega)\\ \delta\Phi^*(\mathbf{r},-\omega)\end{pmatrix} + \begin{pmatrix}P(\omega)\Phi_0(\mathbf{r})\\ P^*(-\omega)\Phi_0^*(\mathbf{r})\end{pmatrix}\\
&+U_0\Phi_0\begin{pmatrix}2\delta\rho(\mathbf{r},\omega)+\delta\kappa(\mathbf{r},\omega)\\ 2\delta\rho^*(\mathbf{r},-\omega)+\delta\kappa^*(\mathbf{r},-\omega)\end{pmatrix}.
\end{aligned} \tag{5.32}$$

At first we shall consider the first term on the right hand side of the above equation. It can be simplified if we expand the mean field fluctuations in terms of the solutions to the BdG equations $\{u_i, v_i\}$. Since we have defined them to be orthogonal to the condensate we will have to include the condensate ground state as additional basis vectors, $u_0 = \phi_0$ and $v_0 = -\phi_0$, to obtain a complete basis for the expansion of $\delta\Phi(\mathbf{r},\omega)$.

$$\begin{pmatrix} \delta\Phi(\mathbf{r},\omega) \\ -\delta\Phi^*(\mathbf{r},-\omega) \end{pmatrix} = \sum_{\pm q} b_q(\omega) \begin{pmatrix} u_q(\mathbf{r}) \\ v_q(\mathbf{r}) \end{pmatrix}, \tag{5.33}$$

which is a compressed matrix notation for

$$\begin{aligned} \delta\Phi(\mathbf{r},\omega) &= \sum_{\pm q} b_q(\omega) u_q(\mathbf{r}) = \sum_q [b_{+q}(\omega) u_{+q}(\mathbf{r}) + b_{-q}(\omega) u_{-q}(\mathbf{r})] \\ &= \sum_q [b_{+q}(\omega) u_{+q}(\mathbf{r}) + b_{-q}(\omega) v^*_{+q}(\mathbf{r})], \\ \delta\Phi(\mathbf{r},-\omega)^* &= \sum_{\pm q} b_q(-\omega) u^*_q(\mathbf{r}) = \sum_q [b_{+q}(-\omega) u^*_{+q}(\mathbf{r}) + b_{-q}(-\omega) u^*_{-q}(\mathbf{r})] \\ &= \sum_q [b_{+q}(-\omega) u^*_{+q}(\mathbf{r}) + b_{-q}(-\omega) v_{+q}(\mathbf{r})]. \end{aligned} \tag{5.34}$$

To form a complete basis the summation over states now includes $p = 0$. We further have used $u_{-p}(\mathbf{r}) = v^*_p(\mathbf{r})$. Since u_p and v_p are solutions of the BdG we can insert the expansion into equation (5.32), multiply from the left with $(u^*_p\ v^*_p)$, integrate, and use $\int d\mathbf{r}(u^*_i u^*_j - v_i v_j) = \delta_{ij}$ to obtain

$$\begin{aligned} \hbar\omega b_p(\omega) = \hbar\omega_p b_p(\omega) \quad &+ \quad \sum_q b_q(\omega) \int d\mathbf{r} \begin{pmatrix} u^*_p & v^*_p \end{pmatrix} \begin{pmatrix} \Delta\mathcal{L} & \Delta\mathcal{M} \\ \Delta\mathcal{M}^* & \Delta\mathcal{L} \end{pmatrix} \begin{pmatrix} u_q \\ v_q \end{pmatrix} \\ &+ \quad \dots, \end{aligned} \tag{5.35}$$

where

$$\begin{aligned} \Delta\mathcal{L}(\mathbf{r}) &= -(\tilde{\mu} - \mu) + 2N_0 U_0 [|\tilde{\Phi}_0|^2 - |\Phi_0|^2] + 2U_0 \rho, \\ \Delta\mathcal{M}(\mathbf{r}) &= N_0 U_0 [\tilde{\Phi}_0^2 - \Phi_0^2] + U_0 \kappa_0, \end{aligned} \tag{5.36}$$

denote the difference between the solutions for the BdG equations and their HFB counterpart, which include the presence of the thermal cloud. The integral over this difference is the same as $\langle p|\Delta H_2 + \Delta H_4|q\rangle$ of the previous section and we therefore write

$$\begin{aligned} \hbar\omega b_p(\omega) = \hbar\omega_p b_p(\omega) \quad &+ \quad \sum_q b_q(\omega) \Big[\Delta E_4(p,q) + \Delta E_\mu(p,q) + \Delta E_{shape}(p,q) \Big] \\ &+ \quad \dots. \end{aligned} \tag{5.37}$$

We now go back to the linearised BdG equation in frequency space, equation (5.32), and consider the term involving the fluctuations,

$$\hbar\omega \begin{pmatrix} \delta\Phi(\mathbf{r},\omega) \\ -\delta\Phi^*(\mathbf{r},-\omega) \end{pmatrix} = \ldots + U_0\Phi_0 \begin{pmatrix} 2\delta\rho(\mathbf{r},\omega) + \delta\kappa(\mathbf{r},\omega) \\ 2\delta\rho^*(\mathbf{r},-\omega) + \delta\kappa^*(\mathbf{r},-\omega) \end{pmatrix}. \quad (5.38)$$

We shall deal with this term in a similar manner to Giorgini. Using the Bogoliubov transformation $\hat{\delta}(\mathbf{r}) = \sum_i [u_i(\mathbf{r})\hat{\beta}_i - v_i^*(\mathbf{r})\hat{\beta}_i^\dagger]$, these quantities can be re-expressed as follows

$$\delta\rho(\mathbf{r},t) = \langle\hat{\delta}^\dagger(\mathbf{r},t)\hat{\delta}(\mathbf{r},t)\rangle = \sum_{ij} \Big\{ u_i(\mathbf{r})u_j(\mathbf{r})g_{ij}(t) + v_i^*(\mathbf{r})v_j^*(\mathbf{r})g_{ij}^*(t)$$
$$+[u_i^*(\mathbf{r})u_j(\mathbf{r}) + v_i^*(\mathbf{r})v_j(\mathbf{r})]f_{ij}(t)\Big\}, \quad (5.39)$$
$$\delta\kappa(\mathbf{r},t) = \langle\hat{\delta}(\mathbf{r},t)\hat{\delta}(\mathbf{r},t)\rangle = \sum_{ij} \Big\{ 2v_i^*(\mathbf{r})u_j(\mathbf{r})f_{ij}(t) + u_i(\mathbf{r})u_j(\mathbf{r})g_{ij}(t)$$
$$+v_i^*(\mathbf{r})u_j^*(\mathbf{r})g_{ij}(t)\Big\}, \quad (5.40)$$

where we have defined $g_{ij}(t) = \langle\hat{\beta}_i(t)\hat{\beta}_j(t)\rangle$, $f_{ij}(t) = \langle\hat{\beta}_i^\dagger(t)\hat{\beta}_j(t)\rangle - \delta_{ij}f_{ii}$, and $f_{ii} = \langle\hat{\beta}_i^\dagger\hat{\beta}_i\rangle = n_i = [e^{e_i/kT} - 1]^{-1}$. The time evolution of the quantities $f_{ij}(t)$ and $g_{ij}(t)$ follow from the commutation with the Hamiltonian and have been written out explicitly by Giorgini (cf. [20], equations (16,17)). In the equations of motion for $f_{ij}(t)$ and $g_{ij}(t)$ we will neglect the terms involving $\delta\rho(\mathbf{r},\omega)$ and $\delta\kappa(\mathbf{r},\omega)$, i.e. in the context of equations (5.39,5.40) neglect the coupling of these quantities to themselves. We further will not include the effect of the external driver onto the time evolution of $\delta\rho(\mathbf{r},\omega)$ and $\delta\kappa(\mathbf{r},\omega)$. Including this effect would allow us to describe the response of the thermal cloud to the external perturbation, independent of the mean field. However, since the coupling of the external perturbation to modes of the trapped system will be proportional to the respective mode populations we can assume that the external driver will predominantly couple to the macroscopically occupied mean field. In turn, the driven mean field will then interact with the thermal cloud, the effects of which are are all contained in above formalism. We thus make the assumption that the direct driving of the thermal cloud will only have a minor effect and thus neglect such contributions altogether. Whether this is actually justified or not can be tested by extending above formalism to include the effect of the driver onto the thermal cloud. A detailed discussion of this form,

[20] S. Giorgini. *Collisionless dynamics of dilute Bose gases: Role of quantum and thermal fluctuations*. Phys. Rev. A 61, 063615 (2000).

however, shall remain beyond the scope of this thesis.

After some lengthy algebra the following expressions for the Fourier components $g^*_{ij}(-\omega)$, $f_{ij}(\omega)$ and $g_{ij}(\omega)$,

$$g^*_{ij}(-\omega) = \frac{-\sqrt{N_0}(1+n_i+n_j)}{\hbar\omega - (\epsilon_j + \epsilon_j)} \sum_q b_q(\omega) A^P_{qji}, \tag{5.41}$$

$$f_{ji}(\omega) = \frac{\sqrt{N_0}(n_j - n_i)}{\hbar\omega - \epsilon_i + \epsilon_j} \sum_q b_q(\omega)[B_{ijq} + B_{iqj}], \tag{5.42}$$

$$g_{ij}(\omega) = \frac{\sqrt{N_0}(1+n_i+n_j)}{\hbar\omega - (\epsilon_j + \epsilon_j)} \sum_q b_q(\omega)[B_{qij} + B_{qji}]^*. \tag{5.43}$$

For A^P_{qji} and B_{ijq} we have used the same notation as in section 5.1. If we insert the above into equations (5.38-??) we arrive at

$$\begin{aligned} \hbar\omega b_p(\omega) &= \hbar\omega_p b_p(\omega) \\ &+ \sum_q b_q(\omega)\Big[\Delta E_4(p,q) + \Delta E_\mu(p,q) + \Delta E_{shape}(p,q)\Big] \\ &+ \int d\mathbf{r}[u^*_p P(\omega)\Phi_0 + v^*_p[P(-\omega)]^*\Phi^*_0] \\ &+ \sum_q b_q(\omega)\Delta E_3(q,\omega), \end{aligned} \tag{5.44}$$

where we have defined $\Delta E_3(q,\omega)$ as in equations (5.25-5.27).

5.4 Fourier transform of the mean-field's response

If only one quasiparticle mode is significantly excited, $b_q(\omega)$ is non-zero for only $p = q$ and above the equation for the Fourier component of the mean-field's excitation simplifies to

$$b_p(\omega) = \frac{\int d\mathbf{r}[u^*_p P(\omega)\Phi_0 + v^*_p[P(-\omega)]^*\Phi^*_0]}{\hbar(\omega - \omega_p) - [\Delta E_4(p) + \Delta E_\lambda(p) + \Delta E_{shape}(p) + \Delta E_3(p,\omega)}, \tag{5.45}$$

which is the product of two Fourier transforms. The numerator of the right hand side is the transform of the driver $P(t)$. The denominator describes the response of the density of the mean field to the external perturbation $P(t)$.

Experimentally, there are various ways of measuring the frequencies and lifetimes of excitations. One technique is akin to resonance spectroscopy. It involves measuring the amplitude of the response of the condensate to an external perturbation of narrowly defined frequency. Scanning the probing perturbation over a range of frequencies then gives a spectrum of the amplitude of the response as a function of frequency. The spectrum obtained by such measurements is given by equation 5.45. A second way of measuring the excitations of a condensate is to excite the system with a broad-band pulse and observe the system evolve in time. The amplitude of the oscillations of the system as a function of time then corresponds to the Fourier transform of the frequency measurement of the previous method.

Both methods have upper limits on their spectral resolution. In the first method the resolution depends on the frequency width of the external perturbation. This, in turn, is limited by the maximal period of time the system can be driven by the perturbation before unwanted effects like heating sufficiently alter the number of atoms in the trap. The second measurement method is also limited by the observation time. The more oscillations of the system that can be observed, the better the frequency resolution. For both methods the upper limit of the observation time is, of course, the lifetime of the condensate itself. In practice, however, the optimal observation time is found as a compromise between maximising observation time and minimising systematic errors of the measurements due to adverse effects like heating etc. For the initial measurements on finite temperature excitations in anisotropic traps the JILA group used both experimental techniques and they gave similar results [5].

We can model the way the finite observation time limits the resolution of the frequency spectrum of the mean field response by considering the quantity

$$\overline{\delta\Phi}(t) = \theta(t)\delta\Phi(t)\theta(T - t). \tag{5.46}$$

$\theta(t)$ and $\theta(T - t)$ are step functions and limit the mean field fluctuations to a time window, which begins with the start of the perturbation and lasts for the period of the observation time. We further define the quantities $\overline{\delta\rho}(t)$ and $\overline{\delta\kappa}(t)$ in the same way. If we multiply the starting point of the second order treatment,

[5] D. S. Jin, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell. *Temperature-dependent damping and frequency shifts in collective excitations of a dilute Bose-Einstein condensate*. Phys. Rev. Lett. 78, 764 (1997).

equation (5.32), with $\theta(t)\theta(T-t)$ we find it simply introduces $\overline{\delta\Psi}(t)$, $\overline{\delta\rho}(t)$, and $\overline{\delta\kappa}(t)$ on the right hand side of the equation and the full analysis of the previous section carries through for the over-lined quantities. The equation of motion of the mean field fluctuation, limited to the time window $[0,T]$ is given by

$$\begin{aligned} i\hbar\frac{d}{dt}\overline{\delta\Phi}(t) = & \; i\hbar\Big[\;\delta(t)\delta\Phi(t)\theta(T-t) + \theta(t)\theta(T-t)\frac{d}{dt}\delta\Phi(t) \\ & + \;\theta(t)\delta\Phi(t)\frac{d}{dt}\theta(T-t)\Big]. \end{aligned} \tag{5.47}$$

Taking the Fourier transform gives

$$\begin{aligned} i\omega\overline{\delta\Phi}(\omega) = & \; i\hbar\Big[\;\delta\Phi(t=0) + \int_{-\infty}^{\infty} dte^{i\omega t}[\theta(t)\theta(T-t)\frac{d}{dt}\delta\Phi(t)] \\ & + \int_{-\infty}^{\infty} dte^{-\omega t}\theta(t)\delta\Phi(t)\frac{d}{dt}\theta(T-t)\Big]. \end{aligned} \tag{5.48}$$

The first term can be taken to be zero since $\delta\Phi(0)=0$. The second term is given by the analysis of the previous section, after substituting the quantities on the right hand side by over-lined ones. Hence we have

$$\begin{aligned} & \hbar\omega\overline{\delta\Phi}(\omega) - i\hbar\int_{-\infty}^{\infty} dte^{i\omega t}\theta(t)\delta\Phi(t)\frac{d}{dt}\theta(T-t) \\ = & \; \mathcal{L}\overline{\delta\Phi}(\omega) + \mathcal{M}\overline{\delta\Phi}^*(-\omega) + \overline{P}(\omega)\Phi_0(\mathbf{r}) + U_0\Phi_0[2\overline{\delta\rho}(\mathbf{r},\omega) + \overline{\delta\kappa}(\mathbf{r},\omega)]. \end{aligned} \tag{5.49}$$

The effect of the limited time window can be modelled by $\theta(T-t)\simeq e^{-t/T}$ which introduces a small imaginary contribution $\gamma = 1/T$ to the scanning frequency ω

$$\begin{aligned} \hbar(\omega+i\gamma)\overline{\delta\Phi}(\omega) = & \; \mathcal{L}\overline{\delta\Phi}(\omega) + \mathcal{M}\overline{\delta\Phi}^*(-\omega) + \overline{P}(\omega)\Phi_0(\mathbf{r}) \\ & + U_0\Phi_0[2\overline{\delta\rho}(\mathbf{r},\omega) + \overline{\delta\kappa}(\mathbf{r},\omega)]. \end{aligned} \tag{5.50}$$

The analysis of the previous section now carries through also for the over-lined quantities. We thus arrive at an expression for the frequency spectrum of the mean field's response to an external perturbation

$$F_p(\omega) \propto \frac{1}{\hbar(\omega+i\gamma) - \hbar\omega_p - [\Delta E_4(p) + \Delta E_\lambda(p) + \Delta E_{shape}(p) + \Delta E_3(p,\omega)]}. \tag{5.51}$$

Assuming the external perturbation $P(t)$ couples predominantly to the mean field, this function corresponds to the experimentally observed amplitude oscillations of the experiments. The next chapter will be concerned with calculating the frequency response, $F_p(\omega)$, for various low-lying excitations in a spherical trap.

CHAPTER 6

EXCITATIONS IN SPHERICALLY SYMMETRIC SYSTEMS

This chapter presents quantitative calculations of excitations in spherical traps based on the second order theory of time dependent mean fields. Experiments in spherical trap geometries have recently become feasible and we present calculations for sets of parameters, which aim to be realistic experimentally.

Most quantitative calculations of finite temperature excitation energies have been performed in a self-consistent fashion [73, 56, 21]. In the following we will not pursue a self-consistent approach, but instead perform purely perturbative calculations. In section 6.1 we test how calculation procedures affects results for energy shifts by comparing perturbative and self-consistent calculations in the HFB-Popov approximation. Both calculations agree to within a few percent of the size of the shifts themselves and we conclude that it is sufficient to calculate the second order theory perturbatively rather than self-consistently.

Previous calculations of excitation lifetimes have been based on the assumption that excitations in trapped systems will exponentially decay in time as their homo-

[73] D. W. Hutchinson, E. Zaremba, and A. Griffin. *Finite temperature excitations of a trapped Bose gas*. Phys. Rev. Lett. 78, 1842 (1997).

[56] R. J. Dodd, M. Edwards, C. W. Clark, and K. Burnett. *Collective excitations of Bose-Einstein-condensed gases at finite temperatures*. Phys. Rev. A 57, R32 (1998).

[21] D. W. Hutchinson, R. J. Dodd, and K. Burnett. *Gapless finite-t theory of collective modes of a trapped gas*. Phys. Rev. Lett. 81, 2198 (1998).

geneous counterparts [22]. In section 6.2 we discuss that we will not make such an assumption from the outset. Instead we explicitly calculate the full second order theory without any further approximations. Systems with rotational symmetries are best described in terms of a basis state decomposition in spherical harmonics. We shall label the excitations in spherical systems by their number of nodes of the radial component, n, and the usual quantum numbers l and m for the angular component. Due to the symmetry of the system the excitations are $(2l+1)$ degenerate in m. In section 6.3 we discuss each of the low lying excitations in turn.

6.1 Perturbative vs. self-consistent calculations: HFB-Popov as a test

Our strategy to calculate the frequency spectrum of the mean field's response at finite temperatures will be follows: We first solve the zero temperature ground state and excitation spectrum, given by the GPE and BdG equations for a value of N_0 corresponding to a given temperature. We then calculate $\rho(\mathbf{r})$ and $\kappa(\mathbf{r})$ and solve the generalised GPE to obtain $\tilde{\phi}_0$ and $\tilde{\mu}_0$. It then is straightforward to evaluate the perturbative correction terms $\Delta E_4(p)$, $\Delta E_{shape}(p)$ and $\Delta E_\mu(p)$, to calculate $\Delta E_3(p,z)$, and obtain the spectrum $F_p(z)$. A more detailed discussion of the numerical procedure will can be found in appendix A.

A self-consistent approach to calculating the second order theory is possible as well. It would again start from the solutions of the zero temperature theory for a given N_0, would calculate the $\rho(\mathbf{r})$ and $\kappa(\mathbf{r})$ to solve the generalised GPE, then construct the matrices of the generalised BdG equations $\mathcal{L}'$ and $\mathcal{M}'$, solve the generalised BdG equations, and determine the new distribution of thermal particles. This then gives a new value of N_0 and the calculation is iterated to convergence. A self-consistent calculation, however, would involve re-calculating the matrix elements of $\Delta E_3(p,z)$ for every step of the iteration and thus is not feasible in practice.

To test the importance of self-consistency we limit our perturbative second order formalism to calculate HFB-Popov energy shifts. This is done by setting $\kappa(\mathbf{r})$ in ΔE_4, ΔE_μ, and ΔE_{shape} to be zero and neglecting ΔE_3 altogether. We

[22] P. O. Fedichev, G. V. Shlyapnikov, and J. T. M. Walraven. *Damping of low-energy excitations of a trapped Bose-Einstein condensate at finite temperatures*. Phys. Rev. Lett. 80, 2269 (1998).

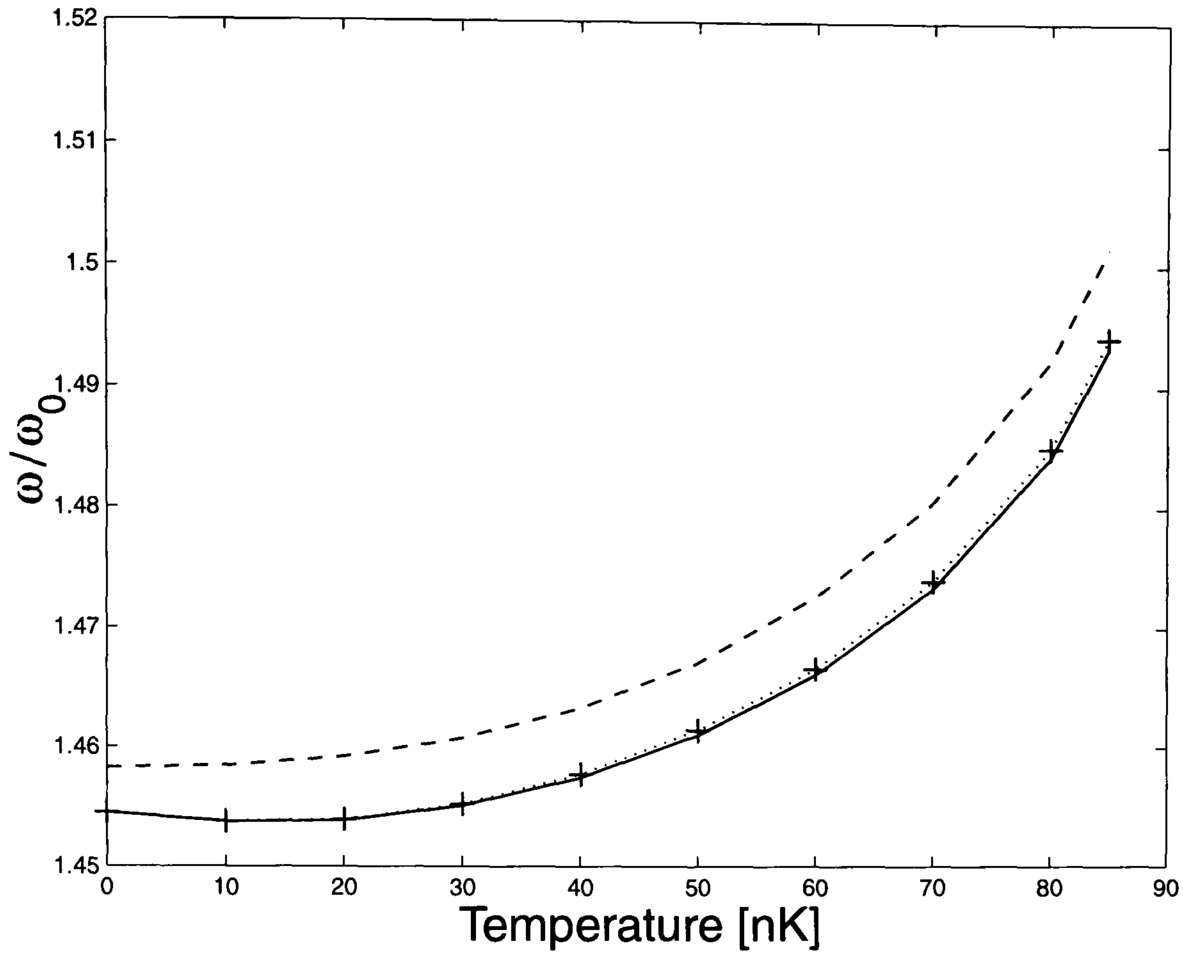

Figure 6.1: HFB-Popov excitation frequency for the (n=0,l=2) mode as a function of temperature, calculated perturbatively (solid line) and self-consistently (+, dotted line). The quadratic theory energy is given by the dashed line.

then compare the perturbative HFB-Popov shifts with results from self-consistent HFB-Popov calculations [73]. We find that the two differ by a maximum of a few percent of the size of the shift itself. As an example, we plot the self-consistent and perturbative HFB-Popov energy of the quadrupole mode (n=0,l=2). The two calculations agree equally well for all other excitations. The good agreement between the two calculations for the HFB-Popov energies shows that it is sufficient to calculate the effects of the thermal cloud perturbatively, rather than self-consistently. It further indicates that we have included all shape effects and energy shifts like ΔE_{shape} and ΔE_{μ}, which account for the presence of the thermal cloud, but never appear explicitly in self-consistent treatments.

[73] D. W. Hutchinson, E. Zaremba, and A. Griffin. *Finite temperature excitations of a trapped Bose gas*. Phys. Rev. Lett. 78, 1842 (1997).

6.2 Decay into continuum or coupling to states?

We discussed earlier, how $\Delta E_3(p, z)$ describes population changes amongst quasiparticle levels and, more specifically, the decay of the particular quasiparticle excitation under consideration. The way a quasiparticle evolves in time depends, in general, on three factors: the number of other states it can couple to, the coupling strength to each of them, given by the overlap integrals of the respective wavefunctions, and finally the energy matches of the various levels involved. All three of these factors strongly depend on the geometry of the system.

Homogeneous systems, unconfined in space, have a continuous spectrum of excitations. Since the energy of a decay channel is given by the energy of sums or differences of quasiparticle energies, any excitation in a homogeneous system couples resonantly to an infinite number of channels and never finds its way back to its initial state, giving an exponential decay of the excitation. In section 4.2.3 we therefore found the exponential decay rate by Fermi's Golden Rule of time-dependent perturbation theory.

Just as the excitation in a homogeneous system is equivalent to an excited atom coupling to the electromagnetic continuum, the trapped system is akin to an excited atom within a high-finesse cavity. The boundary conditions of spatial confinement force the energy levels of the cavity, or equivalently the condensate, to become discrete. The excitation no longer couples to a continuum, but only to a select number of states. Each energy match corresponds to one specific reversible transition. If we have only a small number of energy matches or if the coupling to a select number of modes is far more dominant than all other energy matches, we will observe the reversible transfer between a few coupled modes. From cavity QED experiments it is well known that if the cavity is tuned on resonance the excited atom couples strongly to one mode of the of the electro-magnetic field, leaving the energy quantum oscillating between the atom and the cavity back and forth. Recent experiments have shown that a similar scenario can be found in trapped condensates. The trap can be tuned such that either Landau [76] or Beliaev decay channels [77] couple resonantly to specific excitations. In trapped Bose condensates we therefore cannot assume from the outset that excitations will behave in time

[76] G. Hechenblaikner, O. Maragò, E. Hodby, J. Arlt, *et al.*. *Observation of harmonic generation and non-linear coupling in the collective dynamics of a Bose-Einstein condensate.* Phys. Rev. Lett. 85, 692 (2000).

[77] E. Hodby, G. Hechenblaikner, O. Maragò, and C. Foot. *The experimental observation of Beliaev damping in a Bose condensed gas.* cond-mat/0010157 .

like their homogeneous counterparts. Only in the limit of a large number of energy matches the time evolution will resemble the scenario of the homogeneous gas.

For anisotropic parabolic traps it has been argued that the discrete energy levels are chaotically distributed over the the full range of energies and that the spectrum of decay channels can therefore be approximated to be quasi-continuous. The time evolution of an excitation then again can be dealt with as a decay into a continuum of states [22]. This is valid if we can approximate the second order perturbative term as a slowly varying function, $\Delta E_3(z) \simeq \delta_{E3}(\epsilon_p) + \imath\Gamma_{E3}(\epsilon_p)$. In the spherical trap we find this is not the case. We therefore calculate the spectrum of an excitation to second order as given by equation (5.51), summing over the contributions over individual decay channels, of equations (5.25-5.27). The only approximation involved is due to a high energy, i.e. low population, cut-off of the summation over states when calculating $\Delta E_3(p)$. We show the calculated spectra to be independent of our chosen truncation.

6.3 Second Order Calculations

The following calculations we will be for a system of N_{tot}=10000 ^{87}Rb atoms confined in a spherically symmetric harmonic trap of frequency ω_0=100 Hz, which corresponds to a transition temperature of approximately 90nK. The ground state population N_0 is a function of temperature, determined by the constraint of fixed total number of particles. This set of parameters corresponds to what the Oxford experimental BEC group consider achievable with their TOP trap experiment [78].

We discussed in chapter 5 that we are interested in calculating the frequency spectrum of a given excitation $F_p(z)$ given by equation (5.51). We thus have to evaluate $\Delta E_3(p, z)$ for $z = \omega + i\gamma$ and a range of values of ω in the vicinity of the quadratic energy of the quasiparticle, ϵ_p. The numerically calculated spectra will, of course, depend on the the value of the imaginary component of the scanning frequency, γ, which we identified as a parameter for the experimental resolution of the experiment (see figure 6.2). The resolution of the JILA resonance measurement corresponds to a value for γ of a few 10^{-2} ω_0 [5]. For our calculations we will assume

[22] P. O. Fedichev, G. V. Shlyapnikov, and J. T. M. Walraven. *Damping of low-energy excitations of a trapped Bose-Einstein condensate at finite temperatures*. Phys. Rev. Lett. 80, 2269 (1998).

[78] O. Maragò and C. J. Foot. (private communication) .

[5] D. S. Jin, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell. *Temperature-*

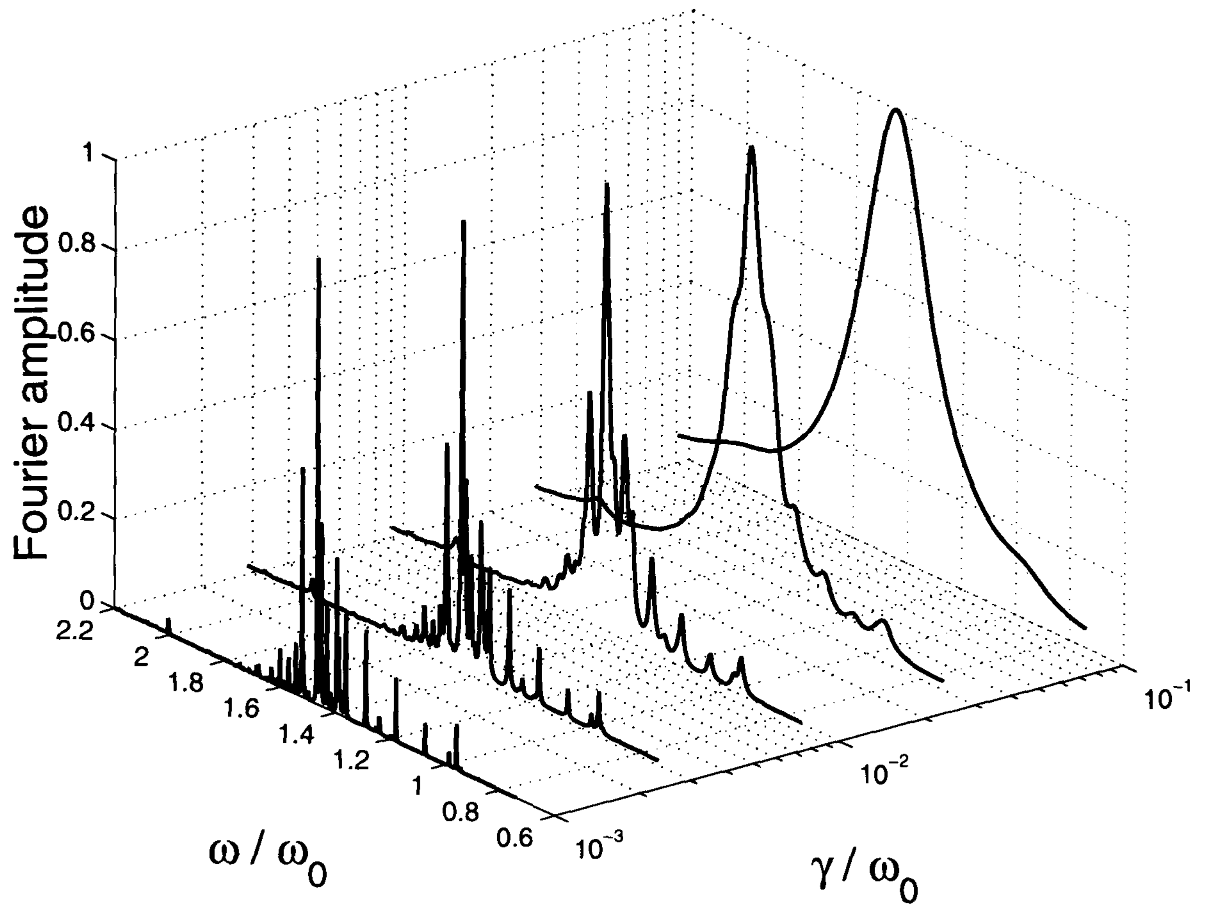

Figure 6.2: The frequency response spectrum $F(\omega + i\gamma)$ of the (n=0,l=2) mode at a temperature of 0.7 T/T_C as a function of the resolution γ.

that experiments in spherical traps γ will take similar values. In spherical systems, we find the spectra of excitations generally are comprised of individual resonances, some of which are well separated. The resonance structure is, of course, due to the second order perturbation term $\Delta E_3(p, z)$ and are a direct consequence of the discrete nature of the trapped system. A detailed study of $\Delta E_3(p, z)$ shows that relatively few decay channels couple strongly to the excitation p, giving rise to large resonances in $\Delta E_3(p, z)$ whenever their energies match the scanning frequency. The contributions of the other decay channels are orders of magnitude smaller and form a negligible background. An analysis of the individual spectra shows that we encounter generally two different types:

The first type of spectrum does display individual resonances, but its over-all shape is approximately of the form of a Lorentzian. We will show that such a spectrum can be analysed in terms of approximate energy shifts and widths. The spectrum of the quadrupole mode, (n = 0, l = 2), is such an example and we will discuss it in greater detail in section 6.3.1. Higher lying modes of (n = 0, l = 3), (n = 0, l = 4), etc. behave in a similar way as the quadrupole mode. Their

dependent damping and frequency shifts in collective excitations of a dilute Bose-Einstein condensate. Phys. Rev. Lett. 78, 764 (1997).

over-all line shape is Lorentzian and can be interpreted in terms of energy shifts and lifetimes.

The second type of spectrum is found for the breathing mode, ($n = 1$, $l = 0$). For this mode the effects of the discreteness of the system are sufficiently pronounced that its spectrum at higher temperatures is not of Lorentzian form. It thus is no longer possible to interpret the spectrum in terms of energy shifts and lifetimes. We will study this mode in detail in section 6.3.1. The dipole mode, incidentally, is one of the two modes, which are not damped for a classical gas confined in a harmonic trap. The other classically undamped mode is the dipole oscillation of the centre-of-mass of the system. Our dipole mode ($n = 0$, $l = 1$) is closely related to, but not exactly the same as this centre-of-mass oscillation. We discuss this matter further in section 6.3.3.

6.3.1 The quadrupole mode ($n = 0$, $l = 2$)

At zero temperature the frequency spectrum $F_p(z)$ of the quadrupole mode ($n = 0$,$l = 2$) is a single peak at the quadratic energy $\epsilon_p = 1.458\omega_0$ with a width corresponding to $\imath\gamma$. The higherlying modes are not thermally occupied and Landau processes therefore do not occur. Due to the lack of suitable energy matches Beliaev damping has no appreciable effect. With rise in temperature, all the other quasiparticle levels get increasingly populated and the spectrum develops further resonance lines signalling the coupling of the excitation to other levels. They are predominantly Landau processes of the type (0,2)+(0,l)$\rightarrow$(0,l+2)+(0,0) and the Beliaev decay (0,2)+(0,0)$\rightarrow$(0,1)+(0,1). This can be seen directly from the resonance structure of $\Delta E_3(z)$, which is plotted in figures 6.3 and 6.4. The same decay processes remain dominant at higher temperatures, but other channels involving higher lying states come into play as well. Due to the limited resolution, given by γ, the individual resonances each have a corresponding width and neighbouring resonances overlap.

The resonances of $\Delta E_3(p, z)$ carry over and give rise to structures in the Fourier amplitude of the frequency response, $F_p(z)$. The additional energy shifts of $\Delta E_4(p)$, $\Delta E_{shape}(p)$, and $\Delta E_\mu(p)$ and the functional form of $F_p(z)$ mean that these resonances do not necessarily occur in the same positions and with the same hights as in $\Delta E_3(p, z)$. This can be seen from direct comparision of figures 6.2 and 6.3. The resonance structure of $\Delta E_3(p, z)$ implies that the time evolution of the quadrupole mode, in principle, follows a complicated pattern. The frequency spectrum $F_p(\omega)$,

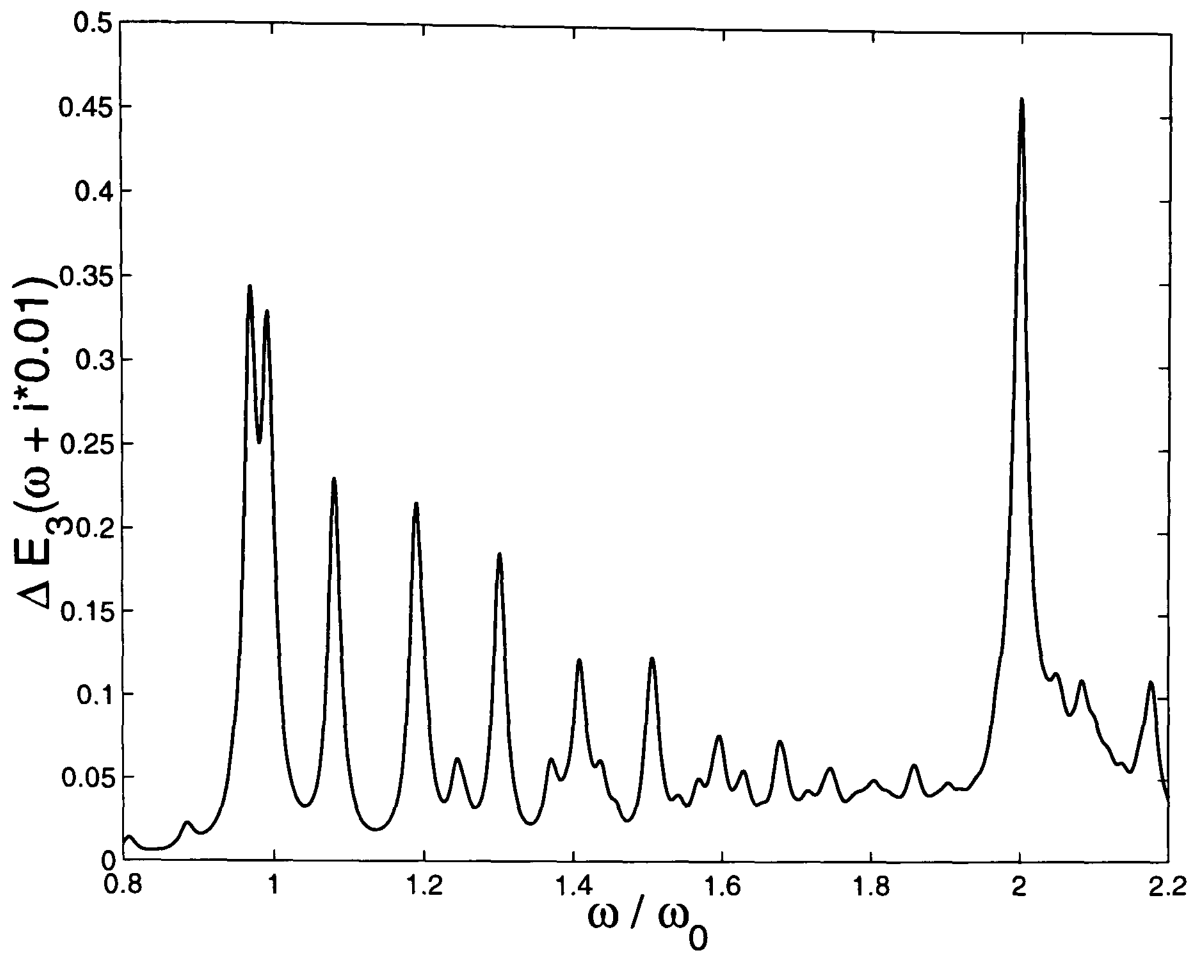

Figure 6.3: $\Delta E_3(\omega + i\gamma)$ of the (n=0,l=2) mode at a temperature of 0.8 T/T_C for a resolution of $\gamma = 10^{-2}\omega_0$.

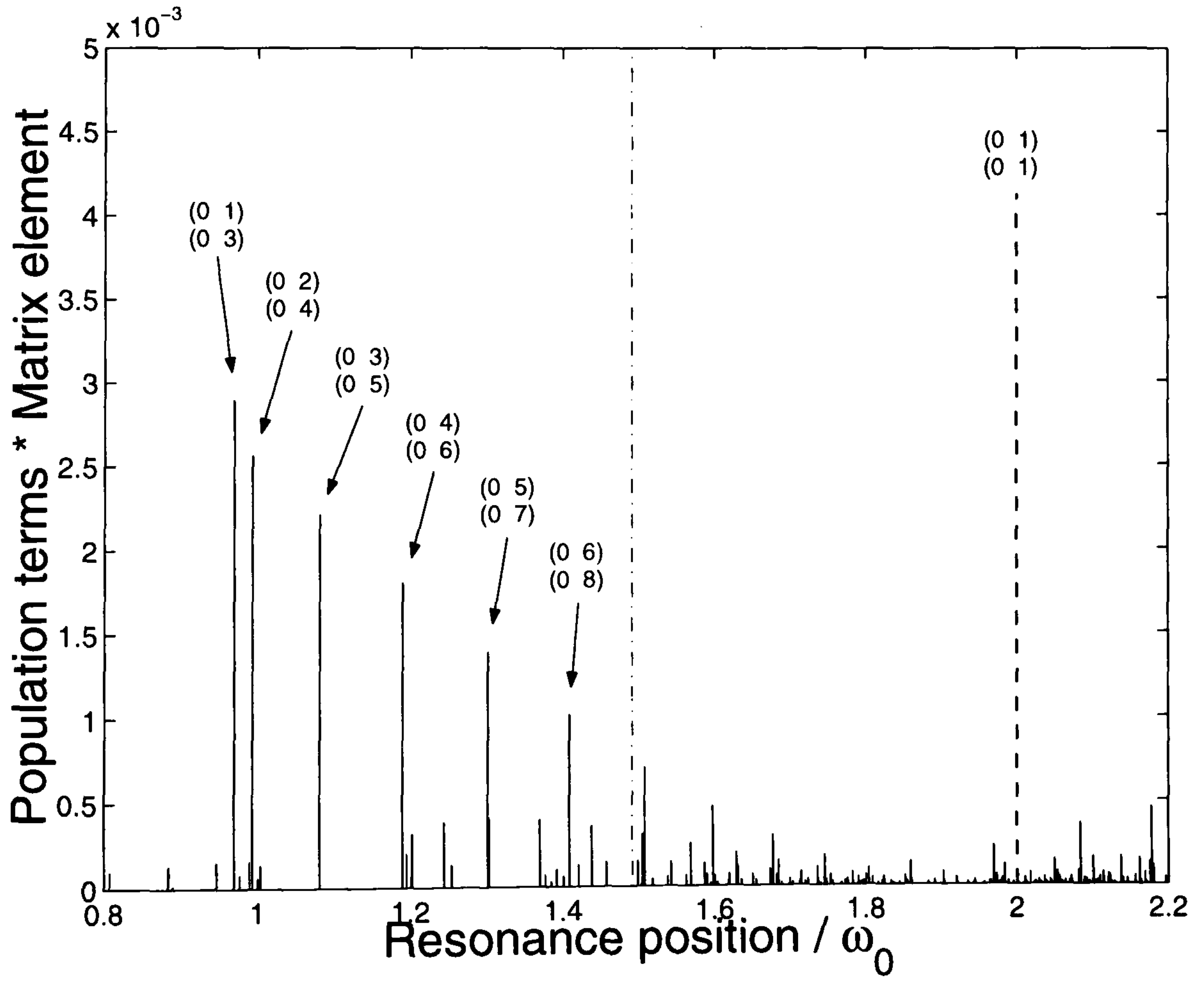

Figure 6.4: The denominators of $\Delta E_3(\omega)$ for (n=0,l=2) mode at a temperature of 0.8 T/T_C are plotted at the positions of their resonance, accorrding to equations (5.25-5.27). The dashed line is the Beliaev process (0,2)+(0,0)→(0,1)+(0,1). The solid lines represent Landau processes, the biggest of which are of the form (0,2)+(0,l)→(0,l+2)+(0,0). The dash-dotted line is of arbitrary height and marks the position of the quadratic theory ϵ_p for the quadrupole mode.

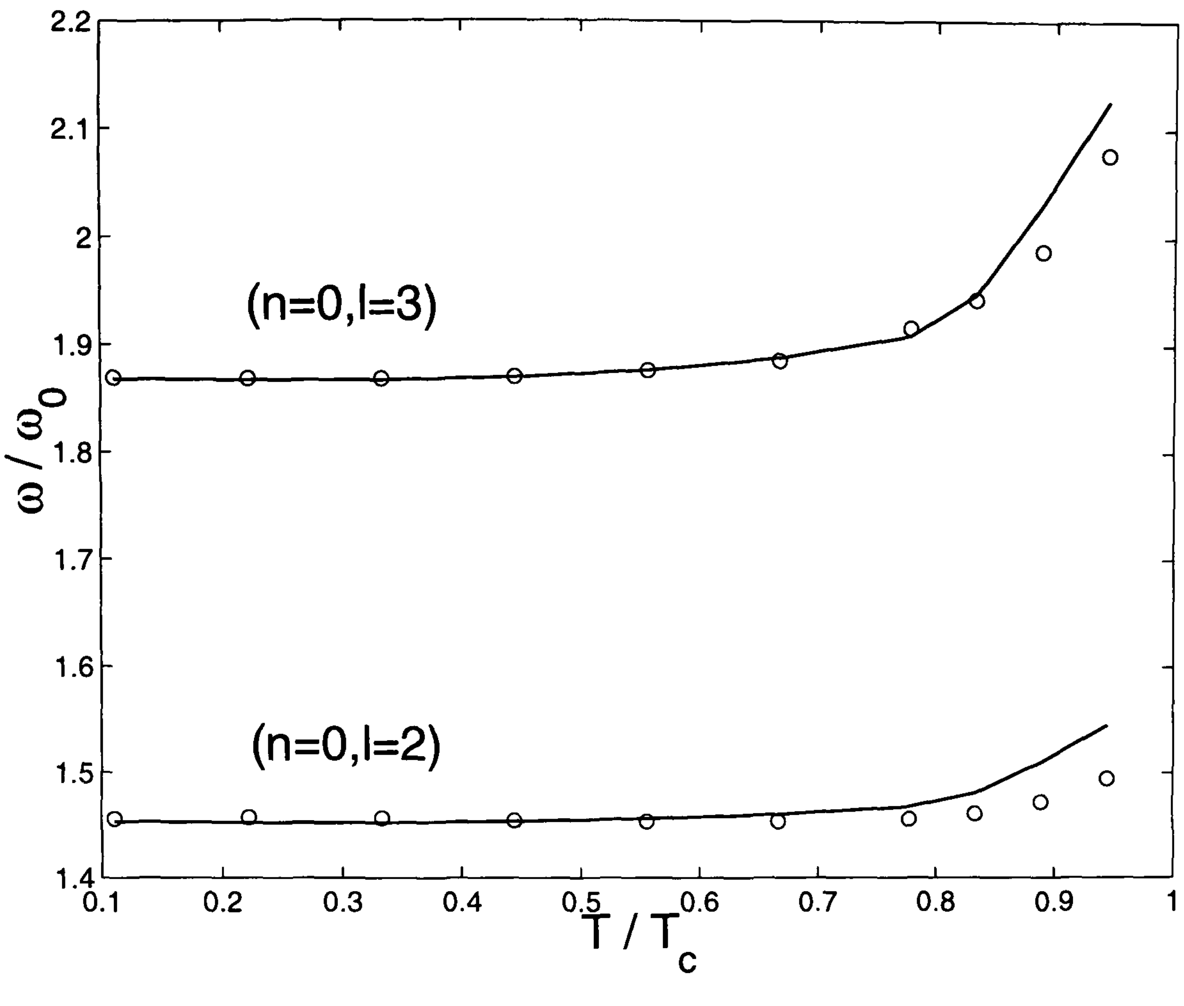

Figure 6.5: Maxima of Lorentzian fits to spectra of (n=0,l=2) and (n=0,l=3) modes. The corresponding HFB-Popov results are plotted as solid lines.

however, is of approximately Lorentzian shape. A Lorentzian lineshape in frequency corresponds to an exponential decay in time. By fitting a Lorentzian to the spectrum we can deduce an approximate mean energy from the position of the maximum. An approximate damping rate Γ is given by the width of Lorentzian fit to the spectra.

As can be seen from figure 6.2, the quality of a Lorentzian fit depends on the resolution. In the range of resolution relevant to experiments, $\gamma = 10^{-1}\omega_0$ to $10^{-2}\omega_0$, the position of the maximum is insensitive to the detailed value of γ. In figure 6.5 we plot the maxima of a least squares fit to the spectrum as a function of temperatures. At low temperatures the maxima of the fit follow the energy shifts of the HFB-Popov theory. At higher temperatures they lie below HFB-Popov by a few percent of the trap frequency. A similar trend was found in recent calculations of gapless HFB theories GHFB calculations, which improve on the HFB-Popov by including anomalous correlations [21].

From figure 6.2 it is obvious that the width of the Lorentzian fit will vary with

[21] D. W. Hutchinson, R. J. Dodd, and K. Burnett. *Gapless finite-t theory of collective modes of a trapped gas*. Phys. Rev. Lett. 81, 2198 (1998).

γ, since it represents the line width of the individual resonances. In figure 6.6 we plot the damping rate Γ of the quadrupole mode as a function of the resolution γ for various temperatures. The measured damping rate depends strongly on the value of the experimental resolution for resolutions of more than γ=$10^{-2}\omega_0$. In the limit of small γ, however, the Lorentzian envelopes of the sectra, and thus also the damping rates, are independent of the value of the resolution. In figure 6.7 we plot the Lorentzian width of the (n = 0, l = 2) spectrum a a function of temperature for various values of γ.

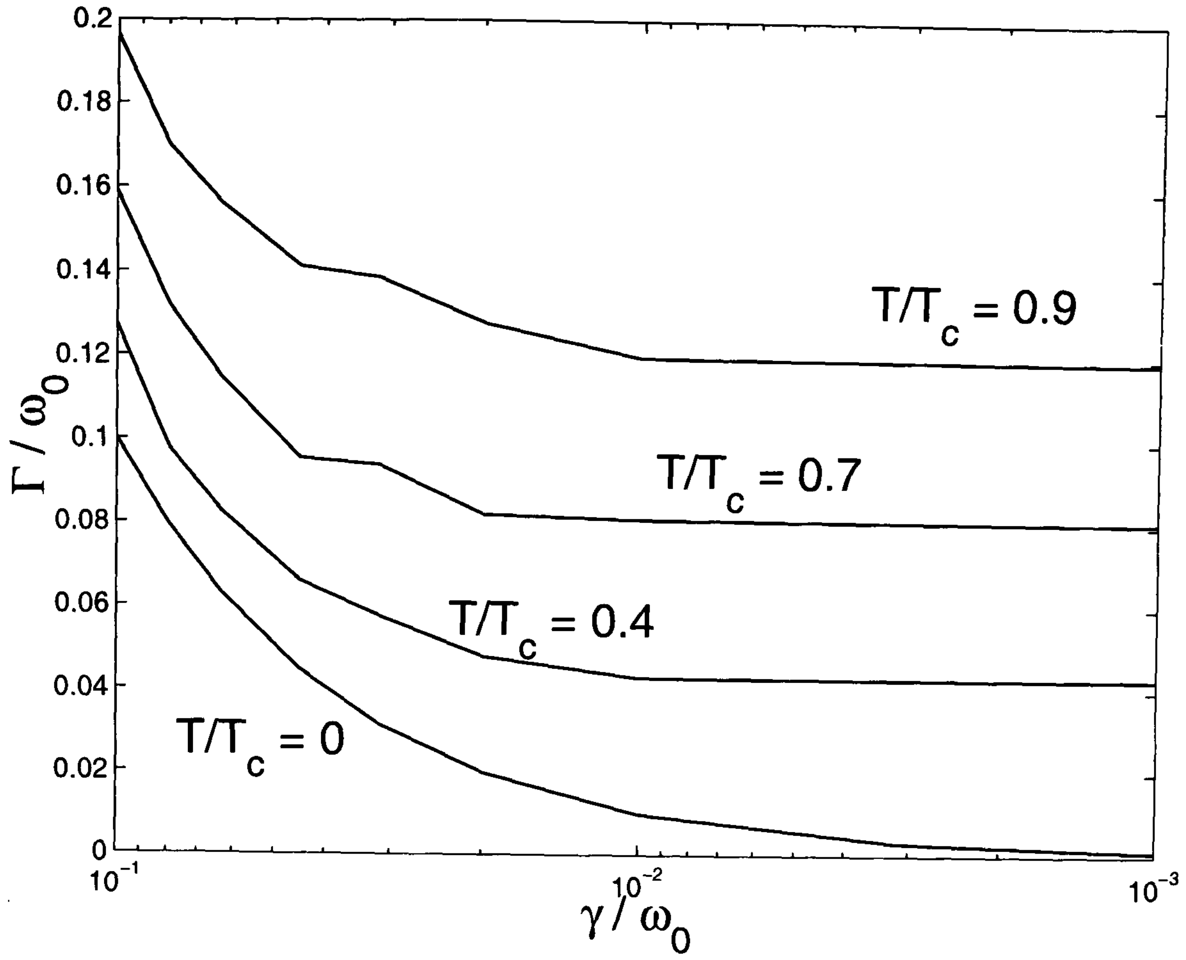

Figure 6.6: The damping rate Γ of the quadrupole as a function of the experimental resolution γ is plotted for a range of temperatures. For an experimental resolution of more than $\gamma = 10^{-2}\omega_0$ the measured damping rate will depend on the experimental resolution. In the limit of small γ, however, the damping rates are independent of the resolution.

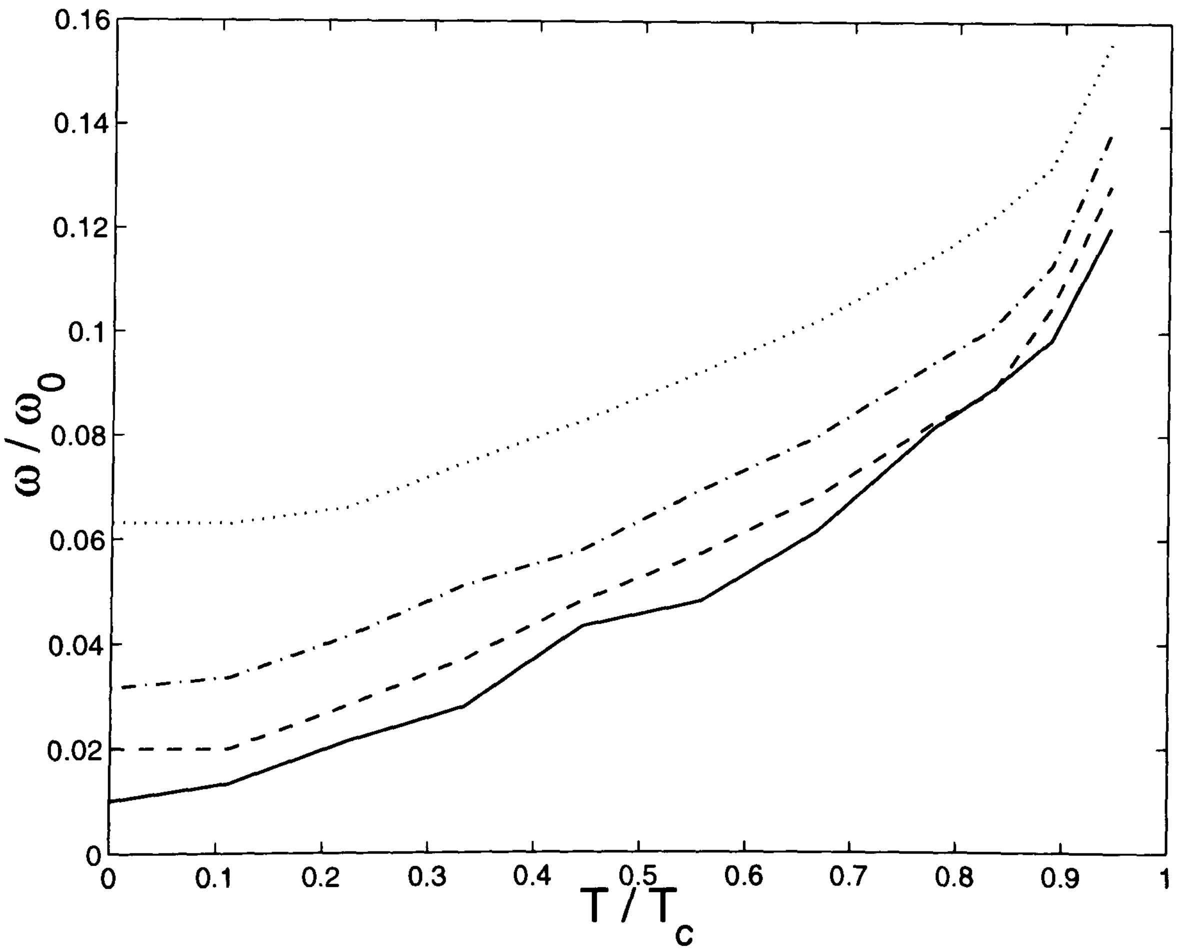

Figure 6.7: Damping rate Γ of the quadrupole mode, (n=0,l=2), as a function of temperature for different resolutions: $\gamma = 10^{-1.25}\omega_0$ (dotted line), $\gamma = 10^{-1.5}\omega_0$ (dashed line), $\gamma = 10^{-1.75}\omega_0$ (dot-dashed line), and $\gamma = 10^{-2}\omega_0$ (solid line).

6.3.2 The monopole or breathing mode ($n = 1$, $l = 0$)

For classical gases confined in spherically symmetric harmonic traps the breathing mode is not damped. This result was initally found by Boltzmann and has recently been re-examined by Guéry-Odelin *et al.* [79]. We shall briefly recall Guéry-Odelin's argument, since it highlights the role of the condensate in collision dynamics, resulting in the classically undamped breathing mode to obtain a finite lifetime. We consider the Boltzmann equation which describes the collisional dynamics of a classical gas

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}_1}{m}\nabla_r + \frac{\mathbf{F}}{m}\nabla_{p1}\right) f_1 = \left(\frac{\partial f_1}{\partial t}\right)_{coll}, \tag{6.1}$$

where $f_1(\mathbf{r}, \mathbf{p}_1, t)$ is the single phase-space distribution function and $\mathbf{F} = -\nabla V_{trap}$ is the force exerted by the harmonic confining potential. In the case of elastic collisions, the collision integral is given by

$$\left(\frac{\partial f_1}{\partial t}\right)_{coll} = \int d\Omega d\mathbf{p}_2 |v_2 - v_1| (d\sigma/d\Omega)[f_1' f_2' - f_1 f_2)]. \tag{6.2}$$

Here we have made the usual assumption of 'molecular chaos', which allows us to assume the colliding particles are uncorrelated so that we can write the two particle correlation function of the collision integral as a simple product of the single particle phase-space distribution functions, $F_{12}(\mathbf{r}, \mathbf{p}_1, \mathbf{p}_2, t) = f_1(\mathbf{r}, \mathbf{p}_1, t) . f_2(\mathbf{r}, \mathbf{p}_2, t)$ [80]. The breathing mode in a spherically symmetric harmonic trap corresponds to a periodic isotropic expansion and contraction of the total system. The time evolution of such an oscillation is given by the variation of the square radius

$$\frac{d}{dt}\langle \mathbf{r}^2 \rangle = 2\langle \mathbf{rv} \rangle, \tag{6.3}$$

which is completed by

$$\frac{d}{dt}\langle \mathbf{rv} \rangle = \langle \mathbf{v}^2 \rangle - \omega_0^2 \langle \mathbf{r}^2 \rangle, \quad \frac{d}{dt}\langle \mathbf{v}^2 \rangle = \omega_0^2 \langle \mathbf{r}^2 \rangle, \tag{6.4}$$

[79] D. Guéry-Odelin, F. Zambelli, J. Dalibard, and S. Stringari. *Collective oscillations of a classical gas confined in harmonic traps*. Phys. Rev. A 60, 4851 (1999).

[80] K. Huang. Statistical Mechanics, 2nd ed. (Wiley, New York, 1987).

to give a closed set of equations. The average of a general quantity $\chi(\mathbf{r},\mathbf{p})$ is given by

$$\langle\chi\rangle = \frac{1}{N}\int d\mathbf{r}d\mathbf{p}f(\mathbf{r},\mathbf{p},t)\chi(\mathbf{r},\mathbf{p}). \tag{6.5}$$

The dynamics of the average of χ are then governed by the Boltzmann equation and effect of collisions is given by the term $\langle\chi(\partial f/\partial t)_{coll}\rangle$. During collisions the total energy and momentum remain unchanged and therefore the collisional term is equal to zero if

$$\chi(\mathbf{r},\mathbf{p}) = a(\mathbf{r}) + b(\mathbf{r})\mathbf{p} + c(\mathbf{r})\mathbf{p}^2, \tag{6.6}$$

where a($\mathbf{r}$), b($\mathbf{r}$), and c($\mathbf{r}$) can be arbitrary position dependent scalars. The equations for the square radius are of the above form and thus the collision term for the square radius is zero. Conservation of energy and momentum ensure that the breathing mode of a classical gas in spherical harmonic trap is not damped. The classical Boltzmann equation only accounts for spontaneous scattering, but does not contain Bose-enhancement factors, representing the stimulated scattering into already occupied states. If the collision term of the classical Boltzmann equation is suitably modified to include the effect of Bose statistics, above result again holds.

For Bose-condensed systems, however, the result no longer is valid. Below the transition temperature mean field effects dominate the dynamics of the breathing mode and the central assumption of the Boltzmann equation that colliding particles are not correlated no longer is valid. Interactions between the collective excitation and the thermal cloud will ensure that the monopole mode is damped. Even at zero temperatures the mode is damped by Beliaev processes, even though this effect is rather small. Second order calculations of the frequency response of the breathing mode again display resonance structure in both $\Delta E_3(z)$ and the frequency response spectrum $F(\omega)$. This is in agreement with a recent study by Guilleumas and Pitaevskii [81]. They calculate the matrix elements of allowed Landau transitions involving the breathing mode and the thermal cloud, the equivalent of ΔE_3, and find similar structure as in figure 6.8. In their ensuing analysis, however, Guilleumas and Pitaevskii differentiate between strongly coupled transitions, which they term 'temperature induced' resonances, and the numerous weaker transitions, which form an almost unresolvable background. For their discussion of lifetimes they only consider the effect of background resonances and thus deal with

[81] M. Guilleumas and L. P. Pitaevskii. *Temperature-induced resonances and Landau damping of collective modes in Bose-Einstein condensed gases in spherical traps*. Phys. Rev. A 61, 013602 (1999).

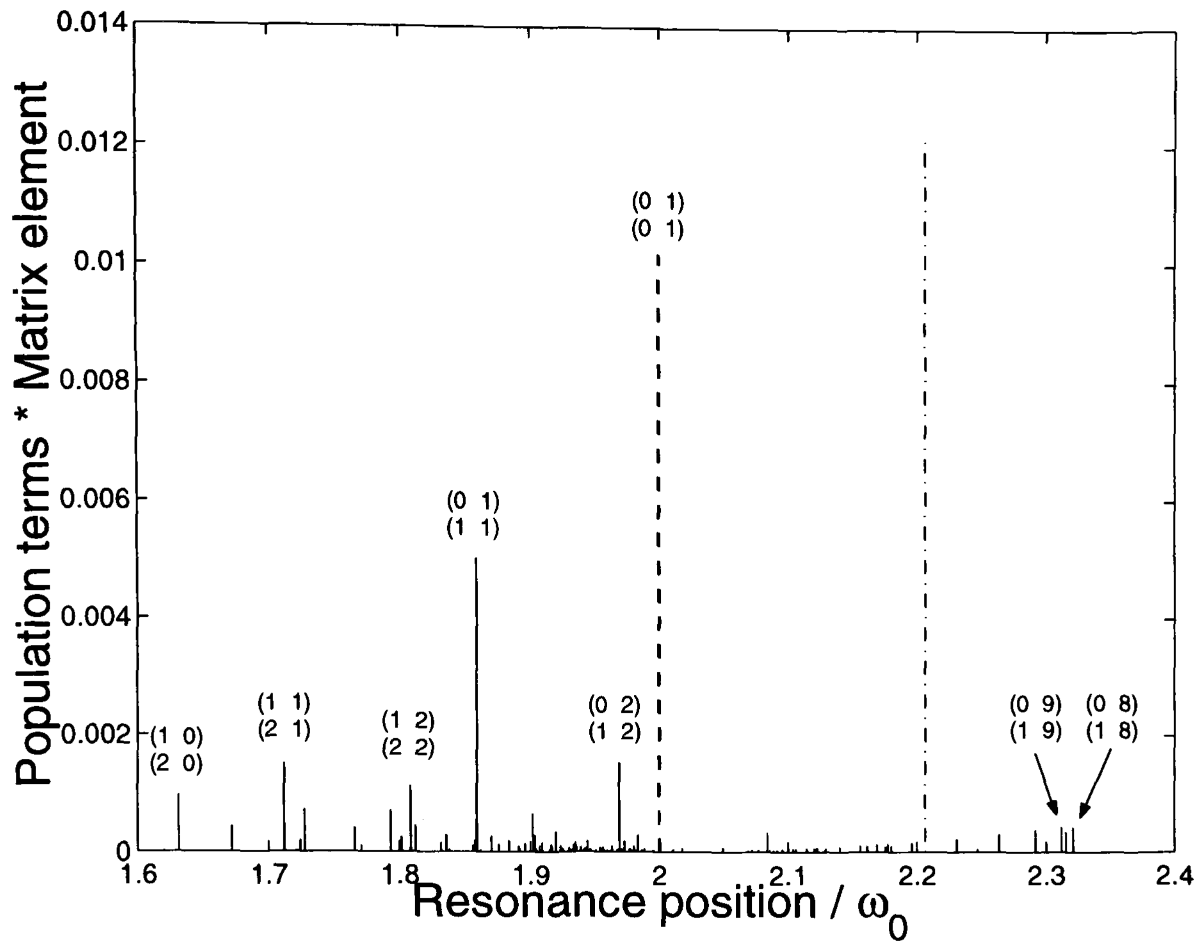

Figure 6.8: Resonance structure of $\Delta E_3(\omega)$ of the monopole mode. Plotted are the denominators of $\Delta E_3(\omega)$ at the positions of their resonance for 0.8 T/T_C. The dashed line is the Beliaev process (1,0)+(0,0)→(0,1)+(0,1). The solid lines represent Landau processes, the biggest of which are of the form (1,0)+(n,l)→(n+1,l)+(0,0). The dash-dotted line is of arbitrary hight and marks the position of the quadratic theory ϵ_p for the quadrupole mode.

the time evolution of the excitation as a decay into a quasi-continuum. The more pronounced 'temperature induced' resonances they treat as separate forms of the system's response to an external perturbation, distinct from the breathing mode itself.

Our treatment of the breathing mode differs in three areas. To begin with, we not only consider Landau processes but also consider Beliaev-type coupling of the mean field to thermally populated excitations. We therefore include the Beliaev process which describes the splitting of the breathing mode into two dipole oscillations, occurring at a frequency of $2\omega_0$. Secondly, we include the first order energy shifts ΔE_μ, ΔE_4, and ΔE_{shape}, as given in equations (5.14-5.16). The positions of the resonances consequently are different relative to those of Guilleumas and Pitaevskii. Finally, in our interpretation of the spectra we do not distinguish between the breathing mode and 'temperature induced' resonances involving the breathing mode as separate entities. Instead we calculate the frequency response of the mean field to an external perturbation of certain geometry. We find the mean

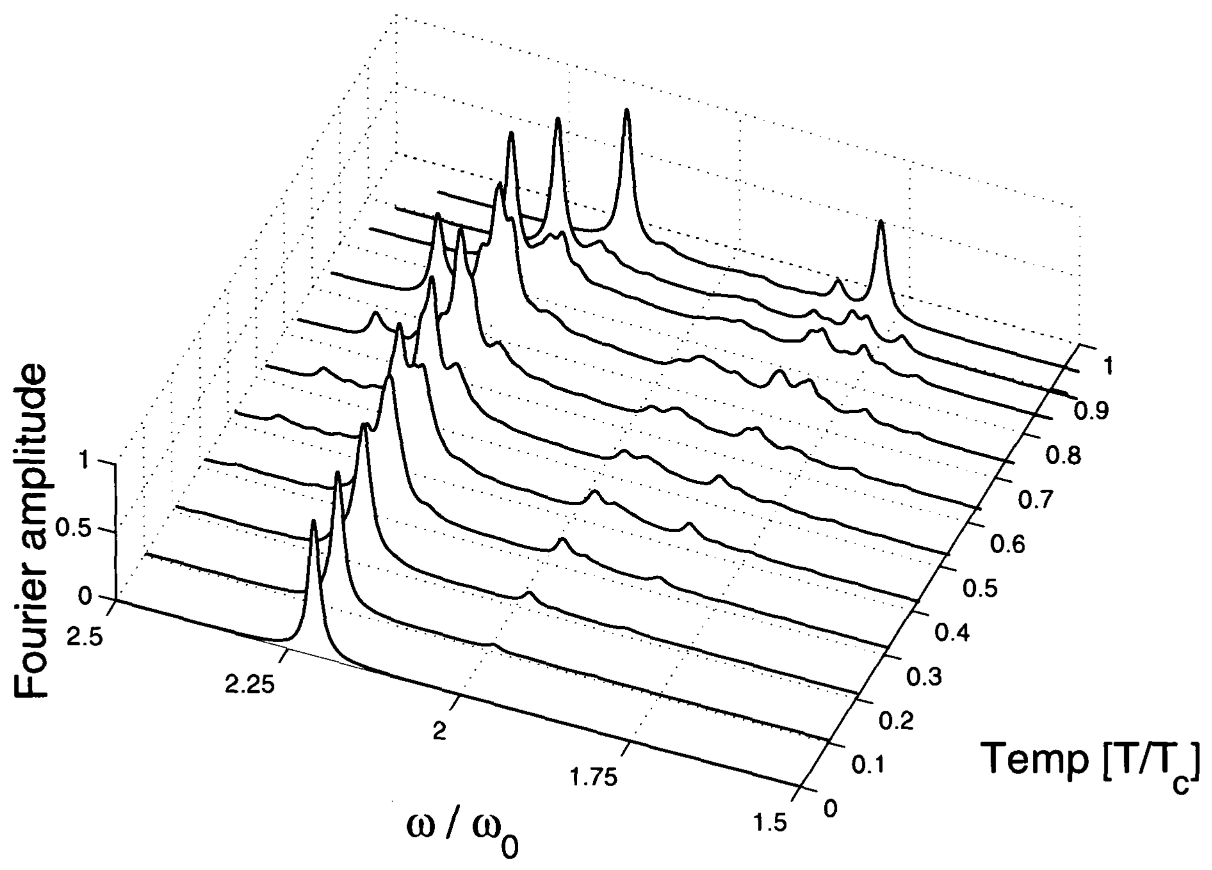

Figure 6.9: The frequency response spectrum $F(\omega)$ of the breathing mode as a function of temperature for a resolution of $\gamma = 10^{-2}\omega_0$.

field responds with a monopolar oscillation not only at the monopole frequency itself, but also whenever the monopole oscillation of the mean field can resonantly excite transitions in the thermal cloud. Since the time evolution of such a monopole oscillation is the Fourier transform of its frequency response we proceed as in the previous section and include the strong resonances in the discussion of the time evolution of the mode.

Unlike the quadrupole mode, the monopole or breathing mode (n=1,l=0) develops resonance structures in two distinct regions, as can be seen in figure 6.9. The main resonance is at $2.216\omega_0$ and shifts upwards with rise in temperature. The dominant Landau processes are (1,0)+(n,l)→(n-1,l)+(0,0), with l=1,2 and give resonances in ΔE_3 in the region around $1.8\omega_0$. The only significant Beliaev process is (1,0)+(0,0)→(0,1)+(0,1), which occurs at $2\omega_0$. The spectra of the monopole and quadrupole excitations are qualitatively so different because the modes differ in two of their properties: For the monopole mode, $(n = 1, l = 0)$, the selection rule $\Delta l = 0$ means that in comparison to the quadrupole mode the number of possible transitions over all is reduced. Individual resonances therefore can have more of an impact on the over-all shape of the spectrum. The second and perhaps more crucial difference is that the monopole mode has far fewer strong transitions in the vicinity of its quadratic quasiparticle energy than the quadrupole mode (compare figures 6.4 and 6.8). When at high temperatures the populations terms add sufficient weight to the transitions of the region of 1.8 to $2\omega_0$, they are unrivalled by any competing processes and can pull the spectrum apart into two distinct structures. Using a Lorentzian fit to assign an approximate energy and a width to the spectrum of figure 6.9 clearly is of little use. Instead we plot the maximum of $F_p(\omega)$, which is the feature experiments are most likely to track as a function of temperature. The detailed structure of the spectrum should be well resolvable in suitable experiments.

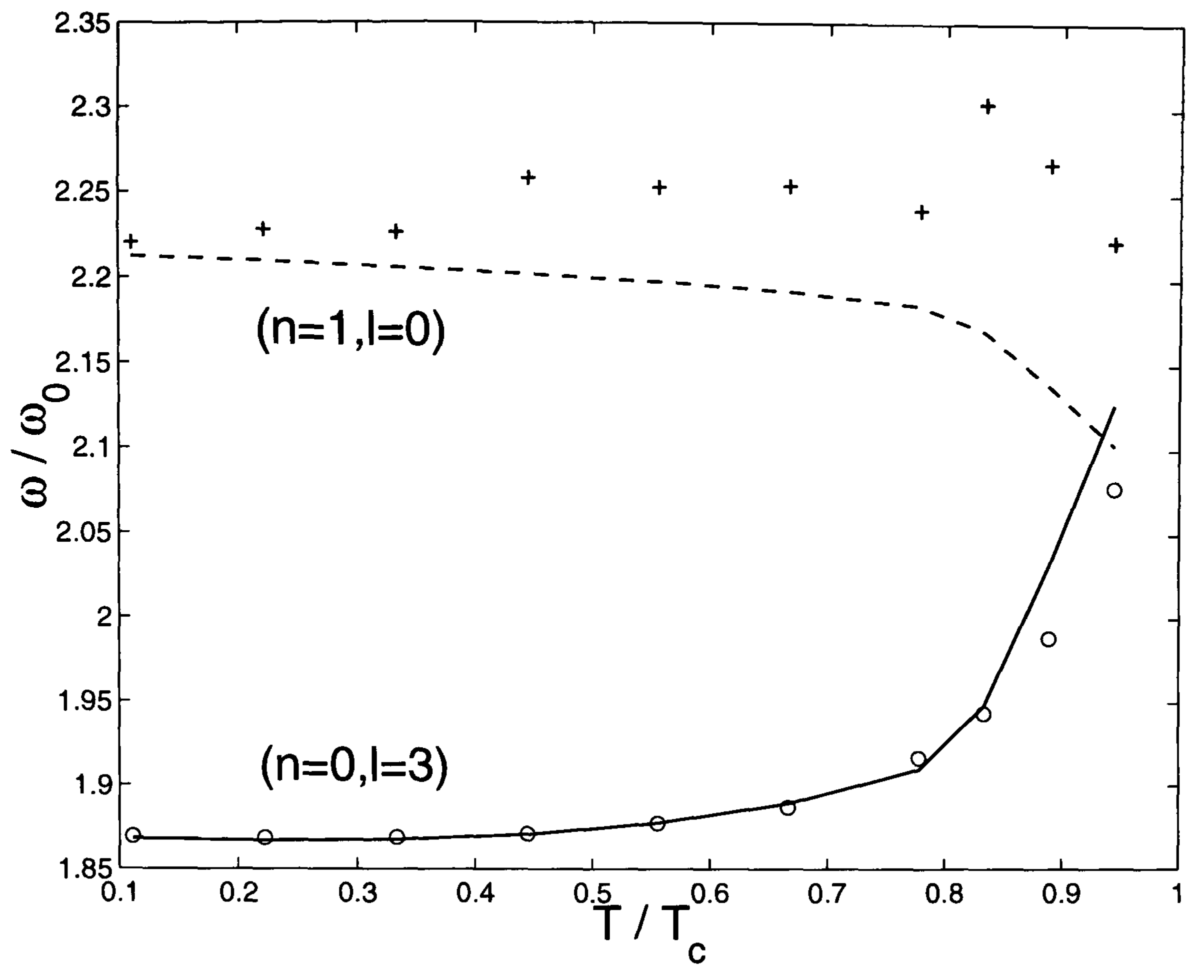

Figure 6.10: Maximum of the spectrum of ($n = 1$,$l = 0$) mode (+) as a function of temperature. The corresponding HFB-Popov energy is give as dashed line. The maximum of Lorentzian fit to the spectrum of (n=0,l=3) mode is given by (o) and its HFB-Popov energy by the solid line. We note that selection rules prohibit that the l=0 and l=3 modes couple to each other. We thus are not observing some form of avoided line crossing.

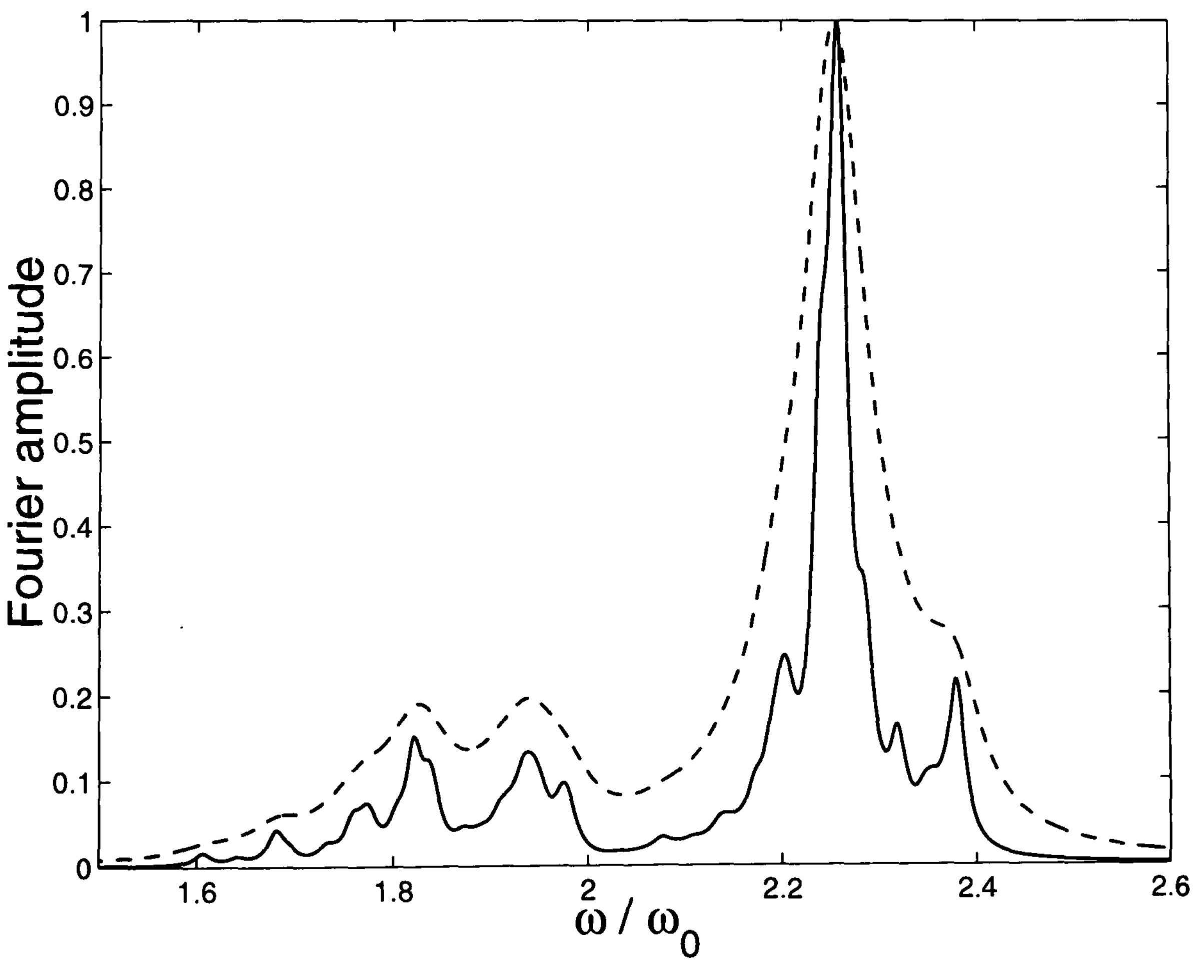

Figure 6.11: The frequency response spectrum $F(\omega + i\gamma)$ of the monopole mode at the temperature of 0.7 T/T_C. The solid line is for a resolution of $\gamma = 10^{-2}$. The dashed line is for a resolution of $\gamma = 10^{-1.5}$. The non-Lorentzian structure of the spectrum should be clearly resolvable in experiments.

6.3.3 The dipole mode ($n = 0$, $l = 1$)

For a classical gas confined in a harmonic trap the dipole oscillation of the centre-of-mass is not damped. This can be seen directly from the Hamiltonian of the system,

$$H = \sum_i^N \left(\frac{1}{2m}\mathbf{p}_i^2 + \frac{m\omega_0^2}{2}\mathbf{r}_i \right) + \sum_{i<j}^N V(\mathbf{r}_i - \mathbf{r}_j). \tag{6.7}$$

The centre-of-mass position is given by $\mathbf{R} = (1/N)\sum_j \mathbf{r}_j$ and the total mass by $M = Nm$. The equations for the evolution of the centre-of-mass position and momentum,

$$\dot{\mathbf{R}} = \mathbf{P}/M \quad \dot{\mathbf{P}} = \sum_i \frac{\partial H}{\partial \mathbf{r}_i} = -M\omega_0^2\mathbf{R}, \tag{6.8}$$

do not depend on the interatomic interaction and the mode therefore is not damped. The centre-of-mass degrees of freedom separate from all other degrees of freedom, giving rise to a collective mode of the system, in which the equilibrium density profile oscillates rigidly back and forth at multiples of the trap frequency ω_0. This simple result holds for any many-body system with momentum-conserving interactions, confined in an isotropic harmonic trap. Any approximate theory put forward to describe a many-body system should, in principle, reproduce the dipole excitation as a centre-of-mass oscillation at the trap frequency [82]. This fact is often referred to as the generalised Kohn theorem and the centre-of-mass oscillation thus is also called the Kohn mode.

In section 3.3 we explained how HFB-Popov treats the effect of the thermal cloud as a change to the static external potential. The effective potential no longer is harmonic and thus the generalised Kohn theorem does not apply for HFB-Popov excitations. In general, the deviation from the harmonic potential is small in the centre of the trap and HFB-Popov gives the frequency of the dipole mode to within one percent of the Kohn mode frequency of ω_0. For sufficiently large systems, however, the two can differ by up to 10 %.

The dipole mode of our second order calculation is not the Kohn mode. What we calculate is the dipolar response of the mean field to an external perturbation. If we neglected any affect of the thermal cloud this then would be equivalent to the centre-of-mass oscillation of the system and we would obtain the excitation frequency of exactly ω_0. Our second order calculation of the mean field response

[82] J. F. Dobson. *Harmonic-potential theorem: implications for approximate many-body theories*. Phys. Rev. Lett. 73, 2244 (1994).

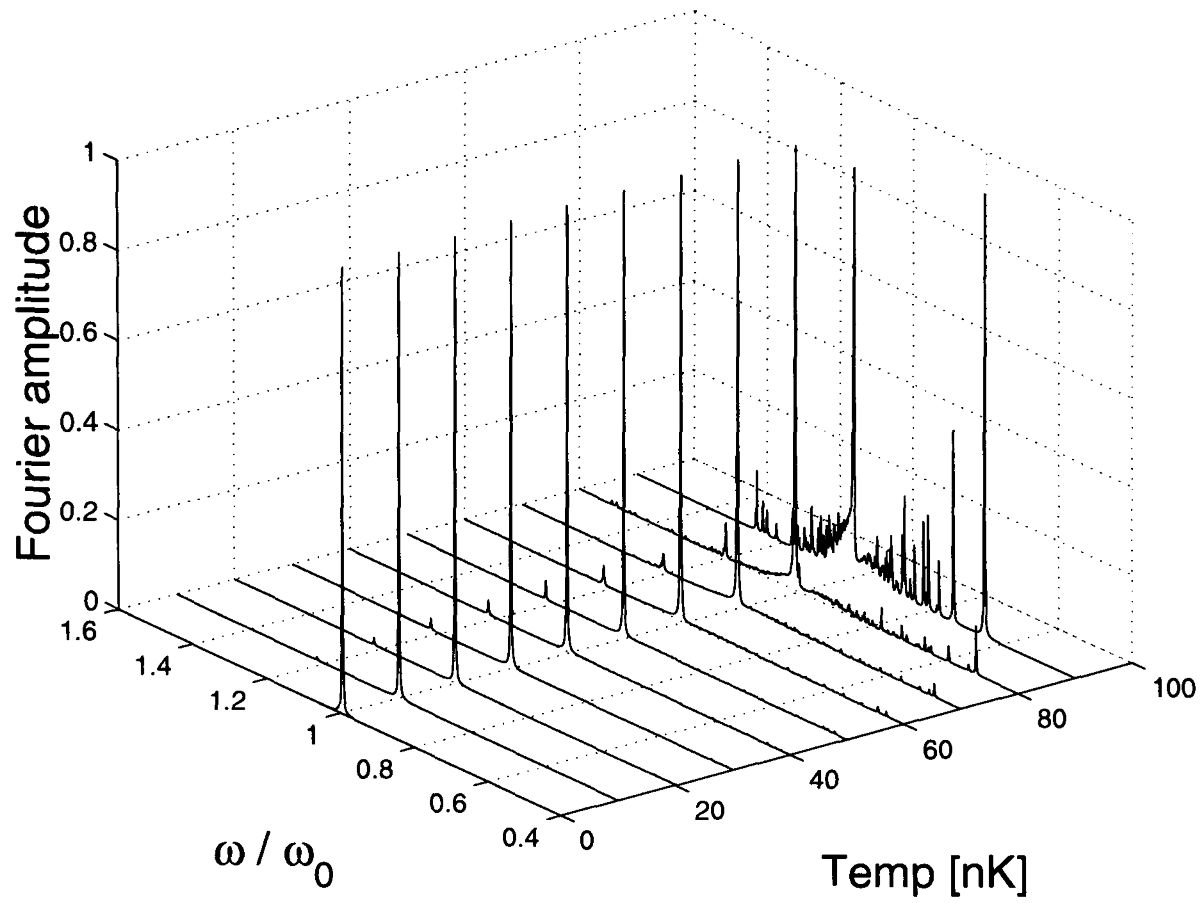

Figure 6.12: The frequency response spectrum $F(\omega)$ of the dipole mode as a function of temperature.

does include the dynamical aspects of the thermal cloud, but only those driven through the mean field itself. We thus deal with a scenario where we start with the condensate sitting in its thermal cloud, excite only the condensate, and then observe how the condensate drives the thermal cloud, which in turn acts back onto the condensate and therefore gives rise to energy shifts and damping of the dipole excitation of the mean field. The dipole mode therefore does couple to other excitations and forms the two final states of the Beliaev decay of the breathing mode.

A linear response analysis of the total system, including the response of the condensed and non-condensed part of the system, should include the Kohn mode as a rigid in-phase centre-of-mass oscillation of the condensate and the thermal cloud.

CHAPTER 7

CONCLUDING REMARKS

7.1 Validity of mean-field theory at finite temperatures

In the course of this thesis we first introduced the concept of the mean-field in the context of condensed systems at zero temperature, at which fluctuations around the mean-field were negligible. We further argued that the mean-field remains valid in the presence of fluctuations, provided they were small enough to be dealt with perturbatively. We then proceed to use the mean-field to calculate the collective excitations of the condensed system for a wide range of temperatures, right up to the transition temperature. This raises the question whether the mean-field picture indeed remains valid at such high temperatures and, if it does so, why.

Our finite temperature treatment of excitations was based on the normal modes of the mean-field, i.e. quasiparticles, given by the zero temperature GPE for a number of condensate particles corresponding to the finite temperature ground state occupation. The effects of the thermal cloud and the further interactions between the quasiparticles we then dealt with using perturbation theory in this quasiparticle basis. Our mean-field theory for excitations therefore fails, when a perturbation expansion in terms of the normal modes of the mean-field becomes ill-defined. This is the case if the perturbative energy shifts and widths become comparable to the spacing of the quasiparticles themselves.

For homogeneous systems a simple estimate for the temperature when shifts become large in comparison to the quadratic energies can be found, when considering the ratio between first and second order terms in the T-matrix expansion of the effective interaction in the same manner as Popov [83]. The leading order term represents the collision of two quasiparticles, whereas the higher order term describes the effect of temperature dependent many-body effects on such a collision. Only if the second order term is small in comparison to the first order one, does mean-field theory give a valid description of finite temperature excitations. Within the V^2 treatment of chapter 4 it is straightforward to derive a the ratio between the second order and first order term of the T-matrix (e.g. equation (4.52)),

$$\frac{2^{nd}}{1^{st}} \simeq \frac{kT}{n_0 U_0}(n_0 a^3)^{1/2}. \tag{7.1}$$

This is equivalent to the validity criterion for second order theories at finite temperatures. At zero temperatures the ratio reduces to $(n_0 a^3)^{1/2}$ which is much smaller than one for the dilute gases of recent experiments as the separation of atoms is much greater than their effective size. The temperature dependence, $kT/(n_0 U_0)$, arises from the thermal population of intermediate states in the collisions of low-energy particles and at sufficiently high temperatures, mean field theories eventually will fail in homogeneous systems.

Above criterion incidentally coincides with the Ginzburg criterion of the theory of critical phenomena. Equation (7.1) scales as one over the square root of the ground state population, $\propto (n_0)^{-(1/2)}$, which near the critical temperature is approximately $n_0 \sim nt$, where $t = (T_C - T)/T_C$. The Ginzburg criterion defines the region near the critical temperature

$$[xt]^{(d-4)/2} \ll 1, \tag{7.2}$$

where where long wavelength fluctuations of the order parameter signal a break down of mean-field theory. d is dimension of the system and x is some positive constant characteristic of it. The Ginzburg criterion states that for dimensions, $d > 4$, mean-field theory remains valid right up to the critical point, beyond which the concept of the mean-field or order parameter becomes meaningless anyway [80]. We discussed earlier that one property of a system critical for the onset of BEC was the density of states. The density of states generally is a function of the dimension and for homogeneous systems goes as $f(\epsilon)d\epsilon \propto \epsilon^{(d-2)/2}d\epsilon$. In this respect the trapped condensates are effectively higher-dimensional. For a 3-d harmonically

[83] N. Popov. Functional integrals and collective excitations (CUP, 1987).

[80] K. Huang. Statistical Mechanics, 2nd ed. (Wiley, New York, 1987).

confined system we obtain $f(\epsilon)d\epsilon \propto \epsilon^2 d\epsilon$, which is equivalent to a six-dimensional homogeneous system. For trapped systems we therefore can expect mean-field theory to remain valid up to the critical temperature.

This is confirmed when considering the ratio of leading and higher order terms in the effective interactions for trapped systems. It becomes

$$\frac{2^{nd}}{1^{st}} \simeq \frac{k_B T}{\hbar\omega_0} \frac{a}{l_{trap}}, \tag{7.3}$$

with l_{trap} as the size of the trap and ω_0 the level spacing. Provided that $a/l_{trap} \ll 1$, mean-field theories for trapped systems will remain valid right up to the transition temperature. This is certainly the case for condensates in dilute atomic vapours.

7.2 Mean-field vs. density response at finite temperatures

In chapter 3 we discussed the difference between elementary excitations and collective excitations (density fluctuations) and showed that the two are identical for a condensed system at zero temperature. The finite temperature treatments of chapters 4, 5, and 6, however, did not deal with either of the two, but instead were concerned with excitations of the time-dependent mean-field. This begs the question of what the relation between collective an elementary excitations for trapped systems at finite temperatures is. Further, one may ask how mean-field fluctuations relate to the two, the density response in particular.

A detailed discussion of the first question is beyond the scope of this thesis. The relation between collective and elementary excitations at finite temperatures has been studied in detail for homogeneous system [84]. To which extent the two agree naturally depends on the level of approximation used for their description. Cheung and Griffin show, that for repulsive interactions and arbitrary values of temperature and wavelength, the single particle Green's function in the second order (Beliaev) approximation has the same poles than the density fluctuation spectrum in the Hartree-Fock approximation [85]. The 'dielectric' formulation of the

[84] A. Griffin. *Theories of excitations of the condensate and non-condensate at finite temperatures.* In Proceedings of the International School of Physics - Enrico Fermi (edited by M. Inguscio, S. Stringari, and C. E. Wieman), p. 1 (IOS Press, 1999).

[85] T. H. Cheung and A. Griffin. *Density fluctuations in an interacting Bose gas.* Phys. Rev.

field-theoretical Green's function formalism features the coincidence of poles of the Green's functions for collective and single-particle excitations as one of the central characteristics of Bose condensed systems [86, 70]. This thesis argues that excitations in trapped systems do not have one single frequency as their homogeneous counterparts, but instead display a more complicated resonance structure in their spectra. Whether or not this affects the hybridisation of elementary and collective excitations, known from homogeneous systems, requires further investigation.

In order to compare the calculations of chapter 6 to actual experiments it is important to explain how the response of the mean field relates to the density response of the system. In experiments collective excitations are usually imparted onto the system by perturbations of the confining potential. Any such perturbation will not only couple to the condensate but will also independently excite the thermal cloud. As pointed out in the derivation of the second order theory of time dependent mean fields of section 5.3 and the discussion of the dipole mode of section 6.3.3, our treatment only considers the effect the external perturbation has on the mean-field. We calculate the response of the mean-field and as such we include how the driven mean-field couples to the themal cloud how the thermal cloud in turn then acts back on the mean-field itself. It is the coupling of the excited mean-field to the thermal cloud which gives rise to temperature dependent coupling to different decay channels. However, we do not include the direct coupling of the external driver to the thermal cloud itself. The response of the mean field therefore is generally not the same as the over-all density response of the system.

The much higher density of the condensate should mean that a perturbation of the trap potential couples predominantly to the condensate. However, one cannot in principle rule out that the perturbation also drives transitions within the thermal component, independent of the condensate. If these processes were of comperable size to the condensate's response they certainly would effect the system's over-all dynamics. Clarification of this issue requires further investigation.

A 4, 237 (1971).

[86] P. Szépfalusy and I. Kondor. *On the dynamics of continuous phase transitions.* Ann. Phys. 82, 1 (1974).

[70] S. H. Payne and A. Griffin. *Goldstone phonons in a Bose-condensed gas at finite temperature: One-loop approximation.* Phys. Rev. B 32, 7199 (1985).

7.3 Spherically symmetric vs. anisotropic Condensates

In chapter 6 we performed calculations for spherically symmetric harmonic traps and showed that measurements of low-lying excitations in these systems should exhibit detailed features in their frequency spectra, which have not been observed previously. With the spectral resolution of previous experiments these should be observable in the breathing mode of the spherical condensate. Experiments in spherical traps have become feasible only recently [78, 87] and we hope the results of this thesis will encourage the study of their finite temperature excitations. Our formalism is by no means limited to spherical systems. It can, in principle, be applied to anisotropic trap geometries as well. The calculations, however, will be computationally more involved.

A significant difference between isotropic and anisotropic trap configurations is the effect they have on the distribution of energy levels. The symmetry of the spherical trap results in a degeneracy in the azimuthal quantum number m, which in turn means that fewer sums and differences of energies match the energy of an excitation. Excitations thus can couple strongly to only relatively few states and the resulting spectra show this in form of distinct features. The good quantum numbers of the anisotropic systems become parity π and the azimuthal quantum number m. The degeneracy in m is lifted and more energy matches are possible. Further, the energies themselves are more evenly distributed [88]. Fedichev *et al.* argue that these two circumstances justify to use an approximation to the density of states and treat the lifetime of the excitation as a decay into a continuum [22]. Our analysis of spherically symmetric systems suggests that such a procedure should in general be valid in anisotropic systems. Even in spherical systems the time evolution of many excitations resembles an exponential decay. In anisotropic systems this then is even more likely to be the case. However, one cannot rule out that a few specific modes may differ in their behaviour even in anisotropic systems.

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[78] O. Maragò and C. J. Foot. (private communication) .

[87] E. A. Cornell. (private communication) .

[88] D. W. Hutchinson and E. Zaremba. *Excitations of a Bose-condensed gas in anisotropic traps.* Phys. Rev. A 57, 1280 (1998).

[22] P. O. Fedichev, G. V. Shlyapnikov, and J. T. M. Walraven. *Damping of low-energy excitations of a trapped Bose-Einstein condensate at finite temperatures.* Phys. Rev. Lett. 80, 2269 (1998).

The only experimental data presently available on finite temperature excitations has been measured for a system of a few thousand ^{87}Rb atoms in an anisotropic axially symmetric harmonic trap of radial frequencies $\omega_{rad} = 129$ Hz and $\omega_{axial} = 365$ Hz [5]. The observed temperature dependence of the frequency shift of the lower-lying $(\pi = +1, m = 2)$ mode has been succesfully predicted by finite temperature theories [21, 23]. The $(\pi = +1, m = 0)$ mode, however, has so far eluded any theoretical description. At temperatures of around 0.6 T_C it was measured to shift upwards almost discontinuously relative to the HFB-Popov prediction. All theories, which sucessfully describe the $(\pi = +1, m = 2)$ mode, fail to reproduce this behaviour, but predict the mode to shift downwards instead.

In section 6.3.2 we discussed that the monopole mode of the spherical system, (n=1,l=0,m=0), has a non-Lorentzian spectrum, the maximum of which moves upwards, relative to the HFB-Popov energy. This behaviour is very similar to the trend observed for the $(\pi = +1, m = 0)$ mode of the anisotropic system of the JILA experiment. One may conjecture that the $m = 0$ mode also comprises a more complicated spectrum, only one feature of which was tracked by the experiment. In our view this the most likely explanation for the anomalous behaviour of the $m = 0$ mode of the JILA experiment. Whether or not the spectra of certain excitations in anisotropic traps display a detailed resonance structure, the $m = 0$ mode in particular, however, remains subject of future work.

[5] D. S. Jin, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell. *Temperature-dependent damping and frequency shifts in collective excitations of a dilute Bose-Einstein condensate.* Phys. Rev. Lett. 78, 764 (1997).

[21] D. W. Hutchinson, R. J. Dodd, and K. Burnett. *Gapless finite-t theory of collective modes of a trapped gas.* Phys. Rev. Lett. 81, 2198 (1998).

[23] J. Reidl, A. Csordás, R. Graham, and P. Szépfalusy. *Shifts and widths of collective excitations in trapped Bose gases by the dielectric effect.* Phys. Rev. A 61, 043606 (2000).

Appendix A

Computational procedure

In the following we outline the computational procedure we use to calculate the finite temperature frequency response of the mean field,

$$F_p(\omega) \propto \frac{1}{\hbar(\omega+i\gamma)-\hbar\omega_p-[\Delta E_4(p)+\Delta E_\lambda(p)+\Delta E_{shape}(p)+\Delta E_3(p,\omega)]}. \tag{A.1}$$

A.1 Quadratic theory

As a first step we calculate the condensate and quasiparticle energies and wavefunctions of the quadratic Bogoliubov theory for an appropriate value of the condensate population N_0. Without loss of generality we can assume the wavefunctions to be real. The condensate ground state and energy is given by the GPE

$$\left[H_{sp}(\mathbf{r})+N_0U_0|\Phi_0(\mathbf{r})|^2\right]\Phi(\mathbf{r})=\mu\Phi_0(\mathbf{r}). \tag{A.2}$$

In spherically symmetric harmonic traps the Hamiltonian is separable and the wave functions take the form $\phi_i(\mathbf{r})=\phi_i(r)Y_{l_i}^{m_i}(\Omega)$, where $Y_{l_i}^{m_i}(\Omega)$ is a spherical harmonic and $\phi_i(r)$ is the solution of the radial equation of the respective wavefunction. Various methods of numerically calculating the ground state of the GPE are known, such as an evolution in imaginary time [89], or a Crank-Nicholson method [90]. For

[89] S. Choi, S. A. Morgan, and K. Burnett. *Phenomenological damping in trapped atomic Bose-Einstein condensates*. Phys. Rev. A 57, 4057 (1998).

[90] P. A. Ruprecht, M. J. Holland, K. Burnett, and M. Edwards. *Time-dependent solution of the nonlinear Schrödinger equation for Bose-condensed trapped neutral atoms*. Phys. Rev.

the calculations of this thesis we employed a shooting method, the general principles of which have been outlined by Edwards and Burnett [34].

For a given temperature T we can calculate the population of quasiparticle levels using the Bose distribution function,

$$n_i = [z^{-1} e^{\epsilon_i / k_B T} - 1]^{-1}. \tag{A.3}$$

The fugacity generally is defined as $z = e^{\mu' / k_B T}$, with μ' as the chemical potential. Our quasiparticle energies are measured relative to the condensate eigenvalue μ so we only have to include the difference between the the two, which is scales as $1/N_0$. In our units z differs from unity only for for very small ground state populations.

The quantities $\rho(\mathbf{r})$ and $\kappa(\mathbf{r})$ we then construct by summing over the the quasiparticle states

$$\rho(\mathbf{r}, t) = \sum_i (|u_i(\mathbf{r})|^2 + |v_i(\mathbf{r})|^2) n_i + |v_i(\mathbf{r})|^2, \tag{A.4}$$

$$\kappa(\mathbf{r}, t) = \sum_i u_i(\mathbf{r}) v_i s(\mathbf{r})(1 + 2n_i). \tag{A.5}$$

The condensate depletion, N_{ex}, is given by the integral over $\rho(\mathbf{r})$ and thus our choice of N_0 and T must be such that it is consistent with total number of particles, $N_{tot} = N_0 + N_{ex}$.

The summation over states in equations (A.4) and (A.5) will inevitably be restricted and we have to be careful not to introduce any truncation errors to the calculation. For high-lying states the quasiparticle wavefunctions go over to their non-interacting limit. $v_i(\mathbf{r})$ quickly tends towards zero, which means that $\kappa(\mathbf{r}, t)$ is unaffected by any reasonable cut-off. $u_i(\mathbf{r})$, however, goes over to the harmonic oscillator states, which means we have non-zero terms above the cut-off contributing to $\rho(\mathbf{r}, t)$. The associated population terms of the individual levels are small but the integral over them is not negligible. To find the correct $\rho(\mathbf{r}, t)$, and thus also the correct number of excited particles, we follow the work of Reidl *et al.* and combine the finite basis state expansion with a semiclassical approximation of the highly excited states [91].

Once the ground state $\phi(\mathbf{r})$ is found the quasiparticle energies and wavefunctions

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can be calculated by solving the BdG equations

$$\begin{aligned}\left[H_{sp}(\mathbf{r}) - \mu + 2N_0U_0\Phi_0(\mathbf{r})^2\right] u_i(\mathbf{r}) + N_0U_0[\Phi_0(\mathbf{r})]^2 v_i(\mathbf{r}), &= \epsilon_i u_i(\mathbf{r}) \\ N_0U_0[\Phi_0(\mathbf{r})]^2 u_i(\mathbf{r}) + \left[H_{sp}(\mathbf{r}) - \mu + 2N_0U_0\Phi_0(\mathbf{r})^2\right] v_i(\mathbf{r}) &= -\epsilon_i v_i(\mathbf{r}), \end{aligned} \quad (A.6)$$

which we do using the method detailed in Hutchinson *et al.* [59].

The finite temperature condensate wavefunction and energy, $\tilde{\psi}_0$ and $\tilde{\mu}$, are found solving the generalised GPE in the same manner as the GPE,

$$i\hbar\frac{d}{dt}\Phi(\mathbf{r},t) = \left(H_{sp} + N_0U_0|\Phi(\mathbf{r},t)|^2 + 2U_0\rho(\mathbf{r},t)\right)\Phi(\mathbf{r},\mathbf{t}) + U_0\kappa(\mathbf{r},t)\Phi(\mathbf{r},t). \quad (A.7)$$

A.2 First order terms

With quadratic theory data at hand, it is straightforward to calculate the first order perturbative shifts $\Delta E^{(1)} = \Delta E_4(p) + \Delta E_\mu(p) + \Delta E_{shape}(p)$,

$$\Delta E_4(p) = U_0 \int d^3\mathbf{r}\, [2\tilde{n}(\mathbf{r})\Delta\rho_p(\mathbf{r}) + \tilde{m}(\mathbf{r})\Delta\kappa_p(\mathbf{r})]\,, \quad (A.8)$$

$$\Delta E_\mu(p) = [\mu - \tilde{\mu}] \int d\mathbf{r}\Delta\rho_p, \quad (A.9)$$

$$\begin{aligned}\Delta E_{shape}(p) = & -N_0U_0\Bigg\{ \int d\mathbf{r}[2\Delta\rho_p(\mathbf{r}) + \Delta\kappa_p(\mathbf{r})][\phi_0^2(\mathbf{r}) - \tilde{\phi}_0^2(\mathbf{r})] \\ & + \int d\mathbf{r}\phi_0^3(\mathbf{r})[u_p(\mathbf{r}) + v_p(\mathbf{r})] \int d\mathbf{r}[\phi_0(\mathbf{r}) - \tilde{\phi}_0(\mathbf{r})][u_p(\mathbf{r}) + v_p(\mathbf{r})]\Bigg\}. \end{aligned} \quad (A.10)$$

where we use $\Delta\rho_p(\mathbf{r}) = (|u_p(\mathbf{r})|^2 + |v_p(\mathbf{r})|^2)$ and $\Delta\kappa_p(\mathbf{r}) = u_p(\mathbf{r})v_p^*(\mathbf{r})$.

A.3 Second order terms

The second order perturbation theory term is given by,

$$\Delta E_3(p,z) = -\sum_{ij\neq 0} \frac{|A^P_{pij}|^2}{2\,(z + \epsilon_i + \epsilon_j)}\,[1 + n_i + n_j] \quad (A.11)$$

[59] D. A. W. Hutchinson, K. Burnett, R. J. Dodd, S. A. Morgan, *et al.*. *Gapless mean-filed theory of Bose-Einstein condensates*. J. Phys. B 33, 3825 (2000).

$$+\sum_{ij\neq 0}\frac{|B_{pij}+B_{pji}|^2}{2\left(z-\epsilon_i-\epsilon_j\right)}\left[1+n_i+n_j\right] \tag{A.12}$$

$$+\sum_{ij\neq 0}\frac{|B_{ijp}+B_{ipj}|^2}{z-\epsilon_i+\epsilon_j}\left[n_j-n_i\right], \tag{A.13}$$

where the matrix elements are defined as

$$\begin{aligned}
A_{ijk} = \quad & \sqrt{N_0}U_0\int d\mathbf{r}\;\phi_0(\mathbf{r})[v_i(\mathbf{r})u_j(\mathbf{r})u_k(\mathbf{r})+u_i(\mathbf{r})v_j(\mathbf{r})v_k(\mathbf{r})],\\
B_{ijk} = \quad & \sqrt{N_0}U_0\int d\mathbf{r}\;\Big\{\phi_0(\mathbf{r})[u_i(\mathbf{r})u_j(\mathbf{r})u_k(\mathbf{r})+v_i(\mathbf{r})v_j(\mathbf{r})u_k(\mathbf{r})+v_i(\mathbf{r})u_j(\mathbf{r})v_k(\mathbf{r})]\\
& +\phi_0(\mathbf{r})[u_i(\mathbf{r})u_j(\mathbf{r})v_k(\mathbf{r})+u_i(\mathbf{r})v_j(\mathbf{r})u_k(\mathbf{r})+v_i(\mathbf{r})v_j(\mathbf{r})v_k(\mathbf{r})]\Big\},
\end{aligned} \tag{A.14}$$

and A^P_{ijk} stands for all permutations of its indices. $\Delta E_3(p,z)$ is calculated by a straightforward summation over all states with non-zero matrix elements. Whether a matrix element is equal to zero follows from the selection rules involved in calculating its angular integrals. To illustrate this we single out one term of the matrix element

$$\begin{aligned}
\int d\mathbf{r}\Phi_0(\mathbf{r})u_i(\mathbf{r})u_j(\mathbf{r})u_k(\mathbf{r}) \;=\; & \int dr\Phi_0(r)u_i(r)u_j(r)u_k(r)\\
& \frac{1}{\sqrt{4\pi}}\int d\Omega Y_{l_i}^{m_i}(\Omega)Y_{l_j}^{m_j}(\Omega)Y_{l_k}^{m_k}(\Omega).
\end{aligned} \tag{A.15}$$

The angular integral is given in terms of Clebsch-Gordan coefficients as

$$\begin{aligned}
& \int d\Omega Y_{l_1}^{m_1}(\Omega)Y_{l_2}^{m_2}(\Omega)Y_{l_3}^{m_3}(\Omega)\\
= \quad & (-1)^{m_3}\sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l_3+1)}}\langle l_1,l_2;0,0|l_3,0\rangle\langle l_1,l_2;m_1,m_2|l_3,-m_3\rangle,
\end{aligned} \tag{A.16}$$

which, of course, is only non-zero if 1) l_1, l_2, and l_3 add up vectorially, 2) $l_1+l_2-l_3$ is even, and 3) $m_1+m_2+m_3=0$. These criteria restrict the size of the summation considerably. The summation over states in ΔE_3 is further simplified by the fact the states are degenerate in m and the angular components of any l subspace add up to unity,

$$\sum_{m=-l_i}^{l_i}\sum_{m=-l_j}^{l_j}|j_1,j_2;m_1,m_2\rangle\langle j_1,j_2;m_1,m_2|=1. \tag{A.17}$$

For non-zero values of the angular integral the radial integral has to be calculated explicitly.

APPENDIX B

EQUATIONS OF MOTION FOR NORMAL AND ANOMALOUS AVERAGES

For convenience, we write out the equation of motion for the pair and triplet averages, which have been derived by Proukakis [66].

They were obtained by commuting the respective product of operators $a_i^\dagger$ and a_i with the Hamiltonian, equation (2.20), taking the expectation value of the resulting equation of motion, and using a decoupling approximation of correlations of four and five fluctuation operators ($\hbar = 1$ henceforth).

$$i\frac{d}{dt}(z_n) = \omega_n z_n + \sum_{ijk}\langle ni|\hat{V}|jk\rangle\left[z_i^* z_j z_k + \kappa_{jk} z_i^* + 2\rho_{ji} z_k + \lambda_{ijk}\right], \tag{B.1}$$

$$\begin{aligned} i\frac{d}{dt}(\rho_{ji}) \;=\;& (\omega_j - \omega_i)\rho_{ji} \\ &+ \sum_r \left[\eta_{jr}\rho_{ri} - \rho_{jr}\eta_{ri}\right] \\ &- \sum_r \left[\kappa_{jr}\Delta^*_{ri} - \Delta_{jr}\kappa^*_{ri}\right] \\ &+ \sum_{rms}\langle jr|\hat{V}|ms\rangle\left(2\lambda^*_{mri} z_s + \lambda_{ims} z_r^*\right) \\ &- \sum_{rms}\langle ms|\hat{V}|ri\rangle\left(2\lambda_{mrj} z_s^* + \lambda^*_{jms} z_r\right), \end{aligned} \tag{B.2}$$

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$$
\begin{aligned}
i\frac{d}{dt}(\kappa_{kj}) &= (\omega_j+\omega_k)\kappa_{kj}+\Delta_{kj} \\
&\quad +\Delta_{kj}+\sum_s\left[\rho_{ks}\Delta_{sj}+\Delta_{ks}\rho^*_{sj}\right] \\
&\quad +\sum_s\left[\eta_{ks}\kappa_{sj}+\kappa_{ks}\eta^*_{sj}\right] \\
&\quad +\sum_{rms}\left\{\langle kr|\hat{V}|ms\rangle\left[2\lambda_{rsj}z_m+\gamma_{msj}z^*_r\right]+(k\leftrightarrow j)\right\}
\end{aligned} \tag{B.3}
$$

$$
\begin{aligned}
i\frac{d}{dt}\lambda_{ijk} &= (\omega_k+\omega_j-\omega_i)\lambda_{ijk}+\sum_{ms}\langle jk|V|ms\rangle_s\left(2\rho_{mi}z_s+\lambda_{ims}\right) \\
&\quad +\sum_{rms}\left\{\langle kr|V|ms\rangle_s\rho_{jr}\left[2\rho_{mi}z_s+\lambda_{ims}\right]+(k\leftrightarrow j)\right\} \\
&\quad -\sum_{rms}\left\{\langle ms|V|ir\rangle_s\rho_{jm}\rho_{ks}z_r+(k\leftrightarrow j)\right\} \\
&\quad +\sum_s\left\{\lambda_{ijs}\eta^*_{sk}+\lambda^*_{jis}\Delta_{sk}+(k\leftrightarrow j)\right\} \\
&\quad -\sum_s\left[\eta^*_{is}\lambda_{sjk}-\Delta^*_{js}\gamma_{sik}\right] \\
&\quad +\sum_{rms}\left\{\langle kr|V|ms\rangle_s 2\rho_{mi}(\kappa_{js}z^*_r+\lambda_{rjs})+(k\leftrightarrow j)\right\} \\
&\quad -\sum_{rms}\langle ms|V|ir\rangle_s\left\{\kappa_{rk}(2\rho_{jm}z^*_s+\lambda^*_{jms})+(k\leftrightarrow j)\right\} \\
&\quad +\sum_{rms}\left\{\langle kr|V|ms\rangle_s\left[2\kappa_{mj}(\kappa^*_{ir}z_s+\lambda^*_{sir})+\kappa^*_{ir}\gamma_{smj}\right]+(k\leftrightarrow j)\right\} \\
&\quad -\sum_{rms}\langle ms|V|ir\rangle_s\left\{2\rho_{jm}\lambda_{skr}+(k\leftrightarrow j)\right\},
\end{aligned} \tag{B.4}
$$

where we define $\gamma_{ijk}=\langle c_ic_jc_k\rangle$. In the above equations, the notation $(k\leftrightarrow j)$ indicates terms with the indices k and j interchanged. We have used the notation

$$
\eta_{jr}=h_{jr}-\langle j|\hat{\Xi}|r\rangle=2\sum_{lt}\langle jl|\hat{V}|tr\rangle(z^*_lz_t+\rho_{tl}) \;, \tag{B.5}
$$

$$
\Delta_{kj}=\sum_{ms}\langle kj|\hat{V}|ms\rangle\left[z_mz_s+\kappa_{ms}\right]. \tag{B.6}
$$

In our V^2 calculation of the homogeneous gas the triplet anomalous average need only include expressions to first order in V, i.e. the first three terms of equation (B.4), excluding the λ_{ims} in the latter two. For our discussion of trapped systems at finite temperatures we again keep only the first three terms of the triplet average, but then do use the recursive expressions which include the λ_{ims}, in order to obtain self-consistent equations. The according expression for the pair anomalous average is given by the first three terms of equation (B.3).

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