



Department of Applied Physics
Coherence and Quantum Technology

Cumulant expansion for an ultracold quantum gas

Bachelors Thesis

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Abstract

Analysis of ultracold quantum gases exists in the domain of many body quantum theory and utilises the formalism of second quantization. This means that many body problems are formulated in terms of creation and annihilation operators [1]. The dynamics of ultracold quantum gases are often formulated in terms of correlated clusters, which assign genuinely correlated atoms. The Heisenberg equation of motion can be written in products of such clusters through a procedure known as the cluster expansion [2]. Using a method first proposed by Fricke in 1996, the equations of motion for the clusters, also known as cumulants, can be approximated as a closed set of ordinary differential equations [3]. Solving these equations gives the dynamics of the cumulants, which can be related to the transition amplitudes of different many body scattering processes within the gas. This cumulant expansion procedure can then be used to describe the full dynamics of an ultracold quantum gas, and can be applied to both bosons and fermions. The resulting equations are suited to predict interesting ultracold phenomena like Bose-Einstein condensation for bosons [4] and formation of cooper pairs for fermions [5].

The practical computation of the cumulant equations is however a time consuming and tedious process when done manually, and is also easily prone to mistakes. It is however a systematic process that should be well suited for automation by a computer script. In this work a Mathematica script is developed that can calculate the cumulant equations for both Bose and Fermi gases at zero temperature, possibly with mixtures of different components. The script relies on the second quantization package SNEG [6]. The cumulant equations are first calculated generally through the cluster expansions, and then simplified under certain assumptions, like the coherent state approximation for Bose gases. The developed script is highly customizable to accept different inputs, and can easily be applied to different many body theories.

This work summarizes results obtained with the developed script up to fourth order, which were obtained within very manageable computation times not exceeding 15 minutes for the most complicated applications. These results are analysed and compared with the relevant literature, which verified the correct operation of the script within the domain in which it was tested. This work also contains an analysis of the cumulant equations as calculated for mixtures. Since the mixture equations can use a host of different initial assumptions, it is a major advantage that this script can quickly provide the user with the dynamics for any desired input.

Contents

Abstract	i
1 Introduction	1
2 Theory	3
2.1 General formalism	3
2.1.1 Second Quantization	3
2.1.2 Many-body Hamiltonian	5
2.1.3 Separable potential	7
2.1.4 Equations of motion	7
2.1.5 Cluster expansion	9
2.2 Condensed Bose gases	11
2.2.1 Coherent state approximation	11
2.2.2 Cumulants	12
2.2.3 Bose mixtures	14
2.2.4 Truncating the cumulant expansion	14
2.3 Fermi gases	16
2.3.1 Fermion Hamiltonian	16
2.3.2 Fermion wave function	16
2.3.3 Cumulants	17
2.3.4 Fermi mixtures	18
3 Model	19
3.1 Model environment	19
3.2 Script operation	20
3.2.1 Species index	20
3.2.2 Preamble	21
3.2.3 Workflow	23
3.3 Custom functions	24
3.3.1 Delta functions	24
3.3.2 Cluster expansion	26
3.3.3 Index simplification	28
3.4 Simplifying the equations	30
3.4.1 Simplifying rulesets	30
3.4.2 Applying simplifications	33
3.4.3 Fricke approximation	35
3.5 Potential issues	35

3.5.1	Error codes	35
3.5.2	Fermion operators	35
3.5.3	Simplifying rule sets	36
3.5.4	Index simplify	36
3.5.5	Computation time	36
4	Results and Discussion	38
4.1	Boson Hartree-Fock Bogoliubov equations	38
4.1.1	Non-interacting mixture	38
4.1.2	Two-Body Schrödinger equation	40
4.1.3	Second order interacting mixtures	40
4.2	Boson third order equations	42
4.2.1	Non-interacting mixture	42
4.2.2	Three-body Schrödinger equation	46
4.2.3	Third order interacting mixtures	47
4.3	Boson fourth order equations	48
4.3.1	Singlets and doublets	48
4.3.2	Four body Schrödinger equation	49
4.4	Fermions	51
4.4.1	Hartree-Fock Bogoliubov equations	51
4.4.2	Interacting fermi mixtures	52
4.4.3	Extending HFB equations	53
5	Conclusion	54
	Bibliography	57

Chapter 1

Introduction

Accurate descriptions of many-particle systems are of interest to a wide range of fields. Historically the dynamics of gases were first described in the context of classical thermodynamics, which provides accurate macroscopic predictions near equilibrium. However the empirical model of thermodynamics is inherently classical, and fails to take into account the quantum mechanical behaviour of particles unveiled in the previous century. This is not an issue at everyday temperatures, where the number of quantized states are closely packed enough to assume a continuous range of energies.

At lower energies or low concentrations however the macroscopic language of classical thermodynamics becomes difficult to reconcile with the microscopic language of quantum theory. Very successful efforts have been made to marry the two descriptions, which manifested in the widely applicable theory of statistical mechanics. Essentially statistical mechanics poses that the stochastic nature of quantum mechanics can be applied macroscopically, where the thermodynamically preferable states will always have the highest probability [7]. Statistical mechanics has proven to be an exceptionally powerful theory for describing physical phenomena. Chief amongst these are the dynamics of phase transitions and the behaviour of Fermi and Bose gasses at low temperatures.

A famous example of a striking prediction made by the field of statistical mechanics is the phase transition postulated by Bose and Einstein between 1924 and 1925, appropriately dubbed Bose-Einstein Condensation (BEC). In this new phase of matter only the ground state of the system is macroscopically occupied with particles. This definition already testifies how such a state can only exist in a quantum mechanical model of the gas, where the particles attain eigenstates with discrete energy levels. From a relatively simple model in which inner particle interactions were neglected statistical mechanics was able to accurately predict the critical temperature at which BEC occurs. To align theory and experimental data more closely though, particle interactions would have to be included. The problem then becomes one of many body quantum physics [2, 8].

The dynamics of many-body quantum systems are most straightforwardly analysed in the formalism of second quantization, which states that all essential information about a certain system state is given by the occupancy of each single particle state. This formalism is convenient since it is inherently suited to deal with identical indistinguishable particles. In fact the formalism of second quantization is built up in such a way that it can easily deal with both fermions and bosons, through the inclusion of fundamental commutation relations. These are enforced through creation and annihilation operators, which form the central basis for all other operators in many body theory [1].

In the last 30 years the analysis of ultracold quantum gases has been in part focused on describing the dynamics of atom clusters, also called cumulants. These identify those atoms in the gas which

are genuinely correlated, and represent the transition amplitudes of certain scattering events within the gas. Knowledge of the dynamics of these cumulants provides the dynamics of the gas under consideration, in the form of the so called cumulant equations. These can be used to predict complex processes in ultracold Fermi and Bose gases, like Bose Einstein condensation, Cooper pairing, quantum depletion and many body scattering processes [4, 5].

The computation of the cumulant equations however often requires tedious operations on indices, which are time consuming and easily prone to errors if done manually. In this work we present a computer script that calculates the cumulant equations automatically, with highly customizable input ensuring that the script can be used for many different theories. This report will both serve as a manual for the use and operation of the script, and conduct analysis on a select set of results which were obtained with the script. After this introductory chapter, chapter 2 will give an overview of the many body theory which forms the backbone of the developed script. The chapter will start with a brief mathematical overview of the formalism of second quantization, which forms the basis for all theory. We then show how one can rewrite the Heisenberg equation in terms of clusters through the cumulant expansion, and show the mathematical advantage of doing so.

Chapter 2 continues with more specific analysis of the cumulant theory surrounding both Bose and Fermi gases. Here we introduce the coherent state approximation for bosons, and show how one can interpret the cumulants as transition amplitudes for scattering processes. Moving on to chapter 3, we explain the script which accompanies this report. The operation of the script is explained in detail, first by giving a general overview of the framework and then by explaining all custom functions that were written for its operation. A large part of the scripts developed in this work focus on the simplification of results. The procedures used for this are also explained in chapter 3.

After the script has been fully introduced and explained, chapter 4 will give an overview of some select results that were obtained during testing. These are analysed and checked against literature to ensure that the script operates correctly. Here we also analyse the cumulant theory as applied to Bose and Fermi mixtures, which is an interesting application of the developed code. Finally chapter 5 concludes by summarizing all results and findings.

Chapter 2

Theory

2.1 General formalism

In this section the quantum mechanical theory for an ultracold quantum gas is developed generally for both bosons and fermions. This theory will form the backbone for the script developed in this work, which aims to make calculations within the theory more efficient and less cumbersome. The calculation and expansion of the cumulant equations is not much different for fermions and bosons, but both types of gases allow for different assumptions and simplifications once the full equations have been calculated. Thus after explaining the general formalism this chapter will focus on both Bose gases and Fermi gases and explain their relevant properties as they relate to the dynamic equations calculated in the script.

The natural language of quantum theory is that of operators, which represent some physical observable and can be interpreted as the mathematical equivalent of the measurement process. In any quantum theory it is convenient to express all physical operators in the same set of basis operators, which have some well defined action on a given state. In more mathematical terms, one looks for a set of operators which form a basis for all other operators in the relevant vector space. In single particle quantum physics these basis operators are the position and momentum operators, which physically represent a measurement of particle positions and momenta respectively. All other operators in single particle quantum theory can be expressed in terms of these operators, which span the single particle Hilbert space.

This thesis considers quantum gases, comprised of arbitrarily large numbers of particles. We require a theory of many body quantum physics that works with arbitrarily large possible interacting systems. The appropriate formalism for such systems is that of second quantization [1].

2.1.1 Second Quantization

Many body systems of identical particles are most easily analyzed using the second quantization formalism. Essentially this formalism exploits the indistinguishability of identical particles to vastly simplify the specification of many particle states. Instead of specifying the state of each particle individually (first quantization), in second quantization only the occupancy of each state is relevant. This means that physical states are only defined uniquely by the occupancy numbers of each single particle state. As was explained at the beginning of this section we require our theory to have a basis set of operators from which we can build up all other physical operators. In second quantization this basis set consists of creation and annihilation operators, which create and annihilate particles

in certain states. In the language of second quantization then, these operators alter the states' occupancy. Any operator written in its second quantization form is written as a combination of creation and annihilation operators. [1, 9].

A large advantage of the second quantization formalism is the ease with which it handles both fermions and bosons. In first quantization one would have to manually (anti)symmetrize the wave function after evaluation. In second quantization however, the symmetry of the wave function is built into the operators via the commutations relations they obey [1, 10]. Let us start by laying the mathematical groundwork for the theory.

We work in some complete basis of orthonormal single particle momentum states $\{|\mathbf{k}\rangle\}$ with momentum $\hbar\mathbf{k}$ in the one particle Hilbert space \mathcal{H}_1 . To further generalise our model we allow the gas to be a mixture of different species with equal atomic mass, denoted by Greek letters. We now have the following properties of completeness and orthonormality.

$$\sum_{\sigma} \sum_{\mathbf{k}} |\mathbf{k}_{\sigma}\rangle\langle\mathbf{k}_{\sigma}| = 1, \quad \langle\mathbf{k}_{\sigma}|\mathbf{q}_{\sigma'}\rangle = \delta_{\mathbf{k}\mathbf{q}}\delta_{\sigma\sigma'}. \quad (2.1)$$

Let us define operators that create and annihilate particles of species σ in momentum state $|\mathbf{k}\rangle$ as

$$\hat{a}_{\sigma,\mathbf{k}}|0\rangle = 0, \quad \langle 0|\hat{a}_{\sigma,\mathbf{k}}^{\dagger} = 0, \quad (2.2)$$

which obey canonical commutation relations as

$$\left[\hat{a}_{\sigma,\mathbf{k}}, \hat{a}_{\sigma',\mathbf{q}}^{\dagger}\right]_{\epsilon} = \delta_{\mathbf{k}\mathbf{q}}\delta_{\sigma\sigma'}, \quad (2.3)$$

$$\left[\hat{a}_{\sigma,\mathbf{k}}, \hat{a}_{\sigma',\mathbf{q}}\right]_{\epsilon} = \left[\hat{a}_{\sigma,\mathbf{k}}^{\dagger}, \hat{a}_{\sigma',\mathbf{q}}^{\dagger}\right]_{\epsilon} = 0. \quad (2.4)$$

Here $\epsilon = -1$ for bosons and $\epsilon = 1$ for fermions [10, 11, 12]. From these commutation relations the appropriate symmetrisation properties for bosons and fermions immediately follow. In the second quantization formalism we define (indistinguishable) particles by their states. This means that a general many-particle (momentum) state in second quantization can be written as

$$|\psi_N\rangle = |\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3 \dots \mathbf{k}_N\rangle \quad (2.5)$$

where \mathbf{k}_j refers to the momentum state of the j th particle in the system. Here the states ψ_n forms a complete basis for the many particle Hilbert space \mathcal{H}_N , with equivalent definitions as those defined for the single particle Hilbert space. Formally this many particle Hilbert space is simply the tensor product of all single particle Hilbert spaces.

Since the creation and annihilation operators alter the number of particles in the gas, they do not operate within a single Hilbert space \mathcal{H}_n , but rather connect Hilbert spaces of different size. To properly define the basis space in which these operators live we work in so called Fock space. A Fock space is defined as the sum of all N particle Hilbert spaces up to an infinite amount of particles. It should be noted that the size of the Fock space is usually truncated somewhat by the physical properties of indistinguishable particles. In the state given by equation 2.5, all particles are indistinguishable which means any interchange of particles should have no measurable effect. This means that any reordering of states is either symmetric or antisymmetric. In theory one could imagine many-particle states which contain mixed symmetric and antissymmetric permutations. In

nature however, one only observes either completely symmetric or completely antisymmetric wave functions, referred to as bosons and fermions respectively. This means that for example the boson Fock space \mathcal{B} only contains fully symmetric many-particle states, and vice versa for the fermion Fock space \mathcal{F} [1, 11]. Completeness in momentum Fock space is expressed mathematically as follows, for the boson Fock space \mathcal{B} .

$$\sum_{N=0}^{\infty} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \dots \mathbf{k}_N}^{\text{symmetric}} |\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \dots \mathbf{k}_N\rangle \langle \mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \dots \mathbf{k}_N| = 1. \quad (2.6)$$

We note that due to the symmetry or asymmetry of a many-particle state as written in equation 2.5, such a state does not singularly define the system. In other words, due to the indistinguishability of particles one could shuffle around the particle numbers without changing the physical state. In second quantization a system is only uniquely defined by the occupation number representation, in which a state is written as

$$|\psi_N\rangle = |n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_3} \dots\rangle \quad (2.7)$$

with $n_{\mathbf{k}_i}$ the occupation of the i th momentum state [11]. We now see how in second quantization system states are only uniquely defined by the occupancy numbers of single particle states, which we also stated at the beginning of this section.

2.1.2 Many-body Hamiltonian

Now that the mathematical basis of second quantization has been defined, some concrete operators can be considered. Here the Hamiltonian which will be used to model the quantum gas will be described, following ref [12]. Let us first consider a single particle operator. According to the completeness relation in equation 2.1 we can write the sum of N single particle operators \hat{H}_0 as

$$\hat{H}_{0,N} = \sum_{i=1}^N \sum_{\sigma\sigma'} \sum_{\mathbf{k}_i, \mathbf{q}_i} |\mathbf{k}_{\sigma,i}\rangle \langle \mathbf{k}_{\sigma,i} | \hat{H}_0^i | \mathbf{k}_{\sigma',i}\rangle \langle \mathbf{k}_{\sigma',i} |, \quad (2.8)$$

where i labels the i th particle in the N particle system. One can now derive that this form is equivalent to the following expression in terms of creation and annihilation operators.

$$\hat{H}_{0,\text{tot}} = \sum_{\sigma\sigma'} \sum_{\mathbf{k}, \mathbf{q}} \langle \mathbf{k}_{\sigma} | \hat{H}_0 | \mathbf{q}_{\sigma'} \rangle \hat{a}_{\sigma, \mathbf{k}}^\dagger \hat{a}_{\sigma', \mathbf{q}}. \quad (2.9)$$

Also again from the completeness relations we can write the sum of two body interaction potentials as

$$\hat{V}_N = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N \sum_{\sigma\sigma'} \sum_{\mathbf{k}_i, \mathbf{q}_i, \mathbf{k}_j, \mathbf{q}_j} |\mathbf{k}_{\sigma,i} \mathbf{k}_{\sigma,j}\rangle \langle \mathbf{k}_{\sigma,i} \mathbf{k}_{\sigma,j} | \hat{V}_{\sigma,\sigma'} | \mathbf{q}_{\sigma',i} \mathbf{q}_{\sigma',j}\rangle \langle \mathbf{q}_{\sigma',i} \mathbf{q}_{\sigma',j} |. \quad (2.10)$$

This can also be rewritten to its second quantized form which gives

$$\hat{V}_{\text{tot}} = \frac{1}{2} \sum_{\sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}'} \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{q}}^{\dagger} \langle \mathbf{k}\mathbf{q} | \hat{V}_{\sigma, \sigma'} | \mathbf{k}'\mathbf{q}' \rangle \hat{a}_{\mathbf{q}'} \hat{a}_{\mathbf{k}'}. \quad (2.11)$$

The proof for these identities in Fock space can be found in for example ref [1] or ref [10]. It is assumed that the single particle operator in the Hamiltonian is diagonal in the basis of momentum states with eigenvalue $\frac{\hbar^2 q^2}{2m}$. In physical terms this means we work in the plane wave basis, and it is assumed that there are no other single particle potentials. This assumption is valid for systems in which the interaction length is much shorter than the oscillator length of any external trapping potential in which the gas is held. Over this region then, the gas is approximately homogeneous [4]. We are now in a position where we can write down the full Hamiltonian. Let us start with the single particle contribution.

$$\begin{aligned} \hat{H}_{0, \text{tot}} &= \sum_{\sigma \sigma'} \sum_{\mathbf{k}, \mathbf{q}} \langle \mathbf{k}_{\sigma} | \hat{H}_0 | \mathbf{q}_{\sigma'} \rangle \hat{a}_{\sigma, \mathbf{k}}^{\dagger} \hat{a}_{\sigma', \mathbf{q}} \\ &= \sum_{\sigma \sigma'} \sum_{\mathbf{k}, \mathbf{q}} \frac{\hbar^2 q^2}{2m} \delta_{\sigma \sigma'} \delta_{\mathbf{k}\mathbf{q}} \hat{a}_{\sigma, \mathbf{k}}^{\dagger} \hat{a}_{\sigma', \mathbf{q}} \\ &= \sum_{\sigma, \mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{a}_{\sigma, \mathbf{k}}^{\dagger} \hat{a}_{\sigma, \mathbf{k}}. \end{aligned} \quad (2.12)$$

Similarly one can derive the two body interaction potential. First we split the momenta into a center of mass and a relative component as follows.

$$\begin{aligned} |\mathbf{k}\mathbf{q}\rangle &= |\mathbf{K}_{\text{cm}}\rangle |\mathbf{K}_{\text{rel}}\rangle, \\ |\mathbf{K}_{\text{cm}}\rangle &= |\mathbf{k} + \mathbf{q}\rangle, \\ |\mathbf{K}_{\text{rel}}\rangle &= \left| \frac{1}{2}(\mathbf{k} - \mathbf{q}) \right\rangle. \end{aligned} \quad (2.13)$$

We assume the interaction potential is diagonal in the center of mass contribution with eigenvalue 1. In other words, we consider translationally invariant interaction potentials which only depend on the relative momenta of the particles. Now we can derive the following general expression.

$$\begin{aligned} \hat{V}_{\text{tot}} &= \frac{1}{2} \sum_{\sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}'} \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{q}}^{\dagger} \left\langle \frac{1}{2}(\mathbf{k} - \mathbf{q}) \left| \hat{V}_{\sigma, \sigma'} \right| \frac{1}{2}(\mathbf{k}' - \mathbf{q}') \right\rangle \delta_{\mathbf{k}+\mathbf{q}, \mathbf{k}'+\mathbf{q}'} \hat{a}_{\mathbf{q}'} \hat{a}_{\mathbf{k}'} \\ &= \frac{1}{2} \sum_{\sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} V_{\sigma, \sigma'} \left(\frac{1}{2}(\mathbf{k} - \mathbf{k}' + 2\mathbf{q}), \frac{1}{2}(\mathbf{k} - \mathbf{k}') \right) \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^{\dagger} \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^{\dagger} \hat{a}_{\sigma', \mathbf{k}'} \hat{a}_{\sigma, \mathbf{k}}. \end{aligned} \quad (2.14)$$

Here we have defined

$$V_{\sigma, \tau}(\mathbf{k}, \mathbf{q}) = \langle \mathbf{k} | \hat{V}_{\sigma, \tau} | \mathbf{q} \rangle \quad (2.15)$$

which will be used throughout this report. Note that in deriving these expressions we have assumed that the interaction potential is always symmetric under exchange of particles. In other words $V_{\sigma, \tau}(\mathbf{k}, \mathbf{q}) = V_{\tau, \sigma}(-\mathbf{k}, -\mathbf{q})$ So our total Hamiltonian becomes

$$\begin{aligned}
\hat{H}_{\text{tot}} &= \hat{H}_{0,\text{tot}} + \hat{V}_{\text{tot}} \\
&= \sum_{\sigma,\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{a}_{\sigma,\mathbf{k}}^\dagger \hat{a}_{\sigma,\mathbf{k}} \\
&\quad + \frac{1}{2} \sum_{\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\sigma,\sigma'}\left(\frac{1}{2}(\mathbf{k}-\mathbf{k}'+\mathbf{2q}), \frac{1}{2}(\mathbf{k}-\mathbf{k}')\right) \hat{a}_{\sigma,\mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma',\mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma',\mathbf{k}'} \hat{a}_{\sigma,\mathbf{k}}.
\end{aligned} \tag{2.16}$$

2.1.3 Separable potential

In deriving the Hamiltonian in equation 2.16 the potential was separated into center of mass and relative components. Sometimes in literature, as in refs [13, 14], an additional assumption is applied. The relative potential operator is then written as

$$\hat{V}_{\text{tot}} = \lambda |\zeta\rangle\langle\zeta|, \tag{2.17}$$

where λ is the effective interaction strength and $|\zeta\rangle$ is the form factor. A potential that can be written in this way is referred to as a separable potential. In the notation of equation 2.15 we can then write

$$V(\mathbf{k}, \mathbf{q}) = \lambda \zeta(\mathbf{k}) \zeta^*(\mathbf{q}). \tag{2.18}$$

Note that writing the mixture potential which we have used up to this point would require more information about the dependence of the form factor ζ on the mixture components. Since the potential in equation 2.15 is more general, it will be used throughout most of this thesis. At the end of the single component script the user can then optionally include a separable potential if this is desired.

2.1.4 Equations of motion

Now that we have our many body Hamiltonian in second quantization, the essential problem becomes the solution of the Schrödinger equation for this Hamiltonian. In the formalism of creation/annihilation operators, it is most useful to work in the Heisenberg picture of quantum theory, since this shifts the time dependence to the operators themselves. We describe the state of a system by a statistical operator or density matrix $\omega(t)$ and the expectation values of all relevant operators or observables.

$$\langle \hat{A} \rangle = \text{Tr}[\omega(t)A]. \tag{2.19}$$

Then with Heisenbergs equation of motion we find for the evolution equations of operators that

$$i\hbar \frac{\partial}{\partial t} \langle \hat{A} \rangle = \langle [\hat{A}, \hat{H}_{\text{tot}}] \rangle. \tag{2.20}$$

Writing down these equations involves simplifying the commutators in the rhs of the EoM. As an example of such a calculation, consider the evolution equation for the creation operator of a particle of species τ in state $|\mathbf{p}\rangle$. In the following derivation the commutator is calculated algebraically.

$$\begin{aligned}
\left[\hat{a}_{\tau, \mathbf{p}}^\dagger, \hat{H}_{tot} \right] &= \left[\hat{a}_{\tau, \mathbf{p}}^\dagger, \hat{H}_{0, tot} + \hat{V}_{tot} \right] \\
&= \left[\hat{a}_{\tau, \mathbf{p}}^\dagger, \hat{H}_{0, tot} \right] + \left[\hat{a}_{\tau, \mathbf{p}}^\dagger, \hat{V}_{tot} \right].
\end{aligned} \tag{2.21}$$

The commutator with both the single particle kinetic energy term and with the interaction potential energy will need to be evaluated. Let us first consider the kinetic energy term

$$\begin{aligned}
\left[\hat{a}_{\tau, \mathbf{p}}^\dagger, \hat{H}_{0, tot} \right] &= \sum_{\sigma, \mathbf{k}} \frac{\hbar^2 k^2}{2m} \left[\hat{a}_{\tau, \mathbf{p}}^\dagger, \hat{a}_{\sigma, \mathbf{k}}^\dagger \hat{a}_{\sigma, \mathbf{k}} \right] \\
&= \sum_{\sigma, \mathbf{k}} \frac{\hbar^2 k^2}{2m} (\hat{a}_{\tau, \mathbf{p}}^\dagger \hat{a}_{\sigma, \mathbf{k}}^\dagger \hat{a}_{\sigma, \mathbf{k}} - \hat{a}_{\sigma, \mathbf{k}}^\dagger \hat{a}_{\sigma, \mathbf{k}} \hat{a}_{\tau, \mathbf{p}}^\dagger) \\
&= \sum_{\sigma, \mathbf{k}} \frac{\hbar^2 k^2}{2m} (\hat{a}_{\tau, \mathbf{p}}^\dagger \hat{a}_{\sigma, \mathbf{k}}^\dagger \hat{a}_{\sigma, \mathbf{k}} - \hat{a}_{\sigma, \mathbf{k}}^\dagger \delta_{\sigma\tau} \delta_{\mathbf{k}\mathbf{p}} - \epsilon^2 \hat{a}_{\tau, \mathbf{p}}^\dagger \hat{a}_{\sigma, \mathbf{k}}^\dagger \hat{a}_{\sigma, \mathbf{k}}) \\
&= - \sum_{\sigma, \mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{a}_{\sigma, \mathbf{k}}^\dagger \delta_{\sigma\tau} \delta_{\mathbf{k}\mathbf{p}} \\
&= - \frac{\hbar^2 p^2}{2m} \hat{a}_{\tau, \mathbf{p}}^\dagger.
\end{aligned} \tag{2.22}$$

To evaluate the commutator with the interaction term, first consider the operator product given as

$$\begin{aligned}
&\hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'} \hat{a}_{\sigma, \mathbf{k}} \hat{a}_{\tau, \mathbf{p}}^\dagger \\
&= \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'} (\delta_{\sigma\tau} \delta_{\mathbf{k}\mathbf{p}} - \epsilon \hat{a}_{\tau, \mathbf{p}}^\dagger \hat{a}_{\sigma, \mathbf{k}}) \\
&= \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger (\hat{a}_{\sigma', \mathbf{k}'} \delta_{\sigma\tau} \delta_{\mathbf{k}\mathbf{p}} - \epsilon (\delta_{\sigma'\tau} \delta_{\mathbf{k}'\mathbf{p}} - \epsilon \hat{a}_{\tau, \mathbf{p}}^\dagger \hat{a}_{\sigma', \mathbf{k}'}) \hat{a}_{\sigma, \mathbf{k}}) \\
&= \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'} \delta_{\sigma\tau} \delta_{\mathbf{k}\mathbf{p}} - \epsilon \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma, \mathbf{k}} \delta_{\sigma'\tau} \delta_{\mathbf{k}'\mathbf{p}} \\
&\quad + \epsilon^4 \hat{a}_{\tau, \mathbf{p}}^\dagger \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'} \hat{a}_{\sigma, \mathbf{k}}.
\end{aligned} \tag{2.23}$$

Using this result we can evaluate the commutator as

$$\begin{aligned}
\left[\hat{a}_{\tau, \mathbf{p}}^\dagger, \hat{V}_{tot} \right] &= \frac{1}{2} \sum_{\sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} V_{\sigma, \sigma'} \left(\frac{1}{2}(\mathbf{k} - \mathbf{k}' + 2\mathbf{q}), \frac{1}{2}(\mathbf{k} - \mathbf{k}') \right) \left[\hat{a}_{\tau, \mathbf{p}}^\dagger, \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'} \hat{a}_{\sigma, \mathbf{k}} \right] \\
&= \frac{1}{2} \sum_{\sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} V_{\sigma, \sigma'} \left(\frac{1}{2}(\mathbf{k} - \mathbf{k}' + 2\mathbf{q}), \frac{1}{2}(\mathbf{k} - \mathbf{k}') \right) \left[\epsilon \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'} \delta_{\sigma\tau} \delta_{\mathbf{k}\mathbf{p}} \right. \\
&\quad \left. - \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma, \mathbf{k}} \delta_{\sigma'\tau} \delta_{\mathbf{k}'\mathbf{p}} \right] \\
&= \frac{1}{2} \sum_{\sigma} \sum_{\mathbf{k}, \mathbf{q}} \left\{ \epsilon V_{\tau, \sigma} \left(\frac{1}{2}(\mathbf{p} - \mathbf{k} + 2\mathbf{q}), \frac{1}{2}(\mathbf{p} - \mathbf{k}) \right) \hat{a}_{\tau, \mathbf{p}+\mathbf{q}}^\dagger \hat{a}_{\sigma, \mathbf{k}-\mathbf{q}}^\dagger \hat{a}_{\sigma, \mathbf{k}} \right. \\
&\quad \left. - V_{\sigma, \tau} \left(\frac{1}{2}(\mathbf{k} - \mathbf{p} + 2\mathbf{q}), \frac{1}{2}(\mathbf{k} - \mathbf{p}) \right) \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\tau, \mathbf{p}-\mathbf{q}}^\dagger \hat{a}_{\sigma, \mathbf{k}} \right\}.
\end{aligned} \tag{2.24}$$

Summarising these results and applying equation 2.20 we now write down the EoM for the creation operator.

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} \hat{a}_{\tau, \mathbf{p}}^\dagger &= -\frac{\hbar^2 p^2}{2m} \hat{a}_{\tau, \mathbf{p}}^\dagger \\
&+ \frac{1}{2} \sum_{\sigma} \sum_{\mathbf{k}, \mathbf{q}} \left\{ \epsilon V_{\sigma, \tau} \left(\frac{1}{2}(\mathbf{p} - \mathbf{k} + 2\mathbf{q}), \frac{1}{2}(\mathbf{p} - \mathbf{k}) \right) \hat{a}_{\tau, \mathbf{p} + \mathbf{q}}^\dagger \hat{a}_{\sigma, \mathbf{k} - \mathbf{q}}^\dagger \hat{a}_{\sigma, \mathbf{k}} \right. \\
&\left. - V_{\sigma, \tau} \left(\frac{1}{2}(\mathbf{k} - \mathbf{p} + 2\mathbf{q}), \frac{1}{2}(\mathbf{k} - \mathbf{p}) \right) \hat{a}_{\sigma, \mathbf{k} + \mathbf{q}}^\dagger \hat{a}_{\tau, \mathbf{p} - \mathbf{q}}^\dagger \hat{a}_{\sigma, \mathbf{k}} \right\}.
\end{aligned} \tag{2.25}$$

2.1.5 Cluster expansion

After writing down Heisenberg's equation we can start working towards a clear system of differential equations in the observables. Since all operators are expressed in creation/annihilation operators, all observables can be found by the expectation values of these operators. As an example, consider the evolution equation for the annihilation operator in a Bose gas, for which the method of calculation is exactly equivalent to the creation operator in the previous section. Taking the expectation value of Heisenberg's equation we find

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} \langle \hat{a}_{\tau, \mathbf{p}} \rangle &= \frac{\hbar^2 p^2}{2m} \langle \hat{a}_{\tau, \mathbf{p}} \rangle \\
&+ \frac{1}{2} \sum_{\sigma} \sum_{\mathbf{k}, \mathbf{q}} V_{\sigma, \tau} \left(\frac{1}{2}(\mathbf{k} - \mathbf{p} + \mathbf{q}), \frac{1}{2}(\mathbf{k} - \mathbf{p} - \mathbf{q}) \right) \langle \hat{a}_{\sigma, \mathbf{k} + \mathbf{q}}^\dagger \hat{a}_{\tau, \mathbf{p} + \mathbf{q}} \hat{a}_{\sigma, \mathbf{k}} \rangle \\
&+ V_{\tau, \sigma} \left(\frac{1}{2}(\mathbf{p} - \mathbf{k} + \mathbf{q}), \frac{1}{2}(\mathbf{p} - \mathbf{k} - \mathbf{q}) \right) \langle \hat{a}_{\sigma, \mathbf{k} - \mathbf{q}}^\dagger \hat{a}_{\tau, \mathbf{p} - \mathbf{q}} \hat{a}_{\sigma, \mathbf{k}} \rangle.
\end{aligned} \tag{2.26}$$

One notices that such an equation is not easily solved or approximated. Ideally we would like to write both expectation values in this equation in terms of the same variables. The equation can then be combined with equations of motion for the other operator products to obtain a system of ordinary differential equations. The canonical way of achieving this is by the cluster expansion, which expands the expectation values in so called cumulants of the operators. These cumulants allow one to rewrite the dynamic equation into a system of ordinary differential equations [3]. The cluster expansion of a set of creation/annihilation operators $\{B_i\}$ is defined as follows

$$\begin{aligned}
\langle \hat{B}_1 \rangle &= \langle \hat{B}_1 \rangle^c, \\
\langle \hat{B}_1 \hat{B}_2 \rangle &= \langle \hat{B}_1 \hat{B}_2 \rangle^c + \langle \hat{B}_1 \rangle^c \langle \hat{B}_2 \rangle^c, \\
\langle \hat{B}_1 \hat{B}_2 \hat{B}_3 \rangle &= \langle \hat{B}_1 \hat{B}_2 \hat{B}_3 \rangle^c + \langle \hat{B}_1 \rangle^c \langle \hat{B}_2 \hat{B}_3 \rangle^c + \langle \hat{B}_2 \rangle^c \langle \hat{B}_1 \hat{B}_3 \rangle^c \\
&\quad + \langle \hat{B}_3 \rangle^c \langle \hat{B}_1 \hat{B}_2 \rangle^c + \langle \hat{B}_1 \rangle^c \langle \hat{B}_2 \rangle^c \langle \hat{B}_3 \rangle^c, \\
&\vdots
\end{aligned} \tag{2.27}$$

The sum runs over all products of partitions of the set of operators $\{\hat{B}_i\}$, where the ordering of operators is conserved inside the cumulants. For fermions one should take care to include a minus

sign if the re-ordering of operators has uneven parity. We define the order of a cumulant as the number of operators it contains. An important property of the cumulants is that for orders $n > 2$ the operators exactly commute or anti-commute for bosons and fermions respectively.

$$\langle \dots B_i B_{i+1} \dots \rangle^c = -\epsilon \langle \dots B_{i+1} B_i \dots \rangle^c. \quad (2.28)$$

Let us define some shorthand notation for cumulants as

$$\begin{aligned} \psi_{\sigma,k} &= \langle \hat{a}_{\sigma,k} \rangle^c, \\ \rho_{\sigma,\sigma',k,\mathbf{q}} &= \langle \hat{a}_{\sigma,k}^\dagger \hat{a}_{\sigma',\mathbf{q}} \rangle^c, \\ \kappa_{\sigma,\sigma',k,\mathbf{q}} &= \langle \hat{a}_{\sigma,k} \hat{a}_{\sigma',\mathbf{q}} \rangle^c \\ T_{\sigma,\sigma',\tau,k,\mathbf{q},\mathbf{k}'}^{1,2} &= \langle \hat{a}_{\sigma,k}^\dagger \hat{a}_{\sigma',\mathbf{q}} \hat{a}_{\tau,\mathbf{k}'} \rangle^c \\ T_{\sigma,\sigma',\tau,k,\mathbf{q},\mathbf{k}'}^{0,3} &= \langle \hat{a}_{\sigma,k} \hat{a}_{\sigma',\mathbf{q}} \hat{a}_{\tau,\mathbf{k}'} \rangle^c. \end{aligned} \quad (2.29)$$

We refer to first, second and third order cumulants as singlets, doublets and triplets respectively. Using this notation the cluster expansion of equation 2.26 was found to equal

$$\begin{aligned} i\hbar\dot{\psi}_{\tau,\mathbf{p}} &= \frac{\hbar^2 b^2}{2m} \psi_{\tau,\mathbf{p}} + \frac{1}{2} \sum_{\sigma} \sum_{\mathbf{k},\mathbf{q}} \left[(V_{\sigma,\tau}(\frac{1}{2}(\mathbf{k}-\mathbf{p}+\mathbf{q}), \frac{1}{2}(\mathbf{k}-\mathbf{p}-\mathbf{q}))) \right. \\ &\quad \left\{ T_{\sigma,\tau,\sigma,k+\mathbf{q},\mathbf{p}+\mathbf{q},\mathbf{k}}^{1,2} + \psi_{\sigma,k+\mathbf{q}}^* \kappa_{\tau,\sigma,\mathbf{p}+\mathbf{q},\mathbf{k}} + \psi_{\tau,\mathbf{p}+\mathbf{q}} \rho_{\sigma,\sigma,k+\mathbf{q},\mathbf{k}} \right. \\ &\quad \left. + \psi_{\sigma,k} \rho_{\sigma,\tau,k+\mathbf{q},\mathbf{p}+\mathbf{q}} + \psi_{\sigma,k+\mathbf{q}}^* \psi_{\tau,\mathbf{p}+\mathbf{q}} \psi_{\sigma,k} \right\} \\ &\quad + V_{\tau,\sigma}(\frac{1}{2}(\mathbf{p}-\mathbf{k}+\mathbf{q}), \frac{1}{2}(\mathbf{p}-\mathbf{k}-\mathbf{q})) \left\{ T_{\sigma,\tau,\sigma,k-\mathbf{q},\mathbf{p}-\mathbf{q},\mathbf{k}}^{1,2} \right. \\ &\quad \left. + \psi_{\sigma,k-\mathbf{q}}^* \kappa_{\tau,\sigma,\mathbf{p}-\mathbf{q},\mathbf{k}} + \psi_{\tau,\mathbf{p}-\mathbf{q}} \rho_{\sigma,\sigma,k-\mathbf{q},\mathbf{k}} + \psi_{\sigma,k} \rho_{\sigma,\tau,k-\mathbf{q},\mathbf{p}-\mathbf{q}} \right. \\ &\quad \left. + \psi_{\sigma,k-\mathbf{q}}^* \psi_{\tau,\mathbf{p}-\mathbf{q}} \psi_{\sigma,k} \right\} \Big]. \end{aligned} \quad (2.30)$$

As an example of a direct application of the previous derivation, lets consider equation 2.30 and neglect all cumulants above first order. This gives

$$\begin{aligned} i\hbar\dot{\psi}_{\tau,\mathbf{p}} &= \frac{\hbar^2 p^2}{2m} \psi_{\tau,\mathbf{p}} \\ &\quad + \frac{1}{2} \sum_{\sigma} \sum_{\mathbf{k},\mathbf{q}} \psi_{\sigma,k} \left\{ V_{\sigma,\tau}(\frac{1}{2}(\mathbf{k}-\mathbf{p}+\mathbf{q}), \frac{1}{2}(\mathbf{k}-\mathbf{p}-\mathbf{q})) \psi_{\sigma,k+\mathbf{q}}^* \psi_{\tau,\mathbf{p}+\mathbf{q}} \right. \\ &\quad \left. + V_{\tau,\sigma}(\frac{1}{2}(\mathbf{p}-\mathbf{k}+\mathbf{q}), \frac{1}{2}(\mathbf{p}-\mathbf{k}-\mathbf{q})) \psi_{\sigma,k-\mathbf{q}}^* \psi_{\tau,\mathbf{p}-\mathbf{q}} \right\}, \end{aligned} \quad (2.31)$$

which is an equivalent to the so called Gross-Pitaevskii equation in the Born approximation. This is a closed ordinary differential equation which one will have to solve as a function of t and \mathbf{p} . The solution can then be used to describe the dynamics of the system provided the gas is dilute and weakly interacting [2, 8]. The mathematical advantage of the cluster expansion method is evident,

but the cumulants also have a well defined physical meaning. To really understand the physical context of the cumulant approach however, we need to more specifically define our quantum gas. So far everything has been essentially general. Now we can start to consider how the formalism can be applied to Bose and Fermi gases.

2.2 Condensed Bose gases

The previous sections have introduced the general framework in which quantum gases can be analyzed. This section will more specifically consider how these methods may be applied to condensed Bose gases. A condensed Bose gas is defined as a boson gas in which (nearly) all particles have condensed to some ground state. Thus the ground state is the only state in the system which is macroscopically occupied, and all particles in this state are so strongly correlated that they are often treated as one macroscopic entity, referred to as the condensate [4].

2.2.1 Coherent state approximation

Let us return to the system modelled at the beginning of this chapter. We have a Bose gas where particle states are described in a complete momentum basis, and particles interact via pairwise interactions. Now let us take a closer look at equation 2.27 which defines the cluster expansion into cumulants. Consider the expansion of the two body operator,

$$\langle \hat{a}_{\sigma,\mathbf{k}}^\dagger \hat{a}_{\sigma,\mathbf{q}} \rangle = \langle \hat{a}_{\sigma,\mathbf{k}}^\dagger \rangle^c \langle \hat{a}_{\sigma,\mathbf{q}} \rangle^c + \langle \hat{a}_{\sigma,\mathbf{k}}^\dagger \hat{a}_{\sigma,\mathbf{q}} \rangle^c. \quad (2.32)$$

We see that the cluster expansion has effectively split the expectation value into a factored product, which defines that part of the expectation value which is classically uncorrelated, and an extra cumulant term. This two atom cluster then defines the actual genuine correlation between the two atoms. For n th order cluster expansions the interpretation is similar, in that all factorizations of cumulants represent classical products between correlated atom clusters while the full n th order cumulant represents the complete correlation between all atoms. In second order such a formulation in terms of clusters is equivalent to Wick's theorem [9].

For a direct physical interpretation of the cumulants let us consider a (nearly) condensed Bose gas where the number of excited atoms is very low. We model the dynamics of such a system by the cumulant expansion method. One problem with this formalism is the condensate itself, which as stated earlier is heavily correlated and acts as one macroscopic entity. Thus if the condensate contains N atoms all N th order correlations must be included. To escape this inefficiency several different approaches have been proposed in literature, though their mathematical representation is practically equivalent.

One suggestion in literature is to switch to the so called excitation picture of Bose-Einstein condensation, where the condensate is assumed to be a vacuum state [15]. In this picture the occupancy of the excited states is kept identical to the "real" system. This means that one can effectively ignore the correlations inside the condensate and only focus on the excitation of atoms into higher states.

The picture of Bose-Einstein condensation adopted here is somewhat different, known as the coherent state approximation. We define the ground state as the state for which $\mathbf{k} = 0$, and assume it is macroscopically occupied. It is assumed that the entire condensate forms a coherent state, which means the condensate wave function is an eigenfunction of the annihilation operator, with eigenvalue ψ_0 . Then mathematically it must hold that

$$\hat{a}_{\sigma,0} |\text{BEC}\rangle = \psi_{\sigma,0} |\text{BEC}\rangle, \quad \langle \hat{a}_{\sigma,0} \rangle = \psi_{\sigma,0}, \quad (2.33)$$

where $|\text{BEC}\rangle$ is the many body wave function for the condensate. Also, in general we can decompose operators as

$$\hat{a}_{\sigma,\mathbf{k}} = \psi_{\sigma,\mathbf{k}} + \delta\hat{a}_{\sigma,\mathbf{k}}, \quad (2.34)$$

with $\langle \hat{a}_{\sigma,\mathbf{k}} \rangle = \psi_{\sigma,\mathbf{k}}$ the expectation value of the operator and $\delta\hat{a}_{\sigma,\mathbf{k}}$ the quantum fluctuations around this expectation value. In a Bose condensed gas only the $\mathbf{k} = 0$ state is macroscopically occupied, so $\psi_{\sigma,\mathbf{k}} = \psi_{\sigma,0} \delta_{\mathbf{k},0}$. Then since it was assumed that the condensate forms a coherent state, $\delta\hat{a}_{\sigma,0} = 0$. In physical terms, the assumption was made that the occupation of the condensate momentum mode does not fluctuate, and that the excited modes are only described by fluctuations and not occupied beyond this. The coherent state approximation is thus essentially a mean field approach to the interactions. The approximation is only valid if the condensate mode is the only macroscopically occupied mode [8, 13].

2.2.2 Cumulants

Now we can start considering the cumulants. Since the Hamiltonian is translationally invariant, as signified by the translationally invariant potential and the absence of trapping potentials, any cumulant must conserve momentum. This means the sum of all wave vectors in the creation operators must equal the wave vector sum in the annihilation operators. Any cumulants which do not obey this condition are not physical and must vanish. Let us now consider some cumulants of the zero momentum mode, as an example.

$$\begin{aligned} \langle \hat{a}_{\sigma,0} \rangle^c &= \langle \hat{a}_{\sigma,0} \rangle = \psi_{\sigma,0} \\ \langle \hat{a}_{\sigma,0} \hat{a}_{\sigma,0} \rangle^c &= \langle \hat{a}_{\sigma,0} \hat{a}_{\sigma,0} \rangle - \langle \hat{a}_{\sigma,0} \rangle^c \langle \hat{a}_{\sigma,0} \rangle^c = 0 \\ \langle \hat{a}_{\sigma,0} \hat{a}_{\sigma,0} \hat{a}_{\sigma,0} \rangle^c &= \langle \hat{a}_{\sigma,0} \hat{a}_{\sigma,0} \hat{a}_{\sigma,0} \rangle - 3 \langle \hat{a}_{\sigma,0} \hat{a}_{\sigma,0} \rangle^c \langle \hat{a}_{\sigma,0} \rangle^c \\ &\quad - \langle \hat{a}_{\sigma,0} \rangle^c \langle \hat{a}_{\sigma,0} \rangle^c \langle \hat{a}_{\sigma,0} \rangle^c = 0 \\ &\vdots \end{aligned} \quad (2.35)$$

Here one can see that the coherent state approximation has eliminated the issue of higher order correlations inside the condensate, which all become trivially zero. The correlations of the excited momentum modes then, are defined as follows. As explained, these cumulants must all obey conservation of momentum.

$$\begin{aligned} \psi_{\sigma,\mathbf{k}} &= \langle \hat{a}_{\sigma,\mathbf{k}} \rangle^c, & T_{\sigma,\mathbf{k},\mathbf{q}}^{1,2} &= \left\langle \hat{a}_{\sigma,\mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma,\mathbf{q}} \hat{a}_{\sigma,\mathbf{k}} \right\rangle^c, \\ \rho_{\sigma,\mathbf{k}} &= \left\langle \hat{a}_{\sigma,\mathbf{k}}^\dagger \hat{a}_{\sigma,\mathbf{k}} \right\rangle^c, & T_{\sigma,\mathbf{k},\mathbf{q}}^{0,3} &= \langle \hat{a}_{\sigma,-\mathbf{k}-\mathbf{q}} \hat{a}_{\sigma,\mathbf{q}} \hat{a}_{\sigma,\mathbf{k}} \rangle^c, \\ \kappa_{\sigma,\mathbf{k}} &= \langle \hat{a}_{\sigma,-\mathbf{k}} \hat{a}_{\sigma,\mathbf{k}} \rangle^c, & Q_{\sigma,\mathbf{k},\mathbf{k}',\mathbf{q}}^{2,2} &= \left\langle \hat{a}_{\sigma,\mathbf{q}}^\dagger \hat{a}_{\sigma,\mathbf{k}'}^\dagger \hat{a}_{\sigma,\mathbf{k}'+\mathbf{k}} \hat{a}_{\sigma,\mathbf{q}-\mathbf{k}} \right\rangle^c, \\ Q_{\sigma,\mathbf{k},\mathbf{k}',\mathbf{q}}^{1,3} &= \left\langle \hat{a}_{\sigma,\mathbf{k}+\mathbf{k}'+\mathbf{q}}^\dagger \hat{a}_{\sigma,\mathbf{k}} \hat{a}_{\sigma,\mathbf{k}'} \hat{a}_{\sigma,\mathbf{q}} \right\rangle^c, & (2.36) \\ Q_{\sigma,\mathbf{k},\mathbf{k}',\mathbf{q}}^{0,4} &= \langle \hat{a}_{\sigma,-\mathbf{k}-\mathbf{k}'-\mathbf{q}} \hat{a}_{\sigma,\mathbf{k}} \hat{a}_{\sigma,\mathbf{k}'} \hat{a}_{\sigma,\mathbf{q}} \rangle^c. \end{aligned}$$

Here we have also included the fourth order cumulants or quadruplets, denoted as Q . Any other cumulants appearing in the expansion are complex conjugates of the cumulants defined above. It should be noted that due to translational invariance $\rho_{-\mathbf{k}} = \rho_{\mathbf{k}}$, with similar relations for the other cumulants.

The first order cumulant $\psi_{\sigma,\mathbf{k}}$ is explained by the coherent state approximation, where it vanishes for all but the zero momentum mode. This cumulant mathematically represents the condensate. $\rho_{\sigma,\mathbf{k}}$ counts the occupation of a certain momentum state, and is thus sometimes referred to as the density matrix. Since only the zero momentum mode is assumed to be macroscopically occupied, this number is always very small.

Continuing down the list, the κ cumulant represents the scattering of two atoms with equal but opposite momenta into the BEC. Note that the complex conjugate of κ gives the opposite process where two atoms in the BEC scatter to form two particles in the excited states \mathbf{k} and $-\mathbf{k}$, also known as quantum depletion. The value of this cumulant is referred to as the transition amplitude of such a scattering event [4]. Following this line of reasoning, the T cumulants also represent scattering processes, where for example $T_{\sigma,\mathbf{k},\mathbf{q}}^{1,2}$ represents the scattering of two excited atoms with one particle transferring all its momentum to the other one. Interestingly one can also imagine two particles scattering with the condensate to excite a third particle which was previously condensed. We thus see that $T^{1,2}$ can be filled by different multiple body scattering processes. Conversely, the $T_{\sigma,\mathbf{k},\mathbf{q}}^{0,3}$ can only represent a three particle scattering process [4]. Figure 2.1 illustrates the points made in this section.

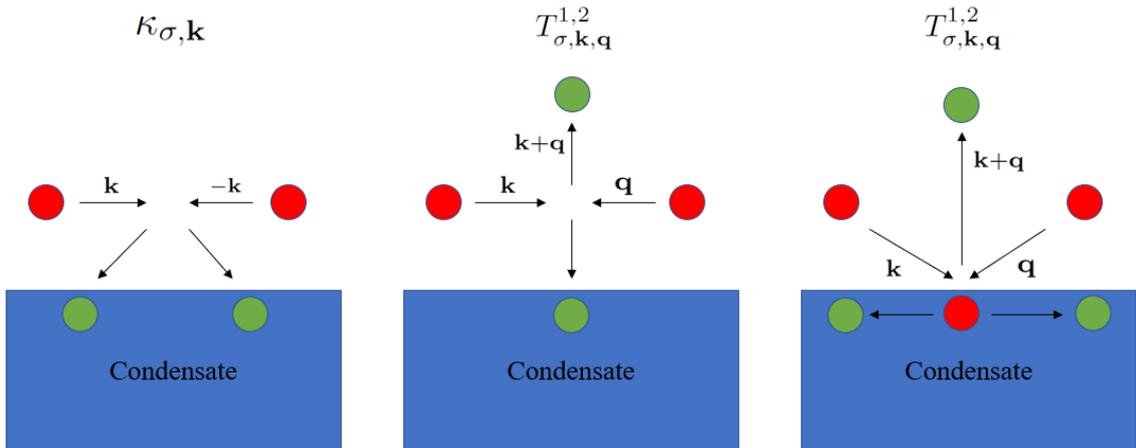


Figure 2.1: Simplified illustration of scattering events with their corresponding cumulants. Note that the $T^{1,2}$ cumulant is filled by both two and three particle scattering. Ingoing and outgoing particles drawn in red and green respectively.

This physical interpretation shows that solving the dynamics of the cumulants provides the dynamics of the entire system, where complex phenomena such as quantum depletion and scattering into the condensate are entirely described. Obviously the expectation value of the operators also contains this information, but it is intermixed with all other correlations of the operator products, which does not allow for such straightforward physical interpretations. The cluster expansion has effectively split the expectation values into cumulants that describe all correlated dynamic processes in the condensate. Since these cumulants also allow us to write the Heisenberg equation as a system of

closed ordinary differential equations, the dynamics of such cumulants can in principal be solved.

2.2.3 Bose mixtures

The momentum conserving cumulants written down in equation 2.36 all act within one component of the gas, specifically the σ component. Stating that these are the only nonzero cumulants in the equations actually makes an assumption about the quantum gas in question. In general, so called mixture cumulants will also exist in the gas, which describe the interactions between different components. Some second and third order mixture cumulants read

$$\begin{aligned} \rho_{\sigma,\tau,\mathbf{k}} &= \langle \hat{a}_{\sigma,\mathbf{k}}^\dagger \hat{a}_{\tau,\mathbf{k}} \rangle^c, & T_{\sigma,\sigma,\tau,\mathbf{k},\mathbf{q}}^{1,2} &= \langle \hat{a}_{\sigma,\mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\tau,\mathbf{q}} \hat{a}_{\tau,\mathbf{k}} \rangle^c, \\ \kappa_{\sigma,\tau,\mathbf{k}} &= \langle \hat{a}_{\sigma,-\mathbf{k}} \hat{a}_{\tau,\mathbf{k}} \rangle^c, & T_{\sigma,\tau,\mathbf{k},\mathbf{q}}^{0,3} &= \langle \hat{a}_{\sigma,-\mathbf{k}-\mathbf{q}} \hat{a}_{\tau,\mathbf{q}} \hat{a}_{\tau,\mathbf{k}} \rangle^c. \end{aligned} \quad (2.37)$$

The specific physical interpretation of these mixture cumulants will depend on the role assigned to the Greek index. In general however a gas consisting of two components σ and τ , will have two coherent condensates represented by $\psi_{\sigma,0}$ and $\psi_{\tau,0}$. Using this we can consider scattering processes that might constitute the mixture cumulants defined in equation 2.37. The $\rho_{\sigma,\tau,\mathbf{k}}$ represents a process in which an excitation of species σ is created at the cost of a particle of species τ . One can imagine a scattering process in which an excited particle of species τ scatters with the σ condensate, thus exciting one particle. The impeding τ particle is then scattered into its own condensate. The mixture $\kappa_{\sigma,\tau,\mathbf{k}}$ cumulant will describe much the same processes as the single component version, although it can now also describe two particle scattering of different species into their respective condensates. For third order cumulants there are obviously many more mixture cumulants that one could write down. Two examples are given in equation 2.37.

The $T_{\sigma,\tau,\mathbf{k},\mathbf{q}}^{1,2}$ cumulant will represent some collision in which two τ particles excite an atom in the σ condensate, transferring all their momenta in the process. Note that this mixture cumulant is always a three body scattering process whereas the single component version could still be filled by two body scattering. $T_{\sigma,\tau,\tau,\mathbf{k},\mathbf{q}}^{0,3}$ can now additionally represent three body scattering between different species.

One should note that different models of study will be interested in different mixture cumulants. For example the $\rho_{\sigma,\sigma',\mathbf{k}}$ cumulant as described above was related to a very specific scattering process. Different models might choose to set such cumulants to zero and thus assume that particles can not scatter in this way. Inclusion of all mixture cumulants will obviously give the most accurate result, but applying smart approximations can lead to much shorter cumulant equations. Ultimately the choice for which mixture cumulants to include can only be answered when a specific system of study has been defined. If one were to exclude all mixture cumulants from the system, then all interspecies scattering processes are ignored. Because of this we will refer to such a system as a "**Non-interacting mixture**" in this work.

2.2.4 Truncating the cumulant expansion

Effectively, the higher order and non number-conserving cumulants represent the deviation from the interaction free model of a quantum gas. This is in agreement with the interpretation of the cumulant expansion as a measure of the correlation between atom clusters. The stronger the interaction, the stronger the correlations and thus the more relevant higher order cumulants become. Usually higher order cumulants are lower in amplitude than their lower order counterparts, although deciding where to truncate the expansion requires careful consideration of the interactions present in the system [2].

Truncating the cumulant expansion is also referred to as breaking the hierarchy. This is because the (unsolvable) exponential growth of clusters with each higher order cumulant equation is dubbed the BBKGY hierarchy in literature [4].

Interaction strength in Bose gases is controlled by the s-wave scattering length a , which is calculated from the number of particles in a scattering volume a^3 . We characterize the interaction length by the diluteness parameter $\bar{n}|a|^3$, with n the particle density [8]. Experimentally this parameter can be tuned by so called Feshbach resonances using a magnetic field. This allows experimentalists to study the Bose gas in different interaction regimes. If the scattering length becomes much larger than the inner particle spacing, all particles become heavily correlated. This is known as the unitarity regime, where strong interactions play the largest role in interacting atoms [13].

In 1996 Fricke suggested a general methodology for "breaking the hierarchy" in the cumulant equations. From equation 2.30 we notice that the equation of motion for a cumulant of order n has cumulants up to order $n + 2$ on the rhs. Fricke proposed that if one seeks all cumulant equations up to a certain order n , then for each EOM neglect all cumulants of order higher than n , and only consider the dynamics of cumulants up to order n . This provides a system of closed ordinary differential equations which one can attempt to solve for the dynamics of the system. [3]. An example of this method was already shown in the previous section, where the cumulant equations were approximated up to order $n = 1$. This yields the Gross-Pitaevski equation which is applicable in the assumption that scattering lengths are relatively small. Additionally, one assumes that the gas is dilute enough so higher order correlations between particles can be neglected [2].

If one were to use Fricke's method up to order $n = 2$ then after calculating the second order cumulant equations one would obtain a closed system of so called Hartree-Fock-Bogoliubov equations. It should be noted that such an approach is equivalent to an expansion in $V\Delta t$ which means the lower order approximations are only valid for short timescales [3].

Obviously the method suggested by Fricke is not the only way to truncate the expansion. Other methods have been proposed which give more accurate dynamics of the multiple scattering processes in quantum gases. However the general idea behind all these methods is to provide a general procedure to break the hierarchy of the dynamic equations, which doesn't allow for any ambiguity in the approximation [2].

Using Fricke's method up to order 1 with the coherent state approximation will then give the dynamics of all first order cumulants, which in the coherent state approximation is only the dynamics of the condensate or ψ_0 .

$$i\hbar\dot{\psi}_{\tau,0} = \sum_{\sigma} V_{\sigma\tau}(\mathbf{0}, \mathbf{0}) |\psi_{\sigma,0}|^2 \psi_{\tau,0}. \quad (2.38)$$

This then is the equivalent of the Gross-Pitaevski equation presented in equation 2.31 for the condensed Bose gas in the coherent state approximation. As was discussed before, this equation can only hold in a Bose gas that is sufficiently dilute for scattering processes to be ignored. This also explains the absence of the ρ and κ cumulants which originate from scattering events. This equation looks very similar to the Schrödinger equation in momentum space and is thus sometimes referred to as the Nonlinear Schrödinger Equation (NLSE) in literature [16]. The natural progression for cumulant theory now is to calculate the equations of motion for higher order cumulants, which would allow for the inclusion of scattering processes. The script developed in this work automates this exact procedure, namely the calculation and proper simplification of the cumulant equations up to higher orders.

2.3 Fermi gases

We now shift our focus from the condensed Bose gas to the general Fermi gas, which only contains fermions. Effectively this means a change of commutations relations and thus statistics, which leads to entirely different behaviour. In particular due to the anti symmetry of the fermion wavefunction the Pauli exclusion principle holds, which states that no two particles can exist in the same quantum state. This then makes a fermion condensate impossible, since the ground state can only house as many fermions as its degeneracy allows. At low temperatures N fermions will then occupy the N single particle states of lowest energy. This energy of the highest state occupied is then referred to as the Fermi level [7].

2.3.1 Fermion Hamiltonian

The antisymmetry of fermion wavefunctions allows us to rewrite the Hamiltonian in equation 2.16 into a more convenient form. In the original Hamiltonian no assumption was made on the symmetry or asymmetry of the matrix elements in the potential. Let us now write an antisymmetrized matrix element with the subscript A . We can define such a matrix element by the following identity [10, 11].

$$\langle \mathbf{kq} | \hat{V} | \mathbf{k}'\mathbf{q}' \rangle_A = \langle \mathbf{kq} | \hat{V} | \mathbf{k}'\mathbf{q}' \rangle - \langle \mathbf{kq} | \hat{V} | \mathbf{q}'\mathbf{k}' \rangle \quad (2.39)$$

By applying the fermion commutation relations we can now write the interaction term for fermions as

$$\hat{V}_{tot} = \frac{1}{4} \sum_{\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}'} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{q}}^\dagger \langle \mathbf{kq} | \hat{V} | \mathbf{k}'\mathbf{q}' \rangle_A \hat{a}_{\mathbf{q}'} \hat{a}_{\mathbf{k}'}. \quad (2.40)$$

The full many body Hamiltonian for fermions then becomes

$$\begin{aligned} \hat{H}_{tot} = & \sum_{\sigma, \mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{a}_{\sigma, \mathbf{k}}^\dagger \hat{a}_{\sigma, \mathbf{k}} \\ & + \frac{1}{4} \sum_{\sigma, \sigma'} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} V_{\sigma, \sigma'}^A \left(\frac{1}{2}(\mathbf{k} - \mathbf{k}' + 2\mathbf{q}), \frac{1}{2}(\mathbf{k} - \mathbf{k}') \right) \hat{a}_{\sigma, \mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\sigma', \mathbf{k}'} \hat{a}_{\sigma, \mathbf{k}}. \end{aligned} \quad (2.41)$$

Use of anti symmetrized matrix elements has altered the interaction term in the Hamiltonian by a factor of $\frac{1}{2}$. Although the difference in the Hamiltonian is minimal, the cumulant equations often contain many expressions like the one on the rhs in 2.39. Thus this definition allows us to shorten the final equations considerably.

2.3.2 Fermion wave function

For the boson gas we introduced the coherent state approximation which allowed us to effectively handle the highly correlated condensate. Obviously in a Fermi gas such an assumption is not necessary and also not physical. In literature different wave functions have been proposed for a many body Fermi gas. Examples of these are Slater determinants, quasi-particle vacuums based on Bogoliubov transformations and generalized density matrices [10, 17]. A simple specific example of a ground state wave function one might use for fermions reads as

$$|\psi\rangle = \prod_{\mathbf{k}} \hat{a}_{\mathbf{k}} |0\rangle, \quad (2.42)$$

where the product runs over all occupied single particle momentum states, which in ground state means all states beneath the Fermi level [18]. In this work however the exact wave function used is further left unspecified, since this has no relevant impact on the calculation of the cumulant expansion. In actuality the choice of wave function will mean different cumulants are required. Changing the input cumulants can easily be done in the script developed in chapter 3.

2.3.3 Cumulants

For fermions we still assume a translationally invariant Hamiltonian, which means all cumulants must conserve momentum, as was the case for bosons.

Due to the coherent state approximation made for bosons 1st order cumulants like $\langle \hat{a}_{\sigma,0} \rangle^c$ had to be included in the cumulant expansion. For fermions these cumulants are always zero and can thus be ignored in all expansions [10]. By extension then, all cumulants of uneven order can be set to zero for fermions. Thus the only relevant cumulants for fermions read

$$\begin{aligned} \rho_{\sigma,\mathbf{k}} &= \langle \hat{a}_{\sigma,\mathbf{k}}^\dagger \hat{a}_{\sigma,\mathbf{k}} \rangle^c, \\ \kappa_{\sigma,-\mathbf{k},\mathbf{k}} &= \langle \hat{a}_{\sigma,-\mathbf{k}} \hat{a}_{\sigma,\mathbf{k}} \rangle^c, \\ Q_{\sigma,\mathbf{q},\mathbf{k},\mathbf{q}-\mathbf{k},\mathbf{k}'+\mathbf{k}}^{2,2} &= \langle \hat{a}_{\sigma,\mathbf{q}}^\dagger \hat{a}_{\sigma,\mathbf{k}'}^\dagger \hat{a}_{\sigma,\mathbf{k}'+\mathbf{k}} \hat{a}_{\sigma,\mathbf{q}-\mathbf{k}} \rangle^c, \\ Q_{\sigma,\mathbf{q},\mathbf{k}',\mathbf{k}}^{1,3} &= \langle \hat{a}_{\sigma,\mathbf{k}+\mathbf{k}'+\mathbf{q}}^\dagger \hat{a}_{\sigma,\mathbf{k}} \hat{a}_{\sigma,\mathbf{k}'} \hat{a}_{\sigma,\mathbf{q}} \rangle^c, \\ Q_{\sigma,\mathbf{q},\mathbf{k}',\mathbf{k}}^{0,4} &= \langle \hat{a}_{\sigma,-\mathbf{k}-\mathbf{k}'-\mathbf{q}} \hat{a}_{\sigma,\mathbf{k}} \hat{a}_{\sigma,\mathbf{k}'} \hat{a}_{\sigma,\mathbf{q}} \rangle^c. \end{aligned} \quad (2.43)$$

As always, researchers can choose to neglect select cumulants to obtain shorter expressions, as was done with $Q^{0,4}$ in ref [5]. The ordering of indices in the above notation has also been kept in accordance with this paper. Note that we no longer use shorthand notation for the wave vectors in κ , and instead explicitly mention the wavevector of each operator. This is because κ is no longer a symmetric matrix. Due to commutation relations we now have $\kappa_{-\mathbf{k},\mathbf{k}} = -\kappa_{\mathbf{k},-\mathbf{k}}$. Because of this it is important to be more specific with the notation.

For fermions the $\kappa_{-\mathbf{k},\mathbf{k}}$ cumulant is also called the pairing tensor, and is related to the formation of correlated Cooper pairs which show very similar behaviour to bosons [19]. Note that the κ cumulant as described above does not necessarily conserve particle number, since two particles are removed from the system with no direct counter. The exact details here however depend on the chosen wave function. For example if the gas is (nearly) in a ground state defined by equation 2.42 with \mathbf{k} a momentum state below the Fermi level, then the κ cumulant would be interpreted as an excitation of a Cooper pair to a state above the Fermi level. Also, since Cooper pairs act as bosons they can form their own condensate. In this way the κ cumulant can be interpreted as excitations from the "Cooper condensate". Obviously the number of Cooper pairs should then be quite large.

The ρ cumulant still counts states in a given momentum mode. Obviously for a single component Fermi gas ρ can never be more than 1.

2.3.4 Fermi mixtures

Similarly to the Bose gas, we can also consider fermion mixture cumulants. Much of the analysis is similar to the Bose gas and won't be repeated here, but one application is of specific interest for Fermi mixtures, namely Fermi gases with particles of different spin. Consider for example a gas consisting of electrons, which have either spin up or spin down. We refer to the spin up state as σ and spin down as τ . Interesting here is the ρ cumulant, which can now describe a process wholly different from scattering. It is well known that electrons will attempt to align their spin (or magnetic dipole moment μ) with an external magnetic field, a phenomena known as paramagnetism. Knowing this, one notices that the $\rho_{\sigma,\tau}$ cumulant could also represent spin flipping under influence of an external magnetic field.

This is a clean example of how cumulant theory and its results can be applied to explore the magnetic behaviour of fermion systems. In literature the formalism has also been used to explore dipole-dipole interactions in denegerate Fermi gases of ^{161}Dy and ^{167}Dy [5], and even in neutron stars [20].

Chapter 3

Model

As shown in the theory section, formulating the dynamic equations becomes a cumbersome task for higher order cumulants, and mistakes can easily creep into manual derivations by the abundance of different indices. This work presents a Mathematica script which calculates the cumulant equations up to arbitrary order automatically, and can print the result simplified under certain assumptions. This means the script can be applied both generally and also to several specific systems. The script can also easily be expanded to write down the cumulant equations for more specialized systems, owing to Mathematica's ease of adaptability.

During the writing of this script the most prevalent challenges that had to be overcome were related to limitations with functions in Mathematica and used packages. Additionally, obtaining results within manageable computation times proved a challenge. Throughout this chapter the developed scripts are explained, and we show how the above challenges were overcome. First the model environment, Mathematica, is introduced. This script heavily relies on a second quantization package for Mathematica called SNEG [6]. Since this package is so important for this script, a short overview of its use will also be given in this section.

The next section will then provide the general framework which the script is based upon, and gives a step by step walk through of the computation. This work relies on several custom functions which expand the SNEG package to work with the cumulant expansion. These custom functions will be introduced and explained in the next section, which gives more detailed insight into the exact workings of the script. Finally, the last section will discuss the way in which the script simplifies the cumulant equations under certain assumptions, which will clearly be dependent on the specific application.

3.1 Model environment

The script was written using Mathematica in its interactive notebook environment. The choice to use Mathematica was made because it is naturally suited to deal with and simplify symbolic expressions, and its output is generally printed in an easily interpreted form. This contrasts with other numeric software that could be applied to this problem like Matlab. Where such software might provide advantages in programmability and computation time, it becomes significantly more difficult to work with complicated symbolic expression in its interfaces. Since the calculation of the cumulant equations will always involve long and symbolically heavy operator expressions, Mathematica was taken to be the optimal choice. Throughout this chapter we notate Mathematica functions as **function**[..] and variables as **variable**.

Next to the functions inherent to Mathematica, the script uses the Mathematica package "SNEG" written by Rok Žitko [6]. This package extends Mathematica to be able to work in the language of second quantization. The reach of SNEG is quite wide in its applications, however for this work only a small subset of its features are important. These are mainly related to the application of commutation relations, the calculation of operator commutators and the simplification of sums over operator expressions. To clearly explain the code, a quick overview of the relevant features in the SNEG package are given here.

Most important in writing down the cumulant equations are operations on creation and annihilation operators. In SNEG such operators are defined by specifying several operator properties. First one defines whether SNEG should treat the operator as if it acts on bosons or fermions. Let us define an operator **a** for bosons and an operator **b** for fermions in the SNEG package as follows.

snegbosonoperators [**a**] , **snegfermionoperators** [**b**] .

To more specifically define creation and annihilation operators SNEG requires function arguments to be given to the allocated variables. The first argument specifies whether the operator is a creation or annihilation operator, while all other arguments are interpreted as indices. So if one would like to define the annihilation operator for boson state $|\mathbf{p}\rangle_\tau$ as it was used throughout the theory section, the corresponding Mathematica code would be **a**[**AN**, τ , **p**]. The first argument can read either AN or CR for annihilation and creation operators respectively. SNEG needs to make a distinction between letters used as indices and those used as normal variables. The indices are specified at the start of the script, by the **snegfreeindexes**[..] function.

The SNEG package allows for calculations with these operators which automatically obey the commutation relations defined in the theory chapter. Such commutative operator products are defined in the SNEG package by the **nc**[..] function, where the multiplied operators can be given as arguments. Care should be taken that SNEG automatically normal orders operator products, in which the commutation relations are applied when necessary. This script also heavily relies on the **sum**[..] function in SNEG, which modifies the native sum function in Mathematica to work properly in the second quantization formalism, and is also better suited to handle symbolic sums. As discussed before, it is important that all indexes in the SNEG sum function are properly defined as indices in the script. One final SNEG function that is central to the operation of this script is the **komutator**[..] function, which simply calculates the commutator between two operator expressions.

3.2 Script operation

Now that the framework in which the script operates has been introduced, it is instructive to consider the general work flow of the script. This section will give a step by step walk through of the entire script starting from the beginning and ending with the final (simplified) cumulant equations. Note that the Mathematica notebook itself also contains comments which give a brief explanation with each step. This section aims to expand on these comments and provide some more detail.

Note that every script is split into two sections, one for bosons and one for fermions. In a lot of ways these two sections operate in similar ways and follow the same structure, but the differences will be clearly highlighted in this chapter.

3.2.1 Species index

In the theory section an extra Greek index was introduced in all creation and annihilation operators, which would specify the specific species of the atom in question. The way this index is handled however, depends on the exact details of the model used in a specific application. To make the

script more widely applicable, several versions were written which deal with the Greek index in a different way. All these scripts are based on the same structure and use the same functions, but differ somewhat in their definitions and rule sets. Each of these three scripts contains a boson and fermion version.

- **Single Component.nb** Here the Greek index is ignored completely. Effectively this means a single component quantum gas is considered. All definitions from chapter 2 still hold but without the extra index. This is the simplest version of the script.
- **Non-Interacting Mixture.nb** Here the Greek index is used, however it is assumed that all cumulants which contain different Greek indices are zero. Physically this script considers a multicomponent gas in which interaction processes between different components (represented by mixture cumulants) are ignored. Note that this name is somewhat misleading since there is still interspecies interaction through the pairwise potential. In this report if we say non-interacting mixture we refer explicitly to the cumulants.
- **Interacting Mixture.nb** Here the index is used generally, without any assumptions made about the gas. Thus all mixture cumulants which describe interaction processes between the components are used in computations. This version of the script is most general, but also gives the longest expressions.

3.2.2 Preamble

Before looking at the entire script, let us consider the blocks of code at the start. Next to the functions inherent to Mathematica and the additional functions supplied by the SNEG package, several custom functions were written which expand the SNEG package to be able to carry out the operations needed for the derivation of the cumulant equations. These functions are defined in the additional Mathematica library "**cuFunctions.nb**". It is essential that the SNEG package and the function library are loaded at the beginning of the script. The very first block takes care of this. During the writing of the script it was often found to be convenient to use slightly different notation in the Mathematica script compared to the conventions used in the report. Also, long expressions printed in Mathematica's notation are often very messy and hard to interpret. Conveniently Mathematica is able to rewrite expression to a form in conventional mathematical notation, which in Mathematica is referred to as the "**TraditionalForm[...]**". At some points in the code **TraditionalForm[...]** notation will be defined for several functions. These do not impact calculation, and whenever the Mathematica form differs from the traditional form it will be mentioned in this chapter.

Before the script starts with actual calculation, the user can define all indices and other variables to be used. This will be referred to as the preamble of the report, and exists of two code blocks. The first is a set of definitions, which are explained in table 3.1.

Function/variable	Description	Default
snegbosonoperators [..]	Define all variables to be used as creation/annihilation operators for bosons	a
snegfermionoperators [..]	Define all variables to be used as creation/annihilation operators for fermions	b
sumwavevectors	Define wave vector indices that are summed over in Hamiltonian	{ k,q,k1,q1 }
sumspecies	Define species indices that are summed over in Hamiltonian	{ $\sigma,\sigma 1$ }
opwavevectors	Define wave vector indices that aren't summed over	{ p,l,g }
opspecies	Define species indices that aren't summed over	{ τ,γ }
ordering [..]	Define the normal ordering for operators, most relevant for fermions.	For bosons: EMPTY For fermions: SEA

Table 3.1: All variables defined and functions run in the preamble of the Mathematica script, with an explanation of their meaning. The third column contains the default values. Note that not all of these appear in all versions of the script.

The last line contains the **ordering**[..] function, which defines the state specific normal ordering SNEG should use for a given operator. This ordering can be defined as **EMPTY**, in which case SNEG assumes that all states are non filled. This is most appropriate for a Bose Einstein Condensate. One could also define the ordering as **SEA**, which assumes that all states up to the Fermi level are filled with atoms, most appropriate for a Fermi gas. Note that in SNEG we notate fermion operators as **b**, while in this report they will always be written as \hat{a} .

The second cell in the preamble only contains two more definitions, but they are central to the operation of the entire script. The first variable "**order**" defines the order of approximation which the script will use. The **order** variable is actually a list containing two values, which gives the user more control over how the equations are calculated. The first number in the list gives the maximum order of cumulant equation that will be calculated. The second number of the list defines the maximum order of cumulant that should be kept on the right hand side of the Heisenberg equation after the cluster expansion. For example, if one were to set the **order** variable to **{2,4}** then the Heisenberg equation would be calculated for all cumulants up to order 2, were the equations themselves can contain cumulants up to order 4. If one aims to use the Fricke method for truncating discussed in section 2.2.4, then the two numbers should be equal.

The second variable **ops** defines a list filled with all operator products of interest. In other words, if one wants to calculate the cumulant equations for certain operator products, they should be defined here. By default the momentum conserving operator products are defined here up to fourth order, but one could change these or add more if desired. As was discussed in chapter 2, the inclusion of certain mixture cumulants heavily depends on the specific model used to describe the gas. This is why this variable is left completely open to user customization.

Note that the **Non-Interacting Mixture.nb** and **Interacting Mixture.nb** script differ mostly in the default definition of the ops list. Specifically the **Non-Interacting Mixture.nb** contains

only cumulants within the same component, which really makes it a more restrictive version of the **Interacting Mixture.nb** script.

The recommended operation of the script then becomes to first draft a model of the gas of interest with all assumptions. Then from these assumptions one can derive which cumulants can be set to zero from the beginning. For example in a mixed Fermi gas without any external magnetic field, one would expect the ρ mixture cumulant to be zero due to the absence of spin flipping. If one has obtained a complete set of cumulants that are relevant to the theory, they can be entered into the operator list **ops** and the corresponding equations can be calculated.

3.2.3 Workflow

Now that all variables and functions have been defined in the preamble, the script can start actual computation. A full overview of the workflow which the script follows to calculate the cumulant equations is shown in figure 3.1.

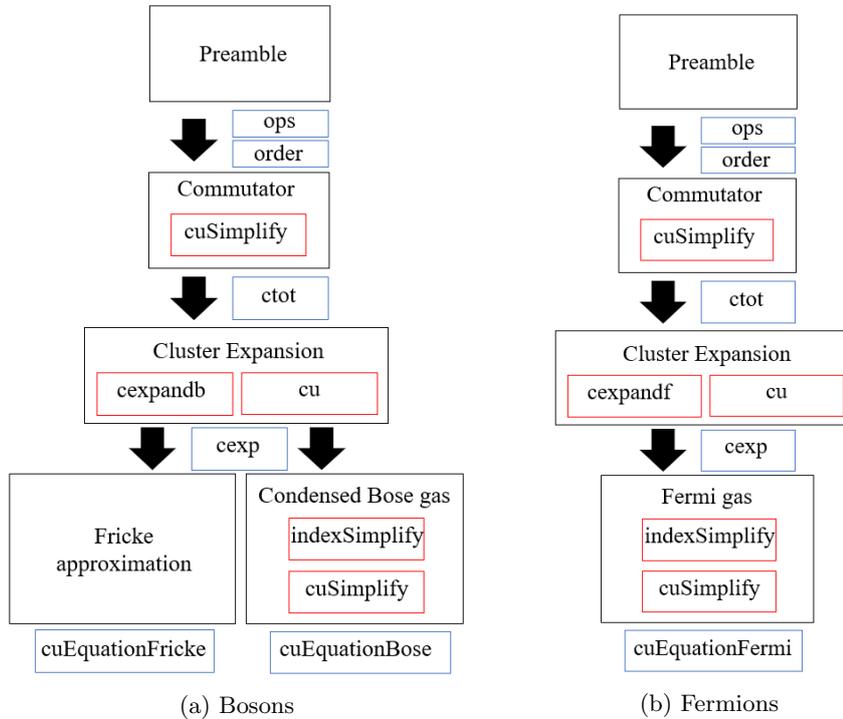


Figure 3.1: Schematic overview of the workflow used in the script. Black boxes represent subsections of the script which should be read from top to bottom. Blue boxes represent results and variables, red boxes represent custom functions used.

This figure shows a schematic representation of the global work flow of the entire script. Each step (black box) will produce certain results saved in a variable, represented by a blue box. The results are produced with the use of SNEG functions and custom functions from the **cuFunctions.nb** library. Any custom functions used are shown with a red box. One notices that the work flow for bosons and fermions is very similar, but diverges somewhat for the last step. This will be explained in more detail later.

The next part of the script after the preamble carries out the first actual computation, namely the commutator of the operator products defined in variable `"ops"` with the Hamiltonian. This is then the right side of the Heisenberg equation as defined in equation 2.20. As seen in section 2.1.4 manual simplification of these commutators becomes cumbersome for longer strings of operator products, and such a process is prone to mistakes. This part of the script carries out the calculation and simplification of the commutator automatically, solving the potential issues with manual evaluation.

To aid in troubleshooting, the single particle terms and interaction terms of the commutator are calculated separately. The basic workings of this part of the code are relatively straightforward. For each element in the operator list `"ops"` the appropriate commutator is calculated and stored in a list called `"ctot"`. Here only the operator products are used which obey the order restriction. One might wonder why a union function is required here for bosons. A quirk in the way SNEG is programmed makes it somewhat difficult to determine the order (length) of an operator product as it is defined by the `nc[...]` function. A simple evaluation of the product length using standard Mathematica functions works for all but the first order product, which requires special treatment. Thus a union function is used which makes sure also first order products are included in the commutators. For fermions this problem is absent, since first order cumulants are automatically zero in a Fermi gas.

Note that at this point in the script we use the same Hamiltonian for both bosons and fermions for calculating the commutators, even though in section 2.3.1 an altered Hamiltonian was introduced for fermions. This choice was made to keep the start of the script as general as possible. Later on in the script then the user can make the choice to introduce anti-symmetrised matrix elements if this is desired. This functionality is explained further in section 3.4.1. Throughout the whole script we notate $V_{\tau,\tau}(\mathbf{k}, \mathbf{p})$ as $V[\{\mathbf{k}, \mathbf{p}\}, \{\tau, \tau\}]$. Also note that at this point we use a placeholder function $f[\mathbf{k}]$ for the kinetic energy.

The list `ctot` now contains the right hand side of the Heisenberg equation for each operator product defined in the preamble. Having this the full Heisenberg equation can easily be defined, and the script can move on to the calculation of the cluster expansion. This is done using the custom function `cexpandb[...]` for bosons or `cexpandf[...]` for fermions. Together with the `cu[...]` function used for notation the full cluster expansion of each commutator is now stored in the variable `"cexp"`. The exact workings of the two cluster expand functions will be explained later in the next section.

In principal the calculation of the cumulant expansion is now finished, and all that remains is the application of simplifying assumptions to shorten them. Before looking at the simplification steps however, it is instructive to take a closer look at the functions used in the previous steps and how they operate. This will be discussed in the next section.

3.3 Custom functions

The script contains several custom functions which either expand SNEG's functionality or solve issues that came up during writing. This section will give an overview of each function and explain its workings in detail. All of these functions are stored in the library `cuFunctions.nb`, and thus it is essential that this library is loaded whenever one works with this script.

3.3.1 Delta functions

As was shown algebraically in section 2.1.4, calculating the commutator gives a sum over the indices containing multiple delta functions. The properties of the delta function then allow one to remove some indices from the summation thus simplifying the final expression. In principle SNEG contains a simplification function that can do this automatically, namely the `sumSimplifyKD[...]` function,

which takes a sum as input and then simplifies all delta functions where possible. In addition to this SNEG also contains other simplification functions. The most general one, `sumSimplify[.]`, simplifies sums in much the same way that the native simplification functions in Mathematica operate, but with some additional rules for symbolic sums.

However several issues with the `sumSimplifyKD[.]` function were found whilst writing the code. The largest issue discovered was SNEG's inability to deal with delta functions containing sums of indices. To illustrate this, let's assume one wants to simplify a sum as

$$\sum_{\mathbf{k}, \mathbf{q}} \delta_{\mathbf{k}+\mathbf{q}, \mathbf{p}} \hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{q}} = \sum_{\mathbf{k}, \mathbf{q}} \delta_{\mathbf{k}, \mathbf{p}-\mathbf{q}} \hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{q}} = \sum_{\mathbf{q}} \hat{a}_{\mathbf{p}-\mathbf{q}} \hat{a}_{\mathbf{q}}. \quad (3.1)$$

Expressions similar to those in equation 3.1 often appear in equations, and thus it is important that they be simplified correctly. The issue with SNEG arises when two dummy summation indices are summed together inside a delta function. Here a choice has to be made to eliminate either \mathbf{k} as done above, or eliminate \mathbf{q} . To force SNEG to make this choice one of the two indices must be isolated inside the delta function, as is done in the first step in equation 3.1. It should be noted that SNEG also encounters issues if the summation index inside the delta function has a minus sign in front.

The library file "`cuFunctions.nb`" contains a function called `deltaSwap[.]`, which applies a permutation to indices inside delta functions to obtain a form which is simplified properly by the `sumSimplifyKD[.]` function. `deltaSwap[.]` takes two arguments, where the first argument is the delta function one aims to rewrite. The second argument is the list of wave vectors that may appear as summation indices, which would by default be the `sumwavevectors` list defined in the preamble. The basic operation of the `deltaSwap[.]` function is as follows.

Input: `{KroneckerDelta[x, y], sumwavevectors}`

For each element `i` in `sumwavevectors`

```

    Solve x = y for i
    If solution is found
        x = i
        y = solution
        Break
    Else
        Break

```

Output: `KroneckerDelta[x, y]`

By this procedure all delta functions are written to a form where a summation vector is isolated. Note that the actual Mathematica functions look quite different at first. This is because iterative `For` statements don't really exist in Mathematica in this form. The operation of the function is essentially the same however, and this is a much cleaner way of writing it. For the remainder of this chapter if we need to write code we will often write it in such "pseudo-code" notation.

The `deltaSwap[.]` function is applied to an expression indirectly through a second parent function, called `cuSimplify[.]`. It also takes two arguments, the first one being the expression that one aims to simplify. If one wishes to apply some assumption related to delta functions then a replacement rule set can also be given as the second argument. This will be useful in the simplification section. The `cuSimplify[.]` code contains three basic operations on delta functions, of which the `deltaSwap[.]` function is one. Their effect is shown in figure 3.2.

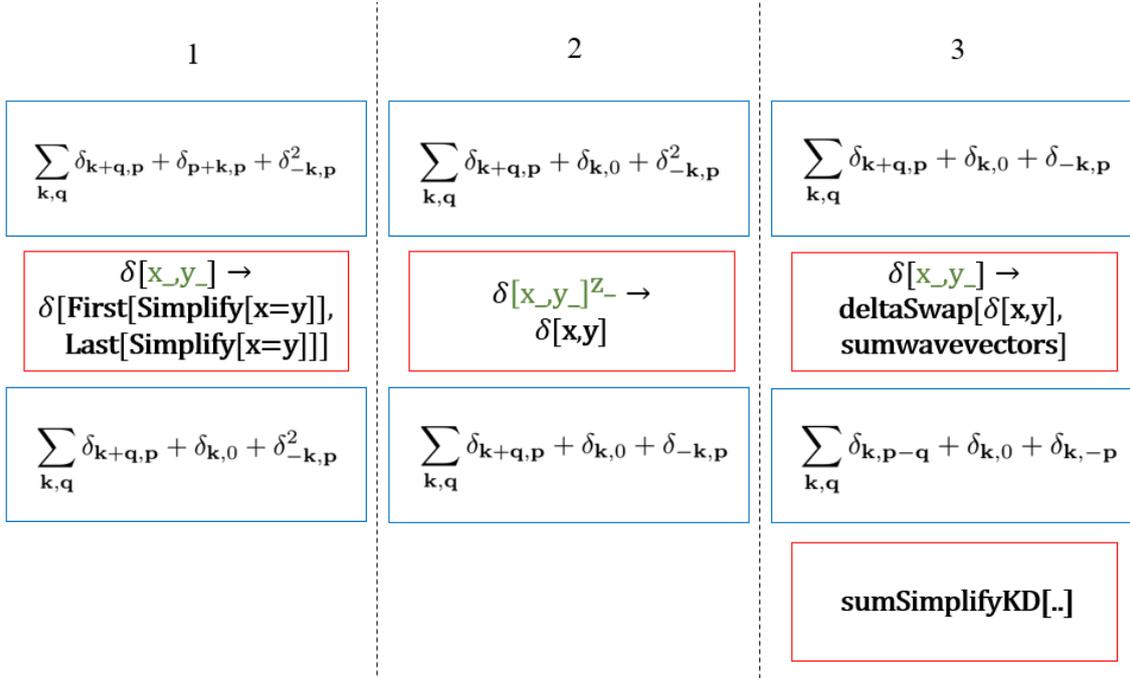


Figure 3.2: Effect of all transformations in the `cuSimplify[.]` function. An example input is shown in the top left, which is rewritten in three steps read from left to right. Each step represents a distinct transformation, read from top to bottom. The final output is then shown in the bottom right. We still represent results by blue boxes and functions/transformations by red boxes.

After these three transformations the `sumSimplifyKD[.]` function can finally be applied for sum simplification. Important to note is that this function is actually mapped over each term instead of applied to the total expression directly. It was found that this simple restriction provides a significant computation time decrease for long sums, which is advantageous for higher order calculations. This may be due to the exponential increase in possible simplifying permutations Mathematica attempts to apply when the sums contain many terms. By only simplifying each term individually this pitfall is avoided. To properly apply the mapping `cuSimplify[.]` contains a line which expands the total sum into individual terms via the `sumExpand[.]` function in SNEG. Several steps in `cuSimplify[.]` are applied twice, which cleans up all residual delta functions that could possibly appear after initial runs. This is especially important for step 2 in figure 3.2.

3.3.2 Cluster expansion

Once the commutator has been calculated and simplified properly, the script starts computing the cluster expansion of all expressions. This part of the script relies on a custom function written for this purpose, called `cexpandb[.]`. This section will explain the operation of this function in detail.

The `cexpandb[.]` function takes an operator product defined by the SNEG function `nc[.]` as input. The function then computes the cluster expansion of the given operator product. This cluster expansion is exactly equivalent to the one defined in equation 2.27.

Computing a cluster expansion involves the computation of all subsets of a given variable set. It turns out however that the `nc[.]` function doesn't easily lend itself to set manipulations, and

thus the first thing the `cexpandb[.]` function does is putting all operators in the product into a list, saved into a local variable **B**. Now we can use all the set manipulations built into Mathematica to compute the cluster expansion. A schematic example of the code as applied to a triple operator product is given in figure 3.3.

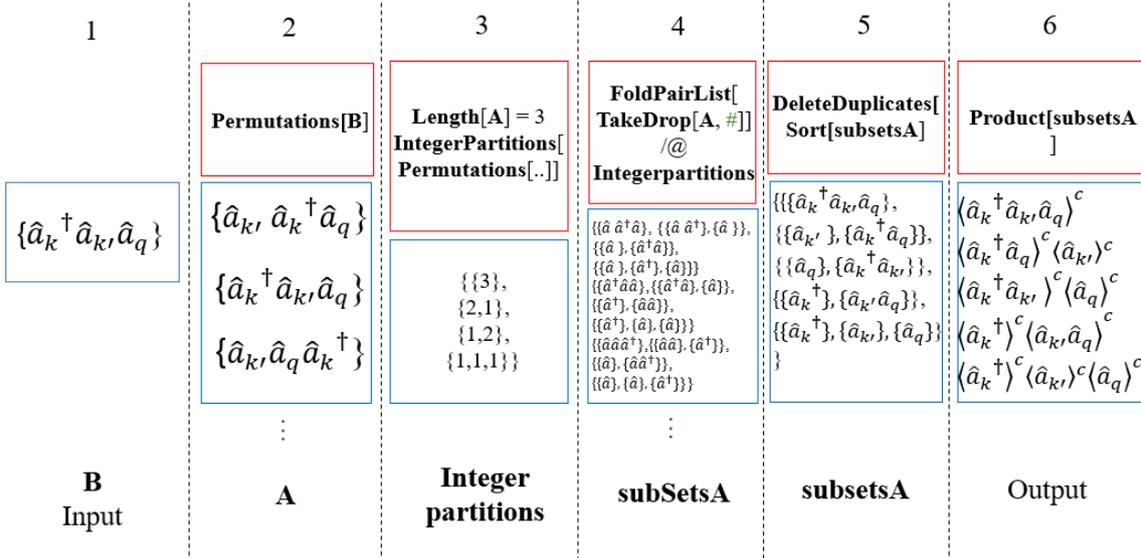


Figure 3.3: Schematic representation of the `cexpandb[.]` function applied to a triple operator product. Operation runs in steps from left to right. Within each step certain functions are applied shown in a red box. The result is then shown in a blue box, with the name of the result given at the bottom. Note that in the second and fourth step not all operator products were written and in the fourth step indices were omitted to save space.

The function code first generates all permutations or orderings of the input set **B** and saves them in set **A**. Then for each element in set **A** all possible partitions are computed. This is done by calculating all possible integer partitions of the length of each permutation in **A**, and splitting every permutation into subsets according to these integer partitions. We have now obtained a set (called "**subSetsA**") containing all possible partitions of all possible permutations of the input operator set. Note that all partitions are appropriately grouped together. An example of such a partition group in figure 3.3 is the group $\{\{\hat{a} \hat{a}\}, \{\hat{a}^\dagger\}\}$

This rather brute force method will generate many duplicate groups of partitions. To figure out which terms appear multiple times, the `Sort[.]` function is applied to each partition in the list. This sorts all operators inside the partitions into canonical order. Then all duplicates can be simply deleted by the `DeleteDuplicates[.]` function. Now within each partition group we can multiply all partitions, with the notation function `cu[.]` applied to each partition. After this all that remains is a summation over all these products. The cluster expansion has now been calculated.

`cexpandb[.]` allows one to calculate the cluster expansion for a boson operator product. For fermions however, one can not just apply the `Sort[.]` function to all partitions without applying the commutation relations in equation 2.28. Also for fermions all cumulants of uneven length are automatically zero. Thus for fermions we use the function `cexpandf[.]`, which slightly alters `cexpandb[.]`. Specifically `cexpandf[.]` first sets all partitions in list **subSetsA** that contain a

product of uneven operators to zero. We now continue along the same lines of the `cexpandb[.]` function, also applying the `Sort[.]` function.

After deleting duplicates, every total partition group is compared to the original operator product with the `FindPermutation[.]` function. This prints the cyclic permutation P required to bring the original product into the order of the total partition group. The length of this cyclic permutation (defined by Mathematica function `Cycles[.]`) can be related to the parity of the permutation by the expression $(-1)^{L_P-1}$, where L_P is the length of the cyclic permutation P . In the script then we simply multiply the product within every partition group with this factor. Then we again sum all partition groups to obtain the appropriate cumulant expansion.

The script supporting `cexpandb[.]` and `cexpandf[.]` simply extracts all operator products from `ctot` into a list called `products`, gives these to `cexpand[.]` as an argument and then plugs the results back into `ctot` with a replacement rule. This gives the full cluster expansion for each equation in a list, referred to as "`cexp`".

3.3.3 Index simplification

In this section we discuss the `indexSimplify[.]` function which was written to further simplify sums in the last section of the script. Consider the following expression,

$$\sum_{\mathbf{k}} \rho_{\tau, \mathbf{p}-\mathbf{k}} V_{\tau, \tau}(\mathbf{k} - \mathbf{p}, \mathbf{p}) + \sum_{\mathbf{k}} \rho_{\tau, \mathbf{k}} V_{\tau, \tau}(-\mathbf{k}, \mathbf{p}). \quad (3.2)$$

At first these two terms seem different, but they are actually equivalent. This is because the first sum can be changed into the second by introducing a change of indices $\mathbf{k} \rightarrow \mathbf{p} - \mathbf{k}$. The first sum is then exactly equal to the second, and the two terms can be combined. By this method significant simplification of the final expression can be achieved.

The `indexSimplify[.]` function automates simplifications of this form. This function works on a sum which contains a potential term multiplied with some other function, which is always a cumulant. This cumulant function must then contain as an argument a summation index summed with an operator index. In equation 3.2, this function is $\rho_{\tau, \mathbf{p}-\mathbf{k}}$.

The `indexSimplify[.]` function takes 4 arguments. The first argument is the sum one aims to simplify, the second argument the summation index, the third argument the operator index and the fourth argument the cumulant function. The operation of this function reads

Input: **sum** expression **x** over indices **y**
 summation index **z**
 operator index **w**
 cumulant function **u**

In u replace **z+w** with **f**
If replacement succeeded
 In x replace **z** with **f-w**
 Break

In u replace **-z+w** with **f**
If replacement succeeded
 In x replace **z** with **-f+w**
 Break

In x replace **f** with **z**

Output: **sum** of expression **x** over indices **y**

The script first replaces all sums of an operator index and a summation index inside the cumulant function with a placeholder **f**. It does this for both the addition and subtraction of operator index and summation index. After both of these replacements, the script checks whether the replacement is successful, i.e. if a cumulant function with argument **f** exists inside the sum. If so all summation indices are replaced by the appropriate solution of the summation. Then the script just replaces the placeholder **f** by the summation index again, and the script finishes, printing the final sum.

To provide a more concrete example, consider the sum in equation 3.2. Here the summation index is **k** and the added operator index is **p**, inside the cumulant function ρ . The function will first attempt the replacement $\mathbf{k} + \mathbf{p} \rightarrow \mathbf{f}$ inside ρ , which will fail. Thus the following **If** statement will fail and the script attempts the replacement $-\mathbf{k} + \mathbf{p} \rightarrow \mathbf{f}$ which will succeed. This provides the script with the information that this is the appropriate sum to replace, and the following **If** statement will evaluate as true. Thus the summation index **k** inside the potential will be replaced with $-\mathbf{f} + \mathbf{p}$. Then **f** will be replaced with **k** and the function is done.

To properly apply the `indexSimplify[.]` function it needs to be given the correct function arguments. Thus it is mapped over an expression by a replacement rule of the following form.

For each **sum** of form $V[...]*n[... , \mathbf{u}+\mathbf{g}, ...]$
 over indices **y**

If **g** is not an element of **sumwavevectors**
 &&
 u is an element of **sumwavevectors**

Apply indexSimplify[.] to **sum** with
 additional arguments $\{\mathbf{y}, \mathbf{g}, \mathbf{n}\}$

We actually apply a set of such rules, which also contains equivalent expressions for negative summation vectors or conjugate cumulant functions. Via these rules the `indexSimplify[.]` function is mapped to each sum containing a product of a cumulant function and a potential matrix element, provided the cumulant function contains a summation index summed with an operator index. Thus

it is important for the input to this replacement rule to be a fully expanded sum.

3.4 Simplifying the equations

In principal the calculation of the cumulant equations is now finished, and all that remains is the application of simplifying assumptions to shorten them. The following sections discuss how these simplifications are applied, starting with the boson scripts. Note that the boson script also allows one to apply just the Fricke truncation method (referred to as the Fricke approximation) without any further assumptions, as seen in figure 3.1a.

3.4.1 Simplifying rulesets

In the previous parts of the script we obtained the rhs of the Heisenberg equation expanded into cumulants. This is the most general way to write the cumulant equations, equivalent in form to equation 2.30. Obviously if this is the form the user is interested in no further computations are required. As discussed in chapter 2 however, the equations become much more useful under certain assumptions. For bosons the most relevant assumption is the coherent state approximation, while fermions allow simplifications through the antisymmetry of the matrix elements. We can thus apply several transformations to the cumulant equations. The script carries out these transformations through several rulesets, which will all be explained in this section.

Before discussing these rulesets however, let us consider the beginning of the "Condensed Bose gas" and "Fermi gas" sections in the script. In section 2.1.5 we defined some shorthand notation for cumulants, which we would like to apply to the list **cexp**. It will later turn out to be useful to also load all these different cumulant functions into a list, which will be called **functions**. Additionally we define each function as numeric with some appropriate notation. For example for the ψ cumulant we write the following.

```
SetAttributes [ $\psi$ , NumericFunction];
Format [ $\psi$  [x--], TraditionalForm] := Subscript [ $\psi$ , x];
```

At this point the notation used in the script in Mathematica notation differs slightly from the theory section, mostly due to Mathematica's difficulty in dealing with superscripts and subscripts within its own notation. Table 3.2 shows the Mathematica form and its equivalent **TraditionalForm**.

Mathematica Form	Traditional Form	Mathematica Form	Traditional Form
$V[\{\mathbf{k}, \mathbf{q}\}, \{\tau, \sigma\}]$	$V_{\tau, \sigma}(k, q)$	$F[\mathbf{k}, \mathbf{q}]$	$T_{k, q}^{\{0, 3\}}$
$\psi[\mathbf{k}]$	ψ_k	$Q[\mathbf{k}, \mathbf{k}', \mathbf{q}]$	$Q_{k, k', q}^{\{2, 2\}}$
$\rho[\mathbf{k}]$	ρ_k	$W[\mathbf{k}, \mathbf{k}', \mathbf{q}]$	$Q_{k, k', q}^{\{1, 3\}}$
$\kappa[\mathbf{k}]$	κ_k	$R[\mathbf{k}, \mathbf{k}', \mathbf{q}]$	$Q_{k, k', q}^{\{0, 4\}}$
$T[\mathbf{k}, \mathbf{q}]$	$T_{k, q}^{\{1, 2\}}$		

Table 3.2: Mathematica form and Traditional form for the cumulant functions.

To avoid the superscripts in notating the triplets and quadruplets different letters are used in Mathematica notation. The **TraditionalForm** however was kept as close to the notation in chapter 2 as possible. Now we move on to the different rulesets that we define. Each ruleset is explained here in the order in which they are defined in the script.

Function rulesets

The two rulesets **AssumpBosePsi** and **AssumpBoseFunc/AssumpFermiFunc** replace all cumulants with the appropriate functions that were defined in the previous section. In the coherent state approximation we require all cumulants to conserve momentum. This condition can be fulfilled by multiplying all expressions with certain delta functions that enforce the condition of momentum conservation. As an example we replace select second and third order cumulants as follows.

$$\begin{aligned} \langle \hat{a}_{\tau,k} \hat{a}_{\sigma,q} \rangle^c &\rightarrow \kappa[\tau, \mathbf{k}] * \mathbf{KroneckerDelta}[\mathbf{k}, -\mathbf{q}] \\ &\quad * \mathbf{KroneckerDelta}[\tau, \sigma] \\ \langle \hat{a}_{\tau,k}^\dagger \hat{a}_{\gamma,k'} \hat{a}_{\sigma,q} \rangle^c &\rightarrow \mathbf{T}[\mathbf{k}, \mathbf{k}', \mathbf{q}] * \mathbf{KroneckerDelta}[\mathbf{k}, \mathbf{k}' + \mathbf{q}] \\ &\quad * \mathbf{KroneckerDelta}[\tau, \gamma] * \mathbf{KroneckerDelta}[\gamma, \sigma] \end{aligned}$$

Equivalent replacement rules are defined for all other cumulant functions. Note that the above ruleset appears in the boson script. As discussed in section 2.3.3 we can no longer use shorthand notation for the cumulant functions for fermions. Thus in the ruleset given above one would have to write $\kappa[\tau, -\mathbf{k}, \mathbf{k}]$.

Also note that at this point the three versions of the script require different rulesets. For the single component script the species index is absent, and thus no extra delta functions are necessary. In the non-interacting mixture the index is there, but it is assumed that only cumulants with the same species index are nonzero. In this case then, we require the replacement rules printed above, with extra delta functions for the Greek index. The full interacting mixture equations then omits these species delta functions again, though obviously the species indices still appear in κ . We define the ψ function separately from the rest of the cumulant functions due to the issues with Mathematica's **Length[.]** function which were discussed earlier. In the **AssumpBoseFunc/AssumpFermiFunc** rulesets we also replace the earlier defined placeholder **f** with the actual momentum eigenvalue $\frac{\hbar^2 q^2}{2m}$.

Delta function ruleset

When applying the function rulesets many new delta functions will appear in the expression. Some of these delta functions only contain indices from the original operator products, i.e. those defined in the **opwavevectors** list. Since by default the original operator products in list **ops** already conserve momentum and these indices are assumed nonzero, all these delta functions automatically vanish. This significantly simplifies the final expression, so here we define a ruleset that automatically sets all delta functions that only contain indices in the **opwavevectors** list to zero. We call this ruleset **AssumpDelta**. Note that in the single component and non-interacting mixtures scripts we can do the same for the operator species saved in list **opspecies**.

Index ruleset

One issue that was observed with the output was the presence of many sums over different dummy indices that could be easily combined into one total sum over the same index. As an example, consider the following identity,

$$\sum_{\mathbf{k}} V(\mathbf{k}, \mathbf{p}) \rho_{\mathbf{k}} + \sum_{\mathbf{k}'} V(\mathbf{k}', \mathbf{p}) \rho_{\mathbf{k}'} = 2 \sum_{\mathbf{k}} V(\mathbf{k}, \mathbf{p}) \rho_{\mathbf{k}}. \quad (3.3)$$

Expressions like the one on the lhs were often found in script results. To properly simplify such expression we use a ruleset called **AssumpIndex**. This essentially rewrites each sum to a sum over

the same (ordered) set of dummy indices, automatically applying the simplification in equation 3.3. Here we again take advantage of the sets **sumwavevectors** and **sumspecies**, which shows why we decided to define these indices separately in the preamble.

Further simplification

Next to the elementary shortening of equations described above we can apply a collection of simplification rules that allow us to shorten the expression further. Specifically, at the start of chapter 2 we assumed a symmetric interaction potential, and our problem is translationally invariant. This allows us to apply some simplifying identities. To this end, we define rulesets called **AssumpBoseSimp/AssumpFermiSimp**. In all scripts these rulesets contain numbers that label different blocks. In the remainder of this section we will outline the simplifying rule belonging to each block.

The blocks labeled (***1***) attempt to shorten the expression via the symmetry of the potential, which holds for both bosons and fermions. This is done by replacing sums of matrix elements that are actually equivalent by symmetry. In the code such a rule takes the following form.

For each **expression** of form

$$V[\{\mathbf{x}, \mathbf{y}\}, \{\mathbf{z}, \mathbf{z}\}] + V[\{\mathbf{w}, \mathbf{l}\}, \{\mathbf{z}, \mathbf{z}\}]$$

If $\{\mathbf{x}, \mathbf{y}\} = -\{\mathbf{w}, \mathbf{l}\}$

Replace expression with $2 * V[\{\mathbf{x}, \mathbf{y}\}, \{\mathbf{z}, \mathbf{z}\}]$

Note that the second list in the argument of V contains the species indices. Obviously in the single component script these indices are absent. Also note that for this rule to apply the species indices must be the same. If they are different, we use the following ruleset.

For each **function** of form

$$V[\{\mathbf{x}, \mathbf{y}\}, \{\mathbf{z}, \mathbf{w}\}]$$

If $\{\mathbf{z}, \mathbf{w}\}$ is **Not Ordered**

Replace function with $V[\{-\mathbf{x}, -\mathbf{y}\}, \{\mathbf{w}, \mathbf{z}\}]$

Which sorts the species indices into canonical order, adding a minus sign to the wavevector indices if a re-ordering is required. Again this rule is not needed for the single component script. By these two rules the symmetry of the potential is properly applied to simplify the final expression.

Moving one to code block (***2***), we apply translational invariance and other symmetries to the cumulant functions. Translational invariance dictates that for example $\rho_{\tau, -\mathbf{k}} = \rho_{\tau, \mathbf{k}}$ for bosons and fermions and $T_{\tau, \mathbf{k}, -\mathbf{q}}^{1,2} = T_{\tau, \mathbf{k}, \mathbf{q}}^{1,2}$ for bosons. Furthermore due to commutation relations we have for example,

<p>Bosons</p> $\kappa_{\tau, -\mathbf{k}} = \kappa_{\tau, \mathbf{k}}$ $T_{\tau, \mathbf{k}, \mathbf{q}}^{1,2} = T_{\tau, \mathbf{q}, \mathbf{k}}^{1,2}$	<p>Fermions</p> $\kappa_{\tau, -\mathbf{k}, \mathbf{k}} = -\kappa_{\tau, \mathbf{k}, -\mathbf{k}}$ $Q_{\tau, \mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}'}^{2,2} = -Q_{\tau, \mathbf{q}, \mathbf{k}, \mathbf{k}', \mathbf{q}'}^{2,2}$	(3.4)
--	---	-------

Ruleset (***2***) uses these properties to attempt to rewrite all cumulant functions to a canonical form, where isolated indices are positive and indices are sorted via **Sort[.]**. By ensuring that as many functions as possible are in this common form, the most effective simplification can be achieved.

A complication in applying translational invariance is that it can also be used to allow further application of the symmetry of the potential. Consider the expression

$$\sum_{\mathbf{k}} \kappa_{\tau, \mathbf{k}} \left[V_{\tau, \tau}(\mathbf{k}, -\mathbf{p}) + V_{\tau, \tau}(\mathbf{k}, \mathbf{p}) \right], \quad (3.5)$$

which will often appear in the cumulant equations. For bosons this expression can be simplified by mapping $\mathbf{k} \rightarrow -\mathbf{k}$ into the first term and applying $\kappa_{\tau, -\mathbf{k}} = \kappa_{\tau, \mathbf{k}}$. This would allow one to combine the two matrix elements by applying potential symmetry. To allow the script to also simplify such equations we use code block (*3*), which contains a rule that reads

For each expression of form

$$V[\{\mathbf{x}, \mathbf{y}\}, \{\mathbf{z}, \mathbf{z}\}] + V[\{\mathbf{w}, \mathbf{l}\}, \{\mathbf{z}, \mathbf{z}\}]$$

In $\{\mathbf{w}, \mathbf{l}\}$ replace `sumwavevectors[[1]]` with `-sumwavevectors[[1]]`

If $\{\mathbf{x}, \mathbf{y}\} = -\{\mathbf{w}, \mathbf{l}\}$ **Or** $\{\mathbf{x}, \mathbf{y}\} = \{\mathbf{w}, \mathbf{l}\}$

Replace expression with `2*V[\{\mathbf{x}, \mathbf{y}\}, \{\mathbf{z}, \mathbf{z}\}]`

which essentially expands the rules in codeblock (*2*) to also allow simplification through mapping of negative summation indices. By default such a replacement is only attempted for the first summation index, since this one appears in sums the most due to the **AssumpIndex** ruleset. At higher orders other summation indices might also appear more often, and the user might choose to also apply this rule for other indices in the list. Note that we do not include codeblock (*3*) for fermions, since mapping like this is not directly allowed without introducing possible minus signs.

For fermions however, we have an additional codeblock (*4*), which uses similar methods to block (*2*) to apply the antisymmetry of fermion matrix elements, which was explained in section 2.3.1. This codeblock is optional, and if used denotes an antisymmetrized matrix element by superscript A, consistent with the theory section.

We have one final code block left, labeled by the number (*5*). This block only exists in the single component script, and allows for the optional application of a separable potential. The details of a separable potential were explained in section 2.1.3. If the user wishes to use this part of the code it can simply be uncommented. Note that we also define a second simplification ruleset **AssumpBoseSimp2/AssumpFermiSimp2**, which just carries out code blocks of the form (*1*), (*3*) and (*4*) but with some arbitrary numeric factor in front of the potential.

3.4.2 Applying simplifications

The second part of the "Condensed Bose gas" and "Fermi gas" sections in the script actually applies all the results defined in the previous section in the appropriate order, and also applies other simplifying steps. This section will summarize these final steps in the order that they are applied.

Breaking the hierarchy

We start with some lines of code that carry out the following operations.

In cexp set **s** to zero

Apply AssumpBosePsi to **cexp**

In cexp set each cumulant of **Length > order[[2]]**
to zero

Apply AssumpBoseFunc to **cexp**

Map cuSimplify[...] over **cexp** with argument **AssumpDelta**

Apply AssumpIndex to **cexp**

First the index **s** is set to zero, which was the index in the first order cumulant inside the **ops** list. This is consistent with applying the coherent state approximation. Thus in the fermion script this step is absent. Next the **AssumpBosePsi** and **AssumpBoseFunc** rulesets are applied, while a condition is given that any cumulants of order higher than the second value in the **order** list are set to zero. This is then the full application of the Fricke method of breaking the hierarchy. Afterwards the **cuSimplify[...]** function is mapped to each equation, which simplifies all delta functions originating from momentum conservation. Note that here we also give **cuSimplify[...]** the ruleset **AssumpDelta** as its second argument. Finally we also apply the **AssumpIndex** ruleset. Here it is convenient that **cuSimplify[...]** has expanded the sum into individual terms, which ensures proper application of **AssumpIndex**.

Further sum simplification

Now that the first couple of rulesets have been applied, the script will carry out several simplifying procedures on the resulting expressions. First we apply **indexSimplify[...]** - now not be confused with **AssumpIndex** - to the expression. The operation of this function was explained in section 3.3.3. Here it is useful that **cuSimplify[...]** has expanded the sum. Note that this is the point in the script where the replacement rules belonging to **indexSimplify[...]** are used.

At this point each individual sum is in its simplest form, and all sums can be collected. We then prepare the expression for application of the further simplification rulesets. This part of the code reads as follows.

For each **sum** of expression **x** over indices **y**

Collect terms in **x** relative to list
functions

Collect terms in **x** relative to list
Conjugate[functions]

Codeblocks (*1*), (*3*) and (*4*) require that all potential terms are collected together as sums to be the most effective. To rewrite the equations in such a form Mathematica's **Collect[...]** function is used, which collects all terms relative to the list **functions**. In other words, all variables in the list **functions** are factored out, which groups the potential terms together. The simplification ruleset can then be applied to maximum effect. To ensure the potential sums are shortened as far as possible the two simplification rulesets are actually applied multiple times through a **Nest[...]** function. The full simplified right hand side of the cumulant equations is now stored in the list **rhsBose** for bosons or **rhsFermi** for fermions.

Lhs cumulant equations

Up to this point, all calculations have been focused on the right hand side of the cumulant equations, which is obviously the most important part for this script. To give a nicer output however, the script also quickly calculates the left hand side of the equation. This is done by taking the original operator product from the **ops** list, applying the appropriate cluster expansion function and applying all relevant simplifying rulesets. We are now in a position to finally print the full cumulant equations, which are saved in the lists **cuEquationBose** for bosons and **cuEquationFermi** for fermions. This list is printed in Mathematica's notation and **TraditionalForm** notation.

3.4.3 Fricke approximation

As discussed before, the boson scripts also give the user the option to just calculate the cumulant equations by the Fricke approximation, without any additional simplifications. This is useful if one is not interested in the coherent state approximation, and no assumption at all is made on the nature of the cumulants. The script for the Fricke approximation follows the same lines as the script for the condensed Bose gas, with several parts omitted. The only rulesets needed for the Fricke approximation are the function rulesets, obviously without the delta functions, and the **AssumpIndex** ruleset. If the user also wishes to include other rulesets here they can obviously be copied over, but by default this part of script is very barebones on purpose. We note that using this part of the script probably also means that one should alter the default starting operator products in the **ops** list, which already implicitly assumed momentum conservation.

3.5 Potential issues

Even though the script will be thoroughly tested in the next chapter, this section will outline some possible issues with the script that users may encounter. We note that these potential issues are mainly related to the final simplification steps and not with the actual computation of the cumulant equations, which is very stable in its operation.

3.5.1 Error codes

Use of the SNEG package with Mathematica version 12.0 gives some compatibility issues. In particular when calculating operator products Mathematica will print errors with, among others, the **LessEqual::nord2** function. As far as we could find these errors never affect the output, and thus the preamble contains commands which turn these error messages off for the remainder of the script. If a user is troubleshooting something with the script it is always advised to check whether these errors may have something to do with it, although such a situation has not yet been found in working with this script.

3.5.2 Fermion operators

As was stated before, the SNEG package automatically sorts operators into normal order when applying the **nc[...]** function. The user should take care of this when defining operators in the **ops** list in the preamble of the script. If the user defines a fermion operator product that is not normal ordered SNEG's permutations could introduce a minus sign in front, which should be avoided. This is because in this case the **Length[...]** function used in the commutator code no longer functions correctly. The user can prevent the minus sign from appearing by simply entering operator products

in their normal order. Since it can sometimes be unclear what Mathematica's canonical order actually is, it is advised to check the output of the `ops` list once and alter the ordering where needed.

3.5.3 Simplifying rule sets

In the previous section we showed what different transformation rules we attempt to apply to the cumulant equations to sort the final expression. Most of these were related to the potential matrix elements which could often be combined by their symmetry. We also used rules that attempted to sort arguments of the cumulant functions into canonical order and make their arguments positive if possible. One major limitation of these procedures is that they become less and less reliable as the order of the equations increases or more mixture cumulants are included. This is mostly because the number of needed replacement rules grows as the number of indices grows. In the scripts that accompany this report some basic replacement rules have been included which work quite well for third order cumulants, but achieving effective simplification for fourth and higher order cumulants would require many more rules.

3.5.4 Index simplify

One other major reason for the decrease in simplification effectiveness, especially for interacting mixtures, is the `indexSimplify[.]` function, which attempted to rewrite sums inside cumulant functions to a single summation index. In the way it is currently programmed however, this function only works on specific sums containing one cumulant function multiplied with an interaction potential matrix element. In the interacting mixture however, we often observe two cumulants multiplied with a matrix element, which could both contain sums of indices. These sums are not grabbed by the replacement rule accompanying `indexSimplify[.]`, and are thus kept in their original form. Obviously one could write a second replacement rule for `indexSimplify[.]` which also grabs such products, but this would just make the issue reappear at even higher orders. Preferable one would want to find a general replacement rule that could apply the `indexSimplify[.]` function correctly to any sum, which may be an interesting point for someone looking to improve the script. We do note that `indexSimplify[.]` itself is essentially general, and only the replacement rule needs to be generalised.

It is comforting that the potential problems described above with the simplifying methods will never lead to wrong output. They just mean that higher order/mixture equations are not always written in as short a form as they could be written, and that some further simplification may have to be done by hand. The calculation of the equations is not affected however, and the results are always still correct.

3.5.5 Computation time

Since the calculation of cumulant equations naturally pushes one to achieve higher and higher orders, it is instructive to consider the computation time of the script. Table 3.3 shows an overview of the approximate computation time of the single component script.

order	Computation time
{2,2}	5 s
{3,3}	27 s
{4,4}	11 m 10s

Table 3.3: Overview of computation times measured when running the single component script for different values of the **order** list. These computation times were measured when running the script on a Windows PC with an INTEL CORE i7-6700HQ cpu clocked at 2.60 GHz backed by 8 gB of internal memory.

Here it is mostly interesting to consider the computation time increase when going to higher orders. We observe that the difference between second and third order is minimal while the elapsed time takes a major jump at fourth order. It was found that the bottleneck was mostly in the **sumSimplifyKD[.]** and **sumExpand[.]/sumCollect[.]** functions that were used when simplifying the cumulant equations. An attempt was already made to make these functions more efficient through the **cuSimplify[.]** function, which already gave a major decrease in computation time. Further improvements however could make going to higher orders more convenient for the user. Still, up to fourth order the time required is still very manageable and definitely much faster than manual derivation of the equations.

Chapter 4

Results and Discussion

This chapter will summarize and analyse some select results obtained from the scripts developed in the previous chapter. We will observe that the cumulant equations become quite lengthy for higher orders, which is why we often define tensors in this chapter which allow us to write the equations in a more compact form. In this chapter the analysis will be mostly focused on the condensed Bose gas, although we will also give a brief overview of fermion results.

We note again that whenever we refer to a non-interacting mixture in this chapter, we are strictly talking about the cumulants. Interaction between species can still occur via the interaction potential. This was explained in more detail in sections 2.2.3 and 3.2.1.

4.1 Boson Hartree-Fock Bogoliubov equations

4.1.1 Non-interacting mixture

Consider the second order equations for a condensed Bose gas in the coherent state approximation, which can be used to describe the dynamics of two particle scattering processes in the gas. Let us first consider the equations for a mixture in which the mixture cumulants are all set to zero. The corresponding cumulant equations can then be calculated by the **Non-Interacting Mixture.nb** script. The $\psi_{\tau,0}$ equation was calculated to equal

$$\begin{aligned} i\hbar\dot{\psi}_{\tau,0} = & \sum_{\mathbf{k}} \psi_{\tau,0}^* \kappa_{\tau,\mathbf{k}} V_{\tau\tau}(0, \mathbf{k}) + \psi_{\tau,0} \left\{ \sum_{\mathbf{k},\sigma} \rho_{\sigma,\mathbf{k}} V_{\sigma\tau}\left(\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}\right) \right. \\ & \left. + \sum_{\mathbf{k}} \rho_{\tau,\mathbf{k}} V_{\tau\tau}\left(\frac{\mathbf{k}}{2}, -\frac{\mathbf{k}}{2}\right) + \sum_{\sigma} |\psi_{\sigma,0}|^2 V_{\sigma,\tau}(0, 0) \right\}, \end{aligned} \quad (4.1)$$

which also follows immediately from equation 2.31 by applying the coherent state approximation [2]. Comparing to the Gross Pitaevskii equation given in equation 2.38 we see that the dynamics of the condensate are now also influenced by the particles scattered into the condensate (κ) and the number of excited particles (ρ). To investigate the exact dynamics of these cumulants, we first define the pairing field $\Delta_{\tau}(\mathbf{p})$ and the Hartree-Fock Hamiltonian $h_{\tau}(\mathbf{p})$ to be consistent with literature as

$$\Delta_{\tau}(\mathbf{p}) = V_{\tau,\tau}(\mathbf{p}, 0)\psi_{\tau,0}^2 + \sum_{\mathbf{k}} V_{\tau,\tau}(\mathbf{p}, \mathbf{k})\kappa_{\tau,\mathbf{k}}, \quad (4.2)$$

$$\begin{aligned}
h_\tau(\mathbf{p}) &= \frac{\hbar^2 p^2}{2m} + \frac{1}{2} \sum_{\mathbf{k}, \sigma} \rho_{\sigma, \mathbf{k}} \left(V_{\sigma, \tau} \left(\frac{\mathbf{k} - \mathbf{p}}{2}, \frac{\mathbf{k} - \mathbf{p}}{2} \right) + V_{\sigma, \tau} \left(\frac{\mathbf{k} + \mathbf{p}}{2}, \frac{\mathbf{k} + \mathbf{p}}{2} \right) \right) \\
&\quad + \sum_{\mathbf{k}} \rho_{\tau, \mathbf{k}} V_{\tau, \tau} \left(\frac{\mathbf{k} + \mathbf{p}}{2}, \frac{1}{2}(-\mathbf{k} - \mathbf{p}) \right) \\
&\quad + \frac{1}{2} \sum_{\sigma} |\psi_{\sigma, 0}|^2 \left(V_{\sigma, \tau} \left(-\frac{\mathbf{p}}{2}, -\frac{\mathbf{p}}{2} \right) + V_{\sigma, \tau} \left(\frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2} \right) \right) \\
&\quad + |\psi_{\tau, 0}|^2 V_{\tau, \tau} \left(\frac{\mathbf{p}}{2}, -\frac{\mathbf{p}}{2} \right).
\end{aligned} \tag{4.3}$$

The pairing field contains the interaction between the excitation with momentum \mathbf{p} and all other excitations. The first term then represents all atoms in the condensate and the second term represent pairing with excited pairs. We note here that summations over \mathbf{k} like the one in equation 4.2 exclude the $\mathbf{k} = 0$ momentum mode, since this term has been effectively separated from the sum via the coherent state approximation [14]. The Hartree-Fock Hamiltonian can be used to calculate the so called Hartree-Fock energy of a certain excitation, which contains its kinetic energy and an additional contribution from pairwise interactions [4]. Now we can write down the calculated cumulant equations for the second order cumulants $\rho_{\tau, \mathbf{p}}$ and $\kappa_{\tau, \mathbf{p}}$ in a compact form which reads

$$i\hbar \dot{\rho}_{\tau, \mathbf{p}} = \Delta_\tau(\mathbf{p}) \kappa_{\tau, \mathbf{p}}^* - \Delta_\tau(\mathbf{p})^* \kappa_{\tau, \mathbf{p}}, \tag{4.4}$$

$$i\hbar \dot{\kappa}_{\tau, \mathbf{p}} = 2h_\tau(\mathbf{p}) \kappa_{\tau, \mathbf{p}} + \Delta_\tau(\mathbf{p})(1 + 2\rho_{\tau, \mathbf{p}}). \tag{4.5}$$

These three equations are collectively known as the Hartree-Fock Bogoliubov (HFB) equations, and match those in the literature. In the cumulant equations it is often instructive to separate the terms according to their function in the dynamics of the cumulants. In equations 4.4 and 4.5 we can distinguish the homogeneous part of the equations from the inhomogeneous part. If one were to consider a system which is initially completely condensed, the so called "quench" scenario, then $\rho(t=0) = \kappa(t=0) = 0$. At this time then, only the inhomogeneous parts of the equations of motion can provide the growth of the cumulant over time, and thus source the dynamics of the cumulant. Because of this we will refer to the inhomogeneous terms as the "source" terms S . The κ equation can be rewritten to separate homogeneous and source terms as

$$\begin{aligned}
i\hbar \dot{\kappa}_{\tau, \mathbf{p}} &= 2h_\tau(\mathbf{p}) \kappa_{\tau, \mathbf{p}} + (1 + 2\rho_{\tau, \mathbf{p}}) \sum_{\mathbf{k}} V_{\tau, \tau}(\mathbf{p}, \mathbf{k}) \kappa_{\tau, \mathbf{k}} \\
&\quad + (1 + 2\rho_{\tau, \mathbf{p}}) V_{\tau, \tau}(\mathbf{p}, 0) \psi_{\tau, 0}^2,
\end{aligned} \tag{4.6}$$

where the first line contains all homogeneous terms and the second line all source terms. Given that the κ cumulant describes scattering of two particles outside the condensate, the source term must be related to excitations of pairs to opposite momentum modes $\{\mathbf{p}, -\mathbf{p}\}$. This can be verified by rewriting the source term as

$$V_{\tau, \tau}(\mathbf{p}, 0) \left[(1 + \rho_{\tau, \mathbf{p}})(1 + \rho_{\tau, -\mathbf{p}}) \psi_{\tau, 0}^2 - \rho_{\tau, \mathbf{p}}^2 \psi_{\tau, 0} \right]. \tag{4.7}$$

This way of writing the equation was taken from ref [14]. Observe that the source contains a term of the form $(1 + \rho_{\tau,\mathbf{p}})$, signifying that the creation of excitation pairs in a certain momentum state is affected if that state is already occupied. Obviously we would not expect anything similar for fermions, where states can only be occupied once. In essence such a term then describes the pairwise interaction between bosons in the same state. We refer to this as Bose enhancement. [4].

Note that the dynamics of the ρ cumulant only contain a source term. This further signifies that the number of excited atoms formed from the κ source term is "counted" by the ρ cumulant, which represents the dynamics of the number operator [4].

4.1.2 Two-Body Schrödinger equation

One interesting property of the cumulant equations can be observed by neglecting all but the homogeneous terms in the κ equation, giving

$$i\hbar\dot{\kappa}_{\tau,\mathbf{p}} = 2h_{\tau}(\mathbf{p})\kappa_{\tau,\mathbf{p}} + (1 + 2\rho_{\tau,\mathbf{p}}) \sum_{\mathbf{k}} V_{\tau,\tau}(\mathbf{p}, \mathbf{k})\kappa_{\tau,\mathbf{k}}. \quad (4.8)$$

Let us make the assumption that the dynamics of κ are much faster than those of ρ and ψ . That means that we can treat these cumulants as approximately stationary. Let us then make the following ansatz for the time dependence of the κ cumulant.

$$\kappa_{\tau,\mathbf{p}} = e^{E_{\nu}t} \phi_{\tau,v}(\mathbf{p}). \quad (4.9)$$

Then equation 4.8 can be written as

$$E_{\nu}\phi_{\tau,\nu}(\mathbf{p}) = 2h_{\tau}(\mathbf{p})\phi_{\tau,\nu}(\mathbf{p}) + (1 + 2\rho_{\tau,\mathbf{p}}) \sum_{\mathbf{k}} V_{\tau,\tau}(\mathbf{p}, \mathbf{k})\phi_{\tau,\nu}(\mathbf{k}), \quad (4.10)$$

which is an eigenvalue equation with eigenvalue E_{ν} and eigenfunction $\phi_{\tau,\nu}(\mathbf{p})$. Note that the factor $i\hbar$ has been absorbed into E_{ν} . This equation is similar in form to the two-body Schrödinger equation, dubbed the Hyperbolic Wannier equation in literature [4]. If we remove all particles from the many body system and go to vacuum, i.e. ρ and ψ both vanish, then the Hartree-Fock energy reduces to the kinetic energy and the potential term is no longer Bose enhanced. In this limit then we find the exact two body Schrödinger equation. Apparently the Hyperbolic Wannier equation generalizes the Schrödinger equation to the presence of a macroscopically occupied condensate, altering both the energy and the pairwise interaction terms. We can use this equation to examine the formation of dimers from the condensate [4, 14].

4.1.3 Second order interacting mixtures

The single component HFB equations look very similar to equations 4.4 and 4.5, obviously without the extra index. More interesting to consider are the full mixture equations, in which we no longer neglect mixture cumulants. These were calculated with the **Interacting Mixture.nb** script. In this case the GP equation reads

$$\begin{aligned}
i\hbar\dot{\psi}_{\tau,0} &= \sum_{\sigma,\mathbf{k}} \left[\frac{1}{2}\psi_{\sigma,0}^* \kappa_{\sigma,\tau,\mathbf{k}} \left(V_{\sigma,\tau}(0, -\mathbf{k}) + V_{\sigma,\tau}(0, \mathbf{k}) \right) + 2\psi_{\tau,0}\rho_{\sigma,\sigma,\mathbf{k}}V_{\sigma\tau}\left(\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}\right) \right. \\
&\quad \left. + \frac{1}{2}\psi_{\sigma,0}\rho_{\sigma,\tau,\mathbf{k}} \left(V_{\sigma,\tau}\left(\frac{\mathbf{k}}{2}, -\frac{\mathbf{k}}{2}\right) + V_{\sigma,\tau}\left(-\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}\right) \right) \right] \\
&\quad + \sum_{\sigma} |\psi_{\sigma,0}|^2 V_{\sigma,\tau}(0, 0)\psi_{\tau,0}.
\end{aligned} \tag{4.11}$$

Comparing to equation 2.38 we see that the GP equation for an interacting mixture looks very similar, with some additional summation over the species index. The second order equations however diverge more significantly. The equation of motion for the $\rho_{\tau,\gamma,\mathbf{p}}$ cumulant for example gains several additional homogeneous terms. To compactly write this EoM we define the mixture pairing field $\Delta_{\gamma,\sigma}(\mathbf{p})$ and the homogeneous terms $\Omega_{\gamma,\sigma}(\mathbf{p})$ and $\Theta_{\gamma,\sigma}(\mathbf{p})$ as

$$\Delta_{\gamma,\sigma}(\mathbf{p}) = V_{\gamma,\sigma}(\mathbf{p}, 0)\psi_{\sigma,0}\psi_{\gamma,0} + \sum_{\mathbf{k}} \kappa_{\gamma,\sigma,\mathbf{k}}V_{\gamma,\sigma}(\mathbf{p}, \mathbf{k}), \tag{4.12}$$

$$\Omega_{\gamma,\sigma}(\mathbf{p}) = V_{\gamma,\sigma}\left(\frac{\mathbf{p}}{2}, -\frac{\mathbf{p}}{2}\right)\psi_{\gamma,0}\psi_{\sigma,0}^* + \sum_{\mathbf{k}} V_{\gamma,\sigma}\left(\frac{\mathbf{p}-\mathbf{k}}{2}, \frac{\mathbf{k}-\mathbf{p}}{2}\right)\rho_{\sigma,\gamma,\mathbf{k}}, \tag{4.13}$$

$$\Theta_{\gamma,\sigma}(\mathbf{p}) = V_{\gamma,\sigma}\left(\frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2}\right)|\psi_{\sigma,0}|^2 + \sum_{\mathbf{k}} V_{\gamma,\sigma}\left(\frac{\mathbf{p}-\mathbf{k}}{2}, \frac{\mathbf{p}-\mathbf{k}}{2}\right)\rho_{\sigma,\sigma,\mathbf{k}}. \tag{4.14}$$

The tensors Ω and Θ seem to represent different types of excitation pairs. In the expression for Ω we observe $\rho_{\sigma,\gamma,\mathbf{k}}$ which suggests that this term represents scattering of an excitation of one species with the condensate of a different species. This is further reinforced by the condensate term, which contains contributions from both the σ and γ condensates. On the other hand the Θ term can be interpreted as a density term, related to the number of excitations of the species σ inside the gas. Now the equation of motion for $\rho_{\tau,\gamma,\mathbf{p}}$ can be written as

$$\begin{aligned}
i\hbar\dot{\rho}_{\tau,\gamma,\mathbf{p}} &= \sum_{\sigma} \left[\Delta_{\gamma,\sigma}(\mathbf{p})\kappa_{\sigma,\tau,\mathbf{p}}^* - \Delta_{\tau,\sigma}(\mathbf{p})^*\kappa_{\sigma,\gamma,\mathbf{p}} \right. \\
&\quad \left. + \Omega_{\gamma,\sigma}(\mathbf{p})\rho_{\tau,\sigma,\mathbf{p}} - \Omega_{\sigma,\tau}(\mathbf{p})\rho_{\sigma,\gamma,\mathbf{p}} \right. \\
&\quad \left. + \rho_{\tau,\gamma,\mathbf{p}}\{\Theta_{\gamma,\sigma}(\mathbf{p}) - \Theta_{\tau,\sigma}(\mathbf{p})\} \right].
\end{aligned} \tag{4.15}$$

We see that if interactions are introduced between the components the ρ dynamics are also influenced by homogeneous terms. This is because in an interacting mixture the ρ cumulant does not just represent the excitation density, but can also be filled by scattering processes between different species, like in the Ω tensor. Note that the extra mixture terms immediately vanish if one sets all mixture cumulants to zero, as is expected.

Next we consider the dynamics of the κ cumulant in an interacting mixture. Again we first define some notation in the form of the mixture Hartree-Fock Hamiltonian

$$h_{\gamma,\tau}(\mathbf{p}) = \frac{\hbar^2 p^2}{2m} + \sum_{\sigma} \frac{1}{2} \left(\Theta_{\gamma,\sigma}(\mathbf{p}) + \Theta_{\sigma,\tau}(\mathbf{p}) \right). \quad (4.16)$$

Now the equation of motion for the κ cumulant was calculated to equal

$$\begin{aligned} i\hbar \dot{\kappa}_{\gamma,\tau,\mathbf{p}} &= 2h_{\gamma,\tau}(\mathbf{p})\kappa_{\gamma,\tau,\mathbf{p}} \\ &+ \sum_{\sigma} \left[\Omega_{\gamma,\sigma}(\mathbf{p})\kappa_{\sigma,\tau,\mathbf{p}} + \Omega_{\sigma,\tau}(\mathbf{p})\kappa_{\gamma,\sigma,\mathbf{p}} \right. \\ &\left. + \Delta_{\gamma,\sigma}(\mathbf{p})\rho_{\sigma,\tau,\mathbf{p}} + \Delta_{\sigma,\tau}(\mathbf{p})\rho_{\sigma,\gamma,\mathbf{p}} \right] + \Delta_{\gamma,\tau}(\mathbf{p}). \end{aligned} \quad (4.17)$$

The first and third line contain terms that were already present in equation 4.5, be it with a somewhat altered Hartree-Fock Hamiltonian and some extra summation over the species index. The second line however contains new terms, expressed in the earlier defined tensor Ω .

4.2 Boson third order equations

4.2.1 Non-interacting mixture

The third order cumulant equations for a condensed Bose gas contain the dynamics of three particle interactions, and are a natural extension of the HFB equations defined in the previous section. These equations can be used to construct a generalized mean-field theory that is both self consistent and includes the kinematics of condensate formation [16]. Let us first consider the third order equations for a non-interacting mixture, as calculated by the **Non-Interacting Mixture.nb** script. Once more we emphasize that this name refers strictly to the cumulants, and interactions between species can still occur via the potential. Again we start with the extension of the Gross-Pitaevski equation including third order correlations,

$$\begin{aligned} i\hbar \dot{\psi}_0(t) &= \sum_{\mathbf{k},\mathbf{q}} V_{\tau,\tau} \left(\frac{\mathbf{k}+\mathbf{q}}{2}, \frac{\mathbf{k}-\mathbf{q}}{2} \right) T_{\tau,\mathbf{k},\mathbf{q}}^{1,2} + \sum_{\mathbf{k}} \psi_{\tau,0}^* \kappa_{\tau,\mathbf{k}} V_{\tau,\tau}(0, -\mathbf{k}) \\ &+ \psi_{\tau,0} \sum_{\sigma} \sum_{\mathbf{k}} \left[\rho_{\sigma,\mathbf{k}} V_{\sigma,\tau} \left(\frac{\mathbf{k}}{2}, -\frac{\mathbf{k}}{2} \right) + \rho_{\tau,\mathbf{k}} V_{\tau,\tau} \left(\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2} \right) \right] \\ &+ \psi_{\tau,0} \sum_{\sigma} |\psi_{\sigma,0}|^2 V_{\sigma,\tau}(0, 0). \end{aligned} \quad (4.18)$$

We see that the third order scattering cumulant $T^{1,2}$ is now also included in the dynamics of the condensate. Now we again define some notation,

$$\begin{aligned} I_{\tau}(\mathbf{p}) &= \sum_{\mathbf{k}} \left[V_{\tau,\tau} \left(\frac{\mathbf{p}}{2}, \mathbf{k} - \frac{\mathbf{p}}{2} \right) T_{\tau,\mathbf{k},\mathbf{p}-\mathbf{k}}^{1,2} \right. \\ &\left. - \left(V_{\tau,\tau} \left(\frac{\mathbf{k}+\mathbf{p}}{2}, \frac{\mathbf{k}-\mathbf{p}}{2} \right) + V_{\tau,\tau} \left(\frac{\mathbf{k}+\mathbf{p}}{2}, \frac{\mathbf{p}-\mathbf{k}}{2} \right) \right) T_{\tau,\mathbf{k},\mathbf{p}}^{1,2} \right]. \end{aligned} \quad (4.19)$$

Expressed in this notation, the equations of motion for the ρ and κ cumulants were calculated to equal

$$i\hbar\dot{\rho}_{\tau,\mathbf{p}} = I_{\tau}(\mathbf{p})\psi_0^* - I_{\tau}(\mathbf{p})^*\psi_0 + \Delta_{\tau}(\mathbf{p})\kappa_{\tau,\mathbf{p}}^* - \Delta_{\tau}(\mathbf{p})^*\kappa_{\tau,\mathbf{p}}, \quad (4.20)$$

$$i\hbar\dot{\kappa}_{\tau,\mathbf{p}} = \sum_{\mathbf{k}} \left[2\psi_{\tau,0}^* V_{\tau,\tau}\left(\frac{\mathbf{p}}{2}, \mathbf{k} + \frac{\mathbf{p}}{2}\right) T_{\tau,\mathbf{k},\mathbf{p}}^{0,3} + \left(2V_{\tau,\tau}\left(\frac{\mathbf{k}}{2} + \mathbf{p}, -\frac{\mathbf{k}}{2}\right) + 2V_{\tau,\tau}\left(\frac{\mathbf{k}}{2} + \mathbf{p}, \frac{\mathbf{k}}{2}\right) \right) T_{\tau,\mathbf{k},\mathbf{p}}^{1,2} \right. \\ \left. + 2h_{\tau}(\mathbf{p})\kappa_{\tau,\mathbf{p}} + \Delta_{\tau}(\mathbf{p})(1 + 2\rho_{\tau,\mathbf{p}}) \right]. \quad (4.21)$$

We see that the ρ and κ cumulants are now also influenced by the 3rd order cumulants $T^{1,2}$ and $T^{0,3}$, which is to be expected since they all relate to the scattering of excited states. For example since a $T^{1,2}$ scattering event alters the occupancy of excited states one would expect its value to alter the number cumulant ρ , which is proven by this equation. Interestingly however, three body scattering events like the one represented by $T^{0,3}$ do not feed the dynamics of ρ .

To obtain a complete picture of third order cumulant theory we require the equation of motion for $T^{1,2}$ and $T^{0,3}$. To write these equations we follow conventions in literature and first define the source terms S [4, 14]. These read

$$S_{\tau,\mathbf{p},\mathbf{l}}^{1,2} = \psi_{\tau,0}\kappa_{\tau,\mathbf{l}+\mathbf{p}}^*\kappa_{\tau,\mathbf{p}} \left(V_{\tau,\tau}\left(\mathbf{l} + \frac{\mathbf{p}}{2}, -\frac{\mathbf{p}}{2}\right) + V_{\tau,\tau}\left(\mathbf{l} + \frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2}\right) \right) \\ + \psi_{\tau,0}^*\kappa_{\tau,\mathbf{p}} \left(V_{\tau,\tau}\left(\frac{\mathbf{l}}{2}, -\mathbf{p} - \frac{\mathbf{l}}{2}\right) + V_{\tau,\tau}\left(\frac{\mathbf{l}}{2}, \mathbf{p} + \frac{\mathbf{l}}{2}\right) \right) (\rho_{\tau,\mathbf{l}+\mathbf{p}} - \rho_{\tau,\mathbf{l}}) \\ + V_{\tau,\tau}\left(\frac{\mathbf{p}-\mathbf{l}}{2}, \frac{\mathbf{l}+\mathbf{p}}{2}\right) \left[\psi_{\tau,0}\rho_{\tau,\mathbf{l}+\mathbf{p}}(1 + \rho_{\tau,\mathbf{p}} + \rho_{\tau,\mathbf{l}}) - \psi_{\tau,0}\rho_{\mathbf{k}}\rho_{\mathbf{l}} \right], \quad (4.22)$$

$$S_{\tau,\mathbf{p},\mathbf{l}}^{0,3} = \kappa_{\tau,\mathbf{p}} \left[\psi_{\tau,0} \left(V_{\tau,\tau}\left(\mathbf{l} + \frac{\mathbf{p}}{2}, -\frac{\mathbf{p}}{2}\right) + V_{\tau,\tau}\left(\mathbf{l} + \frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2}\right) \right) (1 + \rho_{\tau,\mathbf{l}} + \rho_{\tau,\mathbf{p}+\mathbf{l}}) \right. \\ \left. + \left(V_{\tau,\tau}\left(\frac{\mathbf{l}+\mathbf{p}}{2}, \frac{\mathbf{l}-\mathbf{p}}{2}\right) + V_{\tau,\tau}\left(\frac{\mathbf{l}+\mathbf{p}}{2}, \frac{1}{2}(\mathbf{p}-\mathbf{l})\right) \right) \psi_{\tau,0}^*\kappa_{\tau,\mathbf{l}} \right]. \quad (4.23)$$

We then define the total source terms as

$$S_{\text{tot},\tau,\mathbf{p},\mathbf{l}}^{1,2} = S_{\tau,\mathbf{p},\mathbf{l}}^{1,2} + S_{\tau,\mathbf{l},\mathbf{p}}^{1,2}, \quad (4.24)$$

$$S_{\text{tot},\tau,\mathbf{p},\mathbf{l}}^{0,3} = S_{\tau,\mathbf{p},\mathbf{l}}^{0,3} + S_{\tau,-\mathbf{p}-\mathbf{l},\mathbf{p}}^{0,3} + S_{\tau,\mathbf{l},-\mathbf{l}-\mathbf{p}}^{0,3}. \quad (4.25)$$

If the expectation values were expanded according to Wicks theorem these would be the only terms contained in the equations of motion, in other words these are all terms up to second order. In a quenched Bose gas these terms source the initial growth of the third order cumulants as excited states are populated. Note that in these source terms there is no summation over σ , signifying that other components in the gas do not impact the source. Next we define all homogeneous terms H . First $H^{1,2}$ was calculated, which we write with the following distinguished terms, following conventions in ref [14].

$$K_{\tau,\mathbf{p},\mathbf{l}}^{1,2} = \left(f_{\tau}(\mathbf{p}) - f_{\tau}(\mathbf{p} + \mathbf{l}) \right) T_{\tau,\mathbf{p},\mathbf{l}}^{1,2}, \quad (4.26)$$

$$\begin{aligned} V_{\tau,\mathbf{p},\mathbf{l}}^{1,2} &= \frac{1 + \rho_{\tau,\mathbf{p}} + \rho_{\tau,\mathbf{l}}}{2} \sum_{\mathbf{k}} V_{\tau,\tau} \left(\frac{\mathbf{p} - \mathbf{l}}{2}, \frac{2\mathbf{k} - \mathbf{l} - \mathbf{p}}{2} \right) T_{\tau,\mathbf{k},-\mathbf{k}+\mathbf{l}+\mathbf{p}}^{1,2} \\ &+ (\rho_{\tau,\mathbf{p}+\mathbf{l}} - \rho_{\mathbf{l}}) \sum_{\mathbf{k}} \left(V_{\tau,\tau} \left(\frac{\mathbf{p} - \mathbf{k} - \mathbf{l}}{2}, \frac{\mathbf{k} - \mathbf{l} - \mathbf{p}}{2} \right) \right. \\ &\quad \left. + V_{\tau,\tau} \left(\frac{\mathbf{p} - \mathbf{k} - \mathbf{l}}{2}, \frac{-\mathbf{k} + \mathbf{l} + \mathbf{p}}{2} \right) \right) T_{\tau,\mathbf{k},\mathbf{p}}^{1,2}, \end{aligned} \quad (4.27)$$

$$\begin{aligned} P_{\tau,\mathbf{p},\mathbf{l}}^{1,2} &= \Delta_{\tau}(\mathbf{p}) [T_{\tau,\mathbf{p},\mathbf{p}+\mathbf{l}}^{1,2}]^* \\ &+ \sum_{\mathbf{k}} \left\{ \kappa_{\tau,\mathbf{p}} \left[\left(V_{\tau,\tau} \left(\frac{\mathbf{p} - \mathbf{k}}{2}, \frac{-\mathbf{k} - 2\mathbf{l} - \mathbf{p}}{2} \right) \right. \right. \right. \\ &+ \left. \left. \left. V_{\tau,\tau} \left(\frac{\mathbf{p} - \mathbf{k}}{2}, \frac{\mathbf{k} + 2\mathbf{l} + \mathbf{p}}{2} \right) \right) [T_{\tau,\mathbf{k},\mathbf{l}+\mathbf{p}}^{1,2}]^* \right. \right. \\ &\quad \left. \left. + \left(V_{\tau,\tau} \left(\mathbf{k} - \frac{\mathbf{l}}{2}, -\frac{\mathbf{l}}{2} - \mathbf{p} \right) + V_{\tau,\tau} \left(\mathbf{k} - \frac{\mathbf{l}}{2}, \frac{\mathbf{l}}{2} + \mathbf{p} \right) \right) [T_{\tau,\mathbf{k},\mathbf{l}-\mathbf{k}}^{1,2}]^* \right] \right\}. \end{aligned} \quad (4.28)$$

Here a slightly altered Hartree-Fock Hamiltonian $f_{\tau}(\mathbf{p})$ is used that reads

$$\begin{aligned} f_{\tau}(\mathbf{p}) &= \frac{\hbar^2 p^2}{2m} + \sum_{\mathbf{k},\sigma} \rho_{\sigma,\mathbf{k}} V_{\sigma,\tau} \left(\frac{\mathbf{k} - \mathbf{p}}{2}, \frac{\mathbf{k} - \mathbf{p}}{2} \right) \\ &+ \sum_{\mathbf{k}} \rho_{\tau,\mathbf{k}} V_{\tau,\tau} \left(\frac{\mathbf{k} + \mathbf{p}}{2}, \frac{-\mathbf{k} - \mathbf{p}}{2} \right) \\ &+ \sum_{\sigma} |\psi_{\sigma,0}|^2 V_{\sigma,\tau} \left(-\frac{\mathbf{p}}{2}, -\frac{\mathbf{p}}{2} \right) \\ &+ |\psi_{\tau,0}|^2 V_{\tau,\tau} \left(\frac{\mathbf{p}}{2}, -\frac{\mathbf{p}}{2} \right). \end{aligned} \quad (4.29)$$

For a non-interacting mixture we observe that the species index only plays a real role in this Hamiltonian, which is true in the second order equations as well. Specifically one observes that the first line contains a term which counts the total particle density in a certain momentum mode through $\sum_{\sigma} \rho_{\sigma,\mathbf{k}}$. These terms are due to the interaction that still exists between different species through the interaction potential $V_{\sigma,\tau}$. The third term then also includes the influence of the σ condensate on the τ species. We note that in the single component equivalent of these equations the above alteration to the Hartree-Fock Hamiltonian is not necessary. In these equations both the doublets and triplets contain exactly the same Hartree-Fock Hamiltonian.

All homogeneous terms for $T^{1,2}$ can now be written compactly as

$$H_{\text{tot},\tau,\mathbf{p},\mathbf{l}}^{1,2} = K_{\tau,\mathbf{p},\mathbf{l}}^{1,2} + K_{\tau,\mathbf{l},\mathbf{p}}^{1,2} + V_{\tau,\mathbf{p},\mathbf{l}}^{1,2} + V_{\tau,\mathbf{l},\mathbf{p}}^{1,2} + P_{\tau,\mathbf{p},\mathbf{l}}^{1,2} + P_{\tau,\mathbf{l},\mathbf{p}}^{1,2}. \quad (4.30)$$

Here we see the first real example of the sizeable expressions which appear when calculating higher order cumulant equations. This further motivates the creation of a script to automate the calculation

and prevent possible mistakes. We have split the homogeneous terms into three distinct parts, namely the kinetic term $K^{1,2}$, the pairwise interaction term $V^{1,2}$ and the pairing term $^{1,2}P$ [14].

The kinetic terms contain the Hartree-Fock hamiltonian of the two incoming atoms with momenta \mathbf{p} and \mathbf{l} , and the outgoing particle with momentum $\mathbf{p} + \mathbf{l}$. This is in line with the analysis of the $T^{1,2}$ cumulant of section 2.2.2, where two incoming particles could either scatter with a third particle or scatter with each other. Note that the second outgoing particle is scattered into the condensate ($\mathbf{k} = 0$), and thus does not appear in this equation.

In the $V^{1,2}$ term we again observe the Bose enhancement term $(1 + \rho_{\tau, \mathbf{p}})$, signifying that excitation to states is again influenced by the occupation of the state. Also in the $V^{1,2}$ term we observe interactions between the two incoming atoms with momenta \mathbf{p} and \mathbf{l} and the resultant outgoing particle again. This can be seen by considering the arguments inside the interaction potential. In the pairing part $P^{1,2}$ we observe the pairing field defined earlier, for both incoming particles.

Having obtained $H^{1,2}$, we can also consider $H^{0,3}$. This was calculated to equal

$$H_{\tau, \mathbf{p}, \mathbf{l}}^{0,3} = f_{\tau}(\mathbf{p})T_{\tau, \mathbf{p}, \mathbf{l}}^{0,3} + (1 + \rho_{\tau, \mathbf{l}} + \rho_{\tau, \mathbf{p} + \mathbf{l}}) \sum_{\mathbf{k}} V_{\tau, \tau}(\frac{2\mathbf{l} + \mathbf{p}}{2}, \frac{2\mathbf{k} + \mathbf{p}}{2})T_{\tau, \mathbf{p}, \mathbf{k}}^{0,3}, \quad (4.31)$$

$$H_{\text{tot}, \tau, \mathbf{p}, \mathbf{l}}^{0,3} = H_{\tau, \mathbf{p}, \mathbf{l}}^{0,3} + H_{\tau, -\mathbf{p} - \mathbf{l}, \mathbf{p}}^{0,3} + H_{\tau, \mathbf{l}, -\mathbf{p} - \mathbf{l}}^{0,3}. \quad (4.32)$$

We once more observe the Bose enhancement term $(1 + \rho_{\tau, \mathbf{k}})$ appearing, which alters the scattering to populated excited states by $T^{0,3}$ scattering events. Referring back to section 2.2.2, $T^{0,3}$ scattering events were defined as scattering of three excitations into the condensate. For $T_{\tau, \mathbf{p}, \mathbf{l}}^{0,3}$ the three impeding particles have momenta \mathbf{p} , \mathbf{l} and $-\mathbf{p} - \mathbf{l}$. We observe that in $H^{0,3}$ the Hartree-Fock energies of all scattered particles are included, just as was observed for $H^{1,2}$. For the third order equations we have one remaining class of terms, which define the action of the triplets $T^{1,2}$ and $T^{0,3}$ on each other. We refer to these terms as the "back-action" B . Let us first again define the following intermediate terms

$$B_{\tau, \mathbf{p}, \mathbf{l}}^{1,2} = \sum_{\mathbf{k}} V_{\tau, \tau}(\frac{\mathbf{l}}{2} + \mathbf{p}, \mathbf{k} + \frac{\mathbf{l}}{2})\kappa_{\tau, \mathbf{l} + \mathbf{p}}^* T_{\tau, \mathbf{k}, \mathbf{l}}^{0,3} - \frac{1}{2}\Delta(\mathbf{p} + \mathbf{l})^* T_{\tau, \mathbf{p}, \mathbf{l}}^{0,3}, \quad (4.33)$$

$$\begin{aligned} B_{\tau, \mathbf{p}, \mathbf{l}}^{0,3} &= \Delta_{\tau}(\mathbf{l} + \mathbf{p})T_{\tau, \mathbf{p}, \mathbf{l}}^{1,2} \\ &+ \kappa_{\tau, \mathbf{p}} \sum_{\mathbf{k}} \left[V_{\tau, \tau}(-\frac{\mathbf{k}}{2} + \mathbf{l} + \frac{\mathbf{p}}{2}, -\frac{\mathbf{k}}{2} - \frac{\mathbf{p}}{2}) + V_{\tau, \tau}(\frac{-\mathbf{k} + 2\mathbf{l} + \mathbf{p}}{2}, \frac{\mathbf{k} + \mathbf{p}}{2}) \right] T_{\tau, \mathbf{k}, -\mathbf{l} - \mathbf{p}}^{1,2} \\ &+ \left[V_{\tau, \tau}(\frac{\mathbf{k} + 2\mathbf{l} + \mathbf{p}}{2}, \frac{-\mathbf{k} - \mathbf{p}}{2}) + V_{\tau, \tau}(\frac{\mathbf{k} + 2\mathbf{l} + \mathbf{p}}{2}, \frac{\mathbf{k} + \mathbf{p}}{2}) \right] T_{\tau, \mathbf{k}, \mathbf{l}}^{1,2}. \end{aligned} \quad (4.34)$$

Then we write the total back action terms as

$$B_{\text{tot}, \tau, \mathbf{p}, \mathbf{l}}^{1,2} = B_{\tau, \mathbf{p}, \mathbf{l}}^{1,2} + B_{\tau, \mathbf{l}, \mathbf{p}}^{1,2}, \quad (4.35)$$

$$B_{\text{tot}, \tau, \mathbf{p}, \mathbf{l}}^{0,3} = B_{\tau, \mathbf{p}, \mathbf{l}}^{0,3} + B_{\tau, -\mathbf{p} - \mathbf{l}, \mathbf{p}}^{0,3} + B_{\tau, \mathbf{l}, -\mathbf{p} - \mathbf{l}}^{0,3}. \quad (4.36)$$

We see that the triplets influence each other's dynamics partly through the pairing field of the two impeding particles. We can now summarize all results of this section in the following compact equations of motion.

$$i\hbar\dot{T}_{\tau,\mathbf{p},\mathbf{l}}^{1,2} = [S_{\text{tot}}^{1,2} + H_{\text{tot}}^{1,2} + B_{\text{tot}}^{1,2}]_{\tau,\mathbf{p},\mathbf{l}}, \quad (4.37)$$

$$i\hbar\dot{T}_{\tau,\mathbf{p},\mathbf{l}}^{0,3} = [S_{\text{tot}}^{0,3} + H_{\text{tot}}^{0,3} + B_{\text{tot}}^{0,3}]_{\tau,\mathbf{p},\mathbf{l}}. \quad (4.38)$$

The single component equations were checked against ref [16] and found to match. This shows that, at least up to third order, the script works as expected.

4.2.2 Three-body Schrödinger equation

In the HFB equation we could observe the two-body Schrödinger equation. One would thus also expect to find the three-body Schrödinger equation somewhere in the third order equation. As discussed before, the $T^{0,3}$ cumulant describes scattering events between three particles. Let us take its EoM and write only the homogeneous terms, assuming that the entire dynamics is controlled only by three particle interactions. We define permutations

$$P_-^{(3)}O_{ijk} = O_{kij}, \quad P_+^{(3)}O_{ijk} = O_{jki}. \quad (4.39)$$

Given that the three particles in $T^{0,3}$ have momenta \mathbf{p} , \mathbf{l} and $-\mathbf{p} - \mathbf{l}$, we can then compactly write the homogeneous equation as

$$i\hbar\dot{T}_{\tau,\mathbf{p},\mathbf{l}}^{0,3} = \left(1 + P_- + P_+\right) \left\{ f_{\tau}(\mathbf{p})T_{\tau,\mathbf{p},\mathbf{l}}^{0,3} + (1 + \rho_{\tau,\mathbf{l}} + \rho_{\tau,\mathbf{p}+\mathbf{l}}) \sum_{\mathbf{k}} V_{\tau,\tau} \left(\frac{2\mathbf{l} + \mathbf{p}}{2}, \frac{2\mathbf{k} + \mathbf{p}}{2} \right) T_{\tau,\mathbf{p},\mathbf{k}}^{0,3} \right\} \quad (4.40)$$

Again we use an ansatz for the dynamics of $T^{0,3}$, which reads

$$T_{\tau,\mathbf{p},\mathbf{l}}^{0,3} = e^{E_{\nu}t} \Psi_{\tau,\nu}(\mathbf{p}, \mathbf{l}). \quad (4.41)$$

We assume the dynamics of $T^{0,3}$ are much faster than those of ρ and ψ . Then we again formulate an eigenvalue equation of the form

$$E_{\nu} \Psi_{\tau,\nu}(\mathbf{p}, \mathbf{l}) = \left(1 + P_- + P_+\right) \left\{ f_{\tau}(\mathbf{p}) \Psi_{\tau,\nu}(\mathbf{p}, \mathbf{l}) + (1 + \rho_{\tau,\mathbf{l}} + \rho_{\tau,\mathbf{p}+\mathbf{l}}) \sum_{\mathbf{k}} V_{\tau,\tau} \left(\frac{2\mathbf{l} + \mathbf{p}}{2}, \frac{2\mathbf{k} + \mathbf{p}}{2} \right) \Psi_{\tau,\nu}(\mathbf{p}, \mathbf{k}) \right\}, \quad (4.42)$$

with eigenvalue E_{ν} and eigenfunction $\Psi_{\tau,\nu}(\mathbf{p}, \mathbf{l})$. This equation is again similar in form to the three body Schrödinger equation for the three scattered particles [21]. Again we observe that the energy of the particles is altered to the Hartree-Fock energy, and the interaction term is again Bose enhanced by the $(1 + P_- + P_+)(1 + \rho_{\mathbf{k}} + \rho_{\mathbf{k}'})$ term. This eigenvalue equation can be used to examine the dynamics of trimers inside the gas, and the influence of the condensate on the formation of such trimers [14].

4.2.3 Third order interacting mixtures

As was discussed in section 2.2.3, one can formulate many different mixture cumulants in third order cumulant theory. The script developed in this work is programmed in such a way that the user can define what mixture cumulants to include by themselves, which allows for flexible application to different theories on the dynamics of mixed Bose gases. This section will outline some results from the **Interacting Mixture.nb** script when going up to third order.

The simplest result is obviously obtained by only allowing mixture cumulants of second order to be nonzero, and neglecting all third order mixture cumulants. As expected, this would simply extend the second order mixture equations with exactly the same triplets as the non-interacting HFB equations calculated in section 4.2.1. The results become more interesting if we also include a third order mixture cumulant. Taking a look at equations 4.20 and 4.21 we see that the dynamics of ρ and κ in a non-interacting mixture are only influenced by both $T^{1,2}$ and $T^{0,3}$. Note that the ψ equation is not altered by the presence of mixture triplets. Let us then include the mixture cumulant

$$T_{\tau,\gamma}^{1,2} = \langle \hat{a}_\tau^\dagger \hat{a}_\gamma \hat{a}_\gamma \rangle^c. \quad (4.43)$$

Here the momenta indices have been temporarily excluded for brevity. Physically, this cumulant could be filled by the scattering of two γ particles with the τ condensate, exciting one τ atom and condensing both γ excitations. Here we will assume that three particle scattering processes between different species, e.g. $T_{\tau,\gamma,\gamma}^{0,3}$, do not occur. Thus these cumulants can be kept in their original "non-interacting" form. We now find the following resulting dynamics for ρ . The I tensors are altered as

$$\begin{aligned} I_{\gamma,\sigma,\tau}(\mathbf{p}) = \sum_{\mathbf{k}} \left\{ \psi_{\sigma,0}^* \left[V_{\sigma,\tau} \left(\frac{-\mathbf{p}}{2}, \mathbf{k} - \frac{\mathbf{p}}{2} \right) T_{\gamma,\sigma,\mathbf{p}-\mathbf{k},\mathbf{k}}^{1,2} \right. \right. \\ \left. \left. - V_{\gamma,\sigma} \left(\frac{\mathbf{p}-\mathbf{k}}{2}, \frac{\mathbf{k}+\mathbf{p}}{2} \right) T_{\gamma,\sigma,\mathbf{p},\mathbf{k}}^{1,2} \right] \right. \\ \left. - \psi_{\gamma,0}^* V_{\gamma,\sigma} \left(\frac{-\mathbf{k}-\mathbf{p}}{2}, \frac{\mathbf{p}-\mathbf{k}}{2} \right) T_{\sigma,\sigma,\mathbf{p},\mathbf{k}}^{1,2} \right\}. \end{aligned} \quad (4.44)$$

Using this we can again formulate the third order equations for the mixture doublets as

$$\begin{aligned} i\hbar \dot{\rho}_{\tau,\gamma,\mathbf{p}} = I_{\tau,\gamma,\gamma}(\mathbf{p}) - \sum_{\sigma} I_{\gamma,\sigma,\tau}(\mathbf{p})^* \\ + \sum_{\sigma} \left[\Delta_{\gamma,\sigma}(\mathbf{p}) \kappa_{\sigma,\tau,\mathbf{p}}^* - \Delta_{\tau,\sigma}(\mathbf{p})^* \kappa_{\sigma,\gamma,\mathbf{p}} + \Omega_{\gamma,\sigma}(\mathbf{p}) \rho_{\tau,\sigma,\mathbf{p}} - \Omega_{\sigma,\tau}(\mathbf{p}) \rho_{\sigma,\gamma,\mathbf{p}} \right. \\ \left. + \rho_{\tau,\gamma,\mathbf{p}} \{ \Theta_{\gamma,\sigma}(\mathbf{p}) - \Theta_{\tau,\sigma}(\mathbf{p}) \} \right], \end{aligned} \quad (4.45)$$

$$\begin{aligned}
i\hbar\dot{\kappa}_{\gamma,\tau,\mathbf{p}} = & \sum_{\mathbf{k}} V_{\gamma,\tau}(\mathbf{p} - \frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}) \left[\psi_{\tau,0} T_{\gamma,\gamma,\mathbf{k},\mathbf{p}}^{1,2} + \psi_{\gamma,0} T_{\tau,\tau,\mathbf{k},\mathbf{p}}^{1,2} \right] \\
& + \delta_{\gamma,\tau} \sum_{\mathbf{k}} \psi_{\gamma,0}^* \left[V_{\gamma,\gamma}(\frac{\mathbf{p}}{2}, \mathbf{k} - \frac{\mathbf{p}}{2}) + V_{\gamma,\tau}(\frac{\mathbf{p}}{2}, \mathbf{k} + \frac{\mathbf{p}}{2}) \right] T_{\tau,\mathbf{k},\mathbf{p}-\mathbf{k}}^{0,3} \\
& + \delta_{\gamma,\tau} \sum_{\sigma,\mathbf{k}} \psi_{\sigma,0} \left[V_{\sigma,\tau}(\mathbf{p} + \frac{\mathbf{k}}{2}, -\frac{\mathbf{k}}{2}) + V_{\gamma,\sigma}(\mathbf{p} - \frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}) \right] T_{\sigma,\tau,\mathbf{p},\mathbf{k}}^{1,2} \\
& + 2h_{\gamma,\tau}(\mathbf{p})\kappa_{\gamma,\tau,\mathbf{p}} \\
& + \sum_{\sigma} \left[\Omega_{\gamma,\sigma}(\mathbf{p})\kappa_{\sigma,\tau,\mathbf{p}} + \Omega_{\sigma,\tau}(\mathbf{p})\kappa_{\gamma,\sigma,\mathbf{p}} + \Delta_{\gamma,\sigma}(\mathbf{p})\rho_{\sigma,\tau,\mathbf{p}} + \Delta_{\sigma,\tau}(\mathbf{p})\rho_{\sigma,\gamma,\mathbf{p}} \right] + \Delta_{\gamma,\tau}(\mathbf{p}).
\end{aligned} \tag{4.46}$$

Note that compared to the normal third order equations we observe that now several terms are separated where before they could be combined. Interestingly we observe in the equation for κ that if one were to ignore the forming of excitation pairs within the same component entirely, for example if one is only interested in the formation of opposite spin pairs, then several third order terms in the κ equation of motion vanish. This insight could obviously not be gained when only considering the single component cumulants.

One could now also use the interacting mixture script to calculate the equation of motion for $T_{\tau,\gamma}^{1,2}$, which would give an extended version of equation 4.37 in the case of interacting mixtures. We do not analyse this equation here in detail but note that the extensions look very similar to those for the singlets and doublets. For $T_{\tau,\gamma}^{1,2}$ however we do not observe "external" delta functions like the ones we observe in the κ equation.

4.3 Boson fourth order equations

Obviously now that we have considered second and third order cumulant equations the natural next step is the fourth order cumulant theory. Here all quadruplets Q are also included in the equations, meaning that we now start including four particle interactions in the dynamics. Even though the non-interacting mixture can also be used to calculate the fourth order equation, in this section we will switch to the single component script for brevity. We note that even though the third order equations are already of considerable length, the fourth order equations become much too long to completely discuss in this work. This section will pick out some parts of the equations that are interesting to discuss.

4.3.1 Singlets and doublets

Let us first explore the effect of the quadruplets Q on the singlet ψ and doublets ρ and κ . Interestingly the equation of motion for ψ is not influenced by cumulants above third order, signifying that equation 4.18 is exact. The doublets however, are more interesting, and receive some extra inhomogeneous terms. These additional terms read

$$Q_{\mathbf{p}}^{\rho} = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{q}} \left\{ Q_{\mathbf{p}-\mathbf{k}, \mathbf{q}, \mathbf{k}}^{2,2} V\left(\frac{2\mathbf{p}-\mathbf{k}-\mathbf{q}}{2}, \frac{\mathbf{q}-\mathbf{k}}{2}\right) + Q_{\mathbf{q}, \mathbf{k}, \mathbf{p}+\mathbf{q}}^{2,2} V\left(\frac{\mathbf{k}-\mathbf{p}+\mathbf{q}}{2}, \frac{\mathbf{k}-\mathbf{p}-\mathbf{q}}{2}\right) \right. \\ \left. - Q_{\mathbf{q}, \mathbf{k}, \mathbf{p}}^{2,2} \left[V\left(\frac{\mathbf{k}+\mathbf{p}+2\mathbf{q}}{2}, \frac{\mathbf{p}+\mathbf{k}}{2}\right) + V\left(\frac{\mathbf{k}+\mathbf{p}+2\mathbf{q}}{2}, \frac{-\mathbf{p}-\mathbf{k}}{2}\right) \right] \right\}, \quad (4.47)$$

$$Q_{\mathbf{p}}^{\kappa} = 2 \sum_{\mathbf{k}, \mathbf{q}} Q_{\mathbf{p}, \mathbf{q}, \mathbf{k}}^{1,3} V\left(\frac{\mathbf{k}+\mathbf{q}+2\mathbf{p}}{2}, \frac{\mathbf{k}-\mathbf{q}}{2}\right). \quad (4.48)$$

We see that ρ is only influenced by $Q^{2,2}$, which can actually still represent a two body scattering process with two impeding particles altering each others momentum. For $Q_{\mathbf{p}-\mathbf{k}, \mathbf{q}, \mathbf{k}}^{2,2}$ the two incoming particles have momenta \mathbf{p} and $\mathbf{q} - \mathbf{p} + \mathbf{k}$ and the outgoing particles have momenta \mathbf{q} and \mathbf{k} . The potential matrix element for such a scattering event reads

$$\langle \mathbf{p}, \mathbf{q} - \mathbf{p} + \mathbf{k} | \hat{V} | \mathbf{q}, \mathbf{k} \rangle \quad (4.49)$$

which is equivalent to the one in the expression. Similarly the $Q_{\mathbf{q}, \mathbf{k}, \mathbf{p}+\mathbf{q}}^{2,2}$ cumulant is (partially) filled by scattering between two particles of momenta $\mathbf{k} + \mathbf{q}$ and \mathbf{p} to two particles \mathbf{k} and $\mathbf{p} + \mathbf{q}$, which correctly corresponds to the matrix element

$$\langle \mathbf{k} + \mathbf{q}, \mathbf{p} | \hat{V} | \mathbf{k}, \mathbf{p} + \mathbf{q} \rangle \quad (4.50)$$

Note that in two particle $Q^{2,2}$ scattering processes no particles scatter to the condensate. However $Q^{2,2}$ can also be filled by four particle scattering processes in which two particles are scattered into the condensate. If we now take a look at equation 4.48, we see that κ is only influenced by $Q^{1,3}$. Specifically $Q_{\mathbf{p}, \mathbf{q}, \mathbf{k}}^{1,3}$ represents a scattering process in which three particles of momenta \mathbf{p} , \mathbf{k} and \mathbf{q} impede and a single particle with momenta $\mathbf{p} + \mathbf{q} + \mathbf{k}$ leaves, which would imply that three particles have been scattered to the condensate.

4.3.2 Four body Schrödinger equation

One could also continue with the fourth order dynamics of the triplets and quadruplets, which would extend the equations in section 4.2 to fourth order interactions. These equations however are very long, and difficult to check because the literature on this topic is quite sparse. We can however at least partially check the calculated equations by looking for the four body Schrödinger equation. From both the second and third order equation the equivalent many-body Schrödinger equation could be recovered, so one would expect the same to be true for the fourth order equations.

We consider the homogeneous dynamics of the $Q^{0,4}$ cumulant, ensuring that we are only considering four body scattering. Let us first define the single component Hartree-Fock Hamiltonian.

$$h(\mathbf{p}) = \frac{\hbar^2 p^2}{2m} + \sum_{\mathbf{k}} \rho_{\mathbf{k}} \left[V\left(\frac{\mathbf{k}+\mathbf{p}}{2}, \frac{\mathbf{k}+\mathbf{p}}{2}\right) + V\left(\frac{\mathbf{k}+\mathbf{p}}{2}, \frac{-\mathbf{k}-\mathbf{p}}{2}\right) \right] \\ + |\psi_0|^2 \left[V\left(\frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2}\right) + V\left(\frac{\mathbf{p}}{2}, \frac{-\mathbf{p}}{2}\right) \right]. \quad (4.51)$$

Again the homogenous equation is quite lengthy. For convenience of notation we define the following tensor.

$$H_{\mathbf{p},\mathbf{g},\mathbf{l}}^{0,3} = (1 + \rho_{\mathbf{l}} + \rho_{\mathbf{g}+\mathbf{l}+\mathbf{p}}) \sum_{\mathbf{k}} V\left(\frac{2\mathbf{l} + \mathbf{g} + \mathbf{p}}{2}, \frac{2\mathbf{k} + \mathbf{g} + \mathbf{p}}{2}\right) Q_{\mathbf{k},\mathbf{p},\mathbf{g}}^{0,4}. \quad (4.52)$$

If we would like to write the homogeneous terms in a similar form as those for the third order equations we require some extra permutation operators. To save space we also define a total permutation operator P_H .

$$P_-^{(4)} O_{ijkl} = O_{lijk}, \quad P_{23} O_{ijkl} = O_{ikjl}, \quad (4.53)$$

$$P_H = 1 + P_-^{(4)} + P_-^{(4)} P_-^{(4)} + P_{23} P_-^{(4)} + P_-^{(3)} + P_+^{(3)}. \quad (4.54)$$

Note that $P^{(4)}$ permutes the set $\{\mathbf{p}, \mathbf{l}, \mathbf{g}, -\mathbf{g} - \mathbf{l} - \mathbf{p}\}$ whilst $P^{(3)}$ permutes the set $\{\mathbf{p}, \mathbf{l}, \mathbf{g}\}$. Now we are in a position to write the homogeneous equation of motion for $Q^{0,4}$, which reads

$$i\hbar \dot{Q}_{\mathbf{p},\mathbf{g},\mathbf{l}}^{0,4} = h(\mathbf{p}) + h(\mathbf{g}) + h(\mathbf{l}) + h(-\mathbf{g} - \mathbf{l} - \mathbf{p}) Q_{\mathbf{p},\mathbf{g},\mathbf{l}}^{0,4} + P_H H_{\mathbf{p},\mathbf{g},\mathbf{l}}^{0,3}. \quad (4.55)$$

We follow the same procedure as for the second and third order homogeneous equations. Let us define an ansatz

$$Q_{\mathbf{p},\mathbf{g},\mathbf{l}}^{0,4} = e^{E_\nu t} \Phi_{\tau,\nu}(\mathbf{p}, \mathbf{g}, \mathbf{l}). \quad (4.56)$$

Then we can again formulate equation 4.55 as an eigenvalue problem. Here we assume that the dynamics of $Q^{0,4}$ are much faster than those of ρ and ψ , and thus these are assumed stationary. We also write out the $H^{0,3}$ tensor to obtain the most suggestive form of the equation.

$$E_\nu \Phi_{\tau,\nu}(\mathbf{p}, \mathbf{g}, \mathbf{l}) = \left[h(\mathbf{p}) + h(\mathbf{g}) + h(\mathbf{l}) + h(-\mathbf{g} - \mathbf{l} - \mathbf{p}) \right] \Phi_{\tau,\nu}(\mathbf{p}, \mathbf{g}, \mathbf{l}) + P_H \left[(1 + \rho_{\mathbf{l}} + \rho_{\mathbf{g}+\mathbf{l}+\mathbf{p}}) \sum_{\mathbf{k}} V\left(\frac{2\mathbf{l} + \mathbf{g} + \mathbf{p}}{2}, \frac{2\mathbf{k} + \mathbf{g} + \mathbf{p}}{2}\right) \Phi_{\tau,\nu}(\mathbf{k}, \mathbf{p}, \mathbf{g}) \right]. \quad (4.57)$$

The eigenvalue equation obtained above is very similar in form to the four body Schrödinger equation. The fact that this equation appears in the cumulant equations calculated by the script gives at least some indication that the script operates correctly.

The $Q^{0,4}$ cumulant is filled by scattering processes in which four particles of momenta $\mathbf{p}, \mathbf{g}, \mathbf{l}$ and $-\mathbf{p} - \mathbf{g} - \mathbf{l}$ scatter into the condensate. The first four terms of the eigenvalue equation contain the Hartree-Fock energy of the four scattered particles, which reduce to the normal kinetic energy in the vacuum limit $\{\psi, \rho\} \rightarrow 0$. For four particles one would expect the potential part to contain six terms, since a set of 4 particles has $\binom{4}{2} = 6$ unique interacting pairs. Equation 4.57 confirms this,

as it contains 6 interaction terms via the permutation operator P_H . We again observe that each term is Bose enhanced, by a certain combination of ρ cumulants. As an example, consider the term written out in full in equation 4.57, with Bose enhancement factor $(1 + \rho_{\mathbf{l}} + \rho_{\mathbf{g}+\mathbf{l}+\mathbf{p}})$. Writing out the potential matrix element in full we obtain

$$\sum_{\mathbf{k}} \langle \mathbf{l}, -\mathbf{g} - \mathbf{l} - \mathbf{p} | \hat{V} | \mathbf{k}, -\mathbf{k} - \mathbf{g} - \mathbf{p} \rangle, \quad (4.58)$$

which shows that this term represents the interaction between the \mathbf{l} and $-\mathbf{l} - \mathbf{g} - \mathbf{p}$ particles. This is consistent with the Bose enhancement factor, which alters the interaction term if these specific momentum states are already occupied. This analysis can easily be extended to all other interaction terms obtained by applying P_H , and shows that this equation is at least physically consistent. This gives more credence to this expression and thus to the script used to calculate it. Note that the interaction terms also reduce to the equivalent terms in the four body Schrödinger equation in the vacuum limit.

4.4 Fermions

So far the analysis has been focused on the dynamics of condensed Bose gases, which were analysed through the results of the scripts developed in chapter 3. However these script were also developed to handle fermionic operators and can thus also be used to calculate the fermion equivalent of the cumulant equations. This section will outline some results of the fermion scripts and discuss the difference with the results for bosons. As stated earlier, the fermion analysis will not be as elaborate as the one for bosons, which was the principal focus of this chapter. Still we can gain some interesting insight into cumulant theory by a brief look at the fermion equivalents.

4.4.1 Hartree-Fock Bogoliubov equations

Just like for bosons, we begin with the second order equations for a non-interacting mixture, which are also called the Hartree-Fock Bogoliubov (HFB) equations [10]. Note that since all uneven cumulants are automatically zero for fermions, there is no equation of motion for ψ . The HFB equations then describe the dynamics of the ρ and κ cumulants. Let us define a fermion pairing field and Hartree-Fock Hamiltonian that read

$$\Delta_{\tau}(\mathbf{p}) = \frac{1}{2} \sum_{\mathbf{k}} \kappa_{\tau, -\mathbf{k}, \mathbf{k}} V_{\tau, \tau}^A(\mathbf{p}, -\mathbf{k}), \quad (4.59)$$

$$\begin{aligned} h_{\tau}(\mathbf{p}) &= \frac{\hbar^2 p^2}{2m} - \sum_{\mathbf{k}} V_{\tau, \tau}(\frac{\mathbf{p} - \mathbf{k}}{2}, \frac{\mathbf{k} - \mathbf{p}}{2}) \rho_{\tau, \mathbf{k}} \\ &+ \frac{1}{2} \sum_{\sigma, \mathbf{k}} \left[V_{\sigma, \tau}(\frac{\mathbf{k} - \mathbf{p}}{2}, \frac{\mathbf{k} - \mathbf{p}}{2}) + V_{\sigma, \tau}(\frac{\mathbf{p} + \mathbf{k}}{2}, \frac{\mathbf{k} + \mathbf{p}}{2}) \right]. \end{aligned} \quad (4.60)$$

with which we can write the fermion HFB equations as

$$i\hbar \dot{\rho}_{\tau, \mathbf{p}} = \Delta_{\tau}(\mathbf{p})^* \kappa_{\tau, -\mathbf{p}, \mathbf{p}} - \Delta_{\tau}(\mathbf{p}) \kappa_{\tau, -\mathbf{p}, \mathbf{p}}^*, \quad (4.61)$$

$$i\hbar\dot{\kappa}_{\tau,-\mathbf{p},\mathbf{p}} = 2h_{\tau}(\mathbf{p})\kappa_{\tau,-\mathbf{p},\mathbf{p}} + (2\rho_{\tau,\mathbf{p}} - 1)\Delta_{\tau}(\mathbf{p}). \quad (4.62)$$

From a quick look at these equations one already observes several differences with the boson case. For fermions there is no condensate and no ψ cumulant. Thus we observe that all terms that previously involved ψ_0 are now absent. We then find somewhat simpler expressions for the pairing field and Hartree-Fock Hamiltonian. We also see in the equation for κ that we no longer have the Bose enhancement factor. In fact, the occupation of a state now alters the dynamics via a different term $(2\rho_{\tau,\mathbf{p}} - 1)$. Since ρ can be either 1 or 0, we see that the pairing field is added for an occupied state and subtracted for an empty state. This could be a direct manifestation of the Pauli exclusion principle.

Note that we were only able to apply the antisymmetric matrix element in the pairing field. If one were to consider single component equations, i.e. without the Greek index, then we could have also used antisymmetric elements in $h_{\tau}(\mathbf{p})$. Unfortunately for a mixture the terms are separated into different sums. By a similar analysis as was conducted for bosons, one can again discover the two body Schrödinger equation in the homogeneous equation of motion for κ . Since this analysis is so similar to the boson case, we will not repeat it here. The fermion HFB equations were checked with ref [10] and found to match.

4.4.2 Interacting fermi mixtures

An intrinsic property of fermions is that they have half integer spin. An electron for example has either spin $+\frac{1}{2}$ or $-\frac{1}{2}$. Cumulant theory provides the tools to study fermion gases with mixed spins, which may interact via s-wave pairing [22]. This is one interesting application of the **InteractingMixture.nb** script as applied to fermions. This section will summarize some results from this script, again starting with the HFB equations for a multi component Fermi gas. As has now become our standard procedure, we first define the fermion mixture pairing field together with the fermion equivalents of the tensors Ω and Θ .

$$\Delta_{\gamma,\sigma}(\mathbf{p}) = \frac{1}{2} \sum_{\mathbf{k}} V_{\gamma,\sigma}^A(\mathbf{p}, -\mathbf{k}) \kappa_{\gamma,\sigma,-\mathbf{k},\mathbf{k}}, \quad (4.63)$$

$$\Omega_{\gamma,\sigma}(\mathbf{p}) = \sum_{\mathbf{k}} V_{\gamma,\sigma}\left(\frac{\mathbf{p}-\mathbf{k}}{2}, \frac{\mathbf{k}-\mathbf{p}}{2}\right) \rho_{\sigma,\gamma,\mathbf{k}}, \quad (4.64)$$

$$\Theta_{\gamma,\sigma}(\mathbf{p}) = \sum_{\mathbf{k}} V_{\gamma,\sigma}\left(\frac{\mathbf{p}-\mathbf{k}}{2}, \frac{\mathbf{p}-\mathbf{k}}{2}\right) \rho_{\sigma,\sigma,\mathbf{k}}. \quad (4.65)$$

Then the full mixture equation of motion reads

$$\begin{aligned} i\hbar\dot{\rho}_{\tau,\gamma,\mathbf{p}} = & \sum_{\sigma} \left[\Delta_{\tau,\sigma}^*(\mathbf{p}) \kappa_{\sigma,\gamma,-\mathbf{p},\mathbf{p}} - \Delta_{\gamma,\sigma}(\mathbf{p}) \kappa_{\sigma,\tau,-\mathbf{p},\mathbf{p}} \right. \\ & + \Omega_{\sigma,\tau}(\mathbf{p}) \rho_{\sigma,\gamma,\mathbf{p}} - \Omega_{\gamma,\sigma}(\mathbf{p}) \rho_{\tau,\sigma,\mathbf{p}} \\ & \left. + \rho_{\tau,\gamma,\mathbf{p}} \{ \Theta_{\tau,\sigma}(\mathbf{p}) - \Theta_{\gamma,\sigma}(\mathbf{p}) \} \right] \end{aligned} \quad (4.66)$$

We observe that the dynamics for ρ look very similar to the equivalent equation for bosons (4.15), be it with some slight differences. As expected, the condensate is absent again. The $\mathbf{k} = 0$ momentum mode is treated as any other, and is just part of the regular summation. Interestingly we do observe that the sign of the new mixture fermion equation is exactly flipped in comparison to the additional terms in the boson equation. This is probably a straightforward result of the difference in commutation relations. Let us next consider the mixture equation of motion for κ and see if we observe similar differences. We require the mixture Hartree-Fock Hamiltonian, now defined with the fermion tensor Θ as

$$h_{\gamma,\tau}(\mathbf{p}) = \frac{\hbar^2 p^2}{2m} + \sum_{\sigma} \frac{1}{2} \left(\Theta_{\gamma,\sigma}(\mathbf{p}) + \Theta_{\sigma,\tau}(\mathbf{p}) \right). \quad (4.67)$$

Then the κ EoM as calculated by the script reads

$$\begin{aligned} i\hbar\dot{\kappa}_{\tau,\gamma,\mathbf{p}} &= 2h_{\gamma,\tau}(\mathbf{p})\kappa_{\tau,\gamma,\mathbf{p}} \\ &\quad \sum_{\sigma} \left[-\Omega_{\gamma,\sigma}(\mathbf{p})\kappa_{\tau,\sigma,-\mathbf{p},\mathbf{p}} - \Omega_{\sigma,\tau}(\mathbf{p})\kappa_{\tau,\sigma,-\mathbf{p},\mathbf{p}} \right. \\ &\quad \left. + \Delta_{\gamma,\sigma}(\mathbf{p})\rho_{\sigma,\tau,\mathbf{p}} + \Delta_{\sigma,\tau}(\mathbf{p})\rho_{\sigma,\gamma,\mathbf{p}} \right] - \Delta_{\gamma,\tau}(\mathbf{p}) \end{aligned} \quad (4.68)$$

So we again find an equation of very similar form to the boson equation 4.17, however we note that also for κ the additional mixture terms expressed in the tensor Ω have had their sign changed compared to the boson case. These sign changes could be a straightforward consequence of the change in commutation relations between bosons and fermions.

4.4.3 Extending HFB equations

Recently there has been some interest in literature into also extending the fermion HFB equations to include higher order cumulants [5]. Since for fermions the triplets are automatically zero, extending the equations requires the inclusion of quadruplets. The HFB equations for a non-interacting mixture are extended as follows

$$\begin{aligned} i\hbar\dot{\rho}_{\tau,\mathbf{p}} &= \Delta_{\tau}(\mathbf{p})^* \kappa_{\tau,-\mathbf{p},\mathbf{p}} - \Delta_{\tau}(\mathbf{p}) \kappa_{\tau,-\mathbf{p},\mathbf{p}}^* \\ &\quad + \sum_{\mathbf{k},\mathbf{q}} \left[V_{\tau,\tau} \left(\frac{2\mathbf{p} - \mathbf{k} - \mathbf{q}}{2}, \frac{\mathbf{q} - \mathbf{k}}{2} \right) Q_{\tau,\mathbf{q},\mathbf{k},\mathbf{p},\mathbf{k}+\mathbf{q}-\mathbf{p}}^{2,2} \right. \\ &\quad \left. - V_{\tau,\tau} \left(\frac{\mathbf{q} - \mathbf{k}}{2}, \frac{2\mathbf{p} - \mathbf{k} - \mathbf{q}}{2} \right) Q_{\tau,\mathbf{p},\mathbf{k}+\mathbf{q}-\mathbf{p},\mathbf{q},\mathbf{k}}^{2,2} \right], \end{aligned} \quad (4.69)$$

$$\begin{aligned} i\hbar\dot{\kappa}_{\tau,-\mathbf{p},\mathbf{p}} &= 2h_{\tau}(\mathbf{p})\kappa_{\tau,-\mathbf{p},\mathbf{p}} + (2\rho_{\tau,\mathbf{p}} - 1)\Delta_{\tau}(\mathbf{p}) \\ &\quad + \sum_{\mathbf{k}} \left[V_{\tau,\tau} \left(\frac{2\mathbf{p} + \mathbf{q} + \mathbf{k}}{2}, \frac{\mathbf{k} - \mathbf{q}}{2} \right) \right. \\ &\quad \left. - V_{\tau,\tau} \left(\frac{2\mathbf{p} - \mathbf{q} - \mathbf{k}}{2}, \frac{\mathbf{q} - \mathbf{k}}{2} \right) \right] Q_{\tau,\mathbf{p},\mathbf{q},\mathbf{k}}^{1,3} \end{aligned} \quad (4.70)$$

So we observe that the ρ and κ cumulants are influenced by only $Q^{2,2}$ and $Q^{1,3}$ quadruplets respectively, as was the case for bosons. These equations were checked against ref [5] and found to match, again showing that the script works correctly.

Chapter 5

Conclusion

In this work a script was developed capable of calculating the cumulant equations for both bosons and fermions and simplifying these equations to obtain a clear easily interpreted form. The scripts developed in this work run on Mathematica in conjunction with the SNEG package for second quantization. This allows the user to easily modify input and also gives cleaner output in normal mathematical notation. This is very useful for the cumulant equations, which are often quite lengthy. In addition to the functions contained within the SNEG package, several custom functions were written. These functions allow for automatic calculation of different procedures in cumulant theory, like the cluster expansion and index simplification. To widen the applicability of this work, this report is actually accompanied by three Mathematica scripts, which can deal with different kinds of Bose or Fermi mixtures. It was shown that the scripts operate up to fourth order within manageable computation times.

The script first accepts customizable input of operator products, after which each operator product is plugged into the right hand side of the Heisenberg equation. The script then first calculates and simplifies the commutator for each product, after which the resulting expression are expanded via the cluster expansion. The resulting equations are then simplified under customizable assumptions, after which they are combined with the left hand side of the Heisenberg equation to obtain the full equations of motion.

The results of the script were analysed in detail for the condensed Bose gas, which adopts the coherent state approximation. Analysis first focused on the "non-interacting mixture", in which all mixture cumulants are set to zero. In such a gas then interactions between species only occur via the interaction potential. It was shown that the second (Hartree-Fock Bogoliubov) and third order equations match those in the relevant literature, which shows that at least within this domain the script operates properly. The fourth order equations were also analysed, showing that within the dynamics of 4 particles one could find the four body Schrödinger equation in a medium, which is altered by the presence of the condensate. This gives a strong indication that the fourth order equations as calculated by the script are also correct, given that the appropriate many body Schrödinger equation could also be found in second and third order cumulant theory.

Next to analysing the boson equations for a non-interacting mixture, which is easily transformed to a single component gas, this report also analysed the full interacting mixture equations. In a full interacting mixture all mixture cumulants are also taken into account. Here it was observed that the new mixture scattering processes that could fill the ρ cumulants also spawned new terms in the corresponding dynamics. These terms were summarized by defining new tensors, which grouped those terms related to interspecies scattering. A short analysis was also conducted of the third order

equations for an interacting mixture. It was shown that these can also influence the dynamics of the doublets, depending on the specific mixture cumulants considered. It was also shown that the dynamics of the κ cumulant could be shortened significantly if one assumes that only excitation pairs of different species exist. This can for example be applied to study the dynamics of opposite spin pairs, which are often observed in nature. Further analysis of mixture cumulants can also easily be conducted using the scripts developed here, due to the customizability of the code.

This work also conducted a short summary of the equivalent fermion results, including second order interacting mixtures. Here it was observed that the fermion equations for interacting mixtures were extended similarly as those for bosons, although sometimes with a sign change. Also expected differences like the absence of a condensate were all confirmed by the script. The second and fourth order fermion equations for the doublets were calculated for a non-interacting mixture and found to match with literature, thus proving the effectiveness of the script also in this area.

Due to the high customizability of the script it would take much more time to outline all the results one could obtain with it. The scripts developed in this work aim to serve as a basic framework with which a user can perform calculations within cumulant theory and introduce their own assumptions and approximations. This is facilitated by the use of customizable rule sets and input, allowing the script to be quickly adapted to different many body theories. If one were looking to improve the script we advise an extra consideration of the simplification functions, especially those for index simplification. If they could be applied more generally and be more effective with the interacting mixture cumulants the equations could be printed in a shorter form. Also if one were to go above fourth order it could be useful to try and streamline some functions to be more efficient, decreasing computation time. These are just matters of convenience though, and do not impact the correctness of the results. The central initial goal of the script, automating the process of calculating the cumulant equations for both bosons and fermions, has already been achieved.

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