Dynamic Effects of a Feshbach Resonance on Bragg Scattering from a Bose–Einstein Condensate

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A thesis submitted for the degree of Doctor of Philosophy at the University of Otago, Dunedin, New Zealand.

November 2011
**Version history:**

Revised version post-examination: March 2012.
Abstract

The major focus of this thesis is the dynamic effects of Feshbach resonances on Bragg scattering from Bose–Einstein condensates. This work is motivated by the JILA experiment of Papp et al. [Phys. Rev. Lett. 101 (2008)], in which Bragg spectroscopy was used to probe the behaviour of a strongly interacting Bose–Einstein condensate of $^{85}$Rb, near a Feshbach resonance. This experiment was deliberately designed to explore a region of parameter space in which perturbation theory is not expected to be valid. Close to the resonance, the results from this experiment showed significant deviations from the Bragg scattering behaviour predicted by the simplest perturbative and mean-field theories.

We develop a c-field formalism to study Bose–Einstein condensates with interactions altered by a Feshbach resonance. Recognising that the change in scattering length close to the resonance is caused by the existence of a bound state, we formulate a method for treating ultracold Bose gases in terms of coupled atom and molecule fields. We show how to incorporate this atom-molecule model with a truncated Wigner formalism, and derive expressions for the scattering length and binding energy within this formalism. We also demonstrate how to accurately determine the phenomenological parameters in our c-field formalism by relating these to the corresponding experimental parameters.

Using the model of coupled atoms and molecules, we investigate the properties of a strongly interacting Bose–Einstein condensate, and discuss how the results differ from those obtained using a model of structureless atoms. We derive expressions for the condensate profiles in the Thomas–Fermi limit close to a Feshbach resonance, formulate the Bogoliubov theory for excitations in a coupled atom-molecule system, and investigate the case of Bragg scattering from a uniform condensate using Bogoliubov excitations. We show that even when there is very little difference in the condensate appearance between the atom-molecule model and the structureless atom model — as can be seen in the Thomas–Fermi profile — there can be significant changes in the line shifts of the Bragg spectra.

Finally, we perform numerical simulations, modelling the experiment of Papp et al. We describe the numerical techniques used for this purpose, and also outline some of the difficulties encountered in simulating the experiment. The results from these simulations are directly comparable to the results from the experiment, and we show that although the experiment was not designed to test this kind of theory, we obtain quantitative agreement with the experimental results.
Acknowledgements

First and foremost, I wish to thank my supervisor, Professor Crispin Gardiner, who has tirelessly guided me through this project. In Crispin, I have been fortunate enough to have a supervisor who is both brilliant and pleasant, with seemingly endless amounts of time available for discussions. It has been a true privilege to work with such a distinguished mind. This PhD has in many ways been a roller-coaster ride and without Crispin’s steady support, I can safely say that I would not have been able to complete it.

I am grateful to my co-supervisor, Professor Rob Ballagh, for inviting me to do this research project and thereby giving me the opportunity to do my PhD at the University of Otago, as well as for guiding me through the initial stages of this project. I would also like to thank Assoc. Prof. Blair Blakie and Dr. Ashton Bradley for their help at various points during these four years.

I have enjoyed working alongside many of the other staff in the Physics Department, both academic and general. Department Manager Sandy Wilson deserves special mention for all her help, as well as her amazing ability to get things done in a heartbeat.

I would also like thank Professor Tord Johansson at the Division of Nuclear and Particle Physics at Uppsala University in Sweden. As the supervisor of my MSc project, Tord was the one who first introduced me to the world of research; the truly positive experience I had during that project encouraged me to continue down the academic path.

During my time at Otago, I have had the pleasure of getting to know some wonderful people doing research in theoretical atom physics, both at Otago and elsewhere; Dr. Alice Bezett, Dr. Andrew Sykes, Dr. David Hallwood and Andrew Haines have all taught me that it is possible to be a theoretical physicist and still have fun. I am particularly grateful to Alice for her friendship and never-ending support during this experience, initially from the cubicle next to mine in room 524b, and lately from her new homes in Sweden and Holland.

I would also like to thank the other postgraduate students in the Physics Department whom I have gotten to know throughout the years. The experimentalists in the third floor labs have always given me invaluable breaks from my work, in particular Ana Rakonjac, Peter McDowall, Dr. Patrick Ledingham and Dr. David McAuslan who helped me start up the Otago OSA Student Chapter and organise the KOALA conference. I am grateful to them for making so many social events happen (especially karaoke), as well
as for putting up with me bossing them around.

The friends outside of the Physics Department that have stood by me during this experience (both overseas and in New Zealand) are too many to mention here, but I am grateful to each and every one of them. It has been invaluable for me to have friends with whom I have been able to share my PhD experience; Nathalie, Mustafa, Wenzel and Henrik have all been extremely understanding and always willing to offer encouragement to keep me going. I am also grateful for being so lucky as to have had amazing friends in my flatmates, among them Max, who have always given me a different perspective and helped me find my priorities. Rory has proved to be the best friend anyone could wish for, with the patience of a saint and an infinite supply of advice and support; without all our tea breaks, walks and discussions I would surely not have been able to keep sane.

Finally, I am ever grateful to my family — my mum Christina, my sister Lollo, and my brother Magnus — for always believing in me.

*This work was supported by the Marsden Fund of New Zealand under Contract No. UOO509; and the New Zealand Foundation for Research, Science and Technology under Contract No. NERF-UOOX0703.*
Till Mamma
# Contents

1 Introduction .......................................................... 1

1.1 Background .................................................................... 1

1.1.1 Bose–Einstein Condensation ........................................ 1

1.1.2 JILA Experiment ...................................................... 2

1.2 This Work ..................................................................... 3

1.2.1 Outline of Thesis ...................................................... 4

1.2.2 Collaborations ........................................................ 5

1.2.3 Publications ........................................................... 5

2 Background Theory ......................................................... 7

2.1 Bose–Einstein Condensation ............................................ 7

2.1.1 The Gross–Pitaevskii Equation .................................... 7

2.1.2 Interaction Potential ................................................ 8

2.1.3 The Gross–Pitaevskii Equation .................................... 9

2.1.4 Validity of the Gross–Pitaevskii Equation ....................... 10

2.1.5 Healing Length ....................................................... 10

2.1.6 Thomas–Fermi Approximation ................................... 10

2.1.7 Bogoliubov Excitations ............................................. 11

2.1.8 Uniform Condensate ............................................... 12

2.2 Interactions in Bose–Einstein Condensates ......................... 13

2.2.1 Feshbach Resonances ............................................... 13

2.2.2 $^{85}$Rb Feshbach Resonance ..................................... 15

2.3 Three-Body Recombination ............................................ 17

2.3.1 Loss Rate Parameter ............................................... 18

2.3.2 Experimental Evidence of Three-Body Loss .................. 20

2.4 Atom Interactions with Light Fields ................................. 21

2.4.1 Optical Potential in the Gross–Pitaevskii Equation .......... 23

2.4.2 Scattering Regimes .................................................. 25

2.4.3 Raman–Nath Regime ............................................... 25
### 5 Stationary Solutions and Bogoliubov Excitations in Atom-Molecule Systems

- **5.1 Formalism**
  - 5.1.1 Phenomenological Hamiltonian for Atom-Molecule System
  - 5.1.2 Values of Parameters
  - 5.1.3 C-Field Equations
  - 5.1.4 Thomas–Fermi Solutions

- **5.2 Quasiparticle Excitations**
  - 5.2.1 Two-Component Bogoliubov–de Gennes Equations
  - 5.2.2 Orthogonality and Normalisation Conditions

- **5.3 Uniform Condensate**
  - 5.3.1 Eigenvalues of the Bogoliubov–de Gennes Equations
  - 5.3.2 High Momentum Instability
  - 5.3.3 Eigenvectors of the Bogoliubov–de Gennes Equations

- **5.4 Application to Bragg Scattering**
  - 5.4.1 Quasiparticle Evolution
  - 5.4.2 Momentum Transfer from Uniform Condensate

### 6 Numerical Methods

- **6.1 Formalism**
  - 6.1.1 Parameters
  - 6.1.2 Three-Body Loss in the Gross–Pitaevskii Equation

- **6.2 Dimensionless Implementation**
  - 6.2.1 Computational Units
  - 6.2.2 Dimensionless Parameters
  - 6.2.3 Dimensionless Equations

- **6.3 Initial State**
  - 6.3.1 Thomas–Fermi Solutions
  - 6.3.2 Optimisation
  - 6.3.3 Initial Noise

- **6.4 MATLAB Implementation**
  - 6.4.1 Propagation Algorithm
  - 6.4.2 Discretised Grids
  - 6.4.3 Projectors
  - 6.4.4 Aliasing
  - 6.4.5 Discretised Time

- **6.5 Momentum Space Truncation**
  - 6.5.1 General method
  - 6.5.2 Four Significant Bands
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.5.3</td>
<td>Validity of Band Truncation</td>
<td>98</td>
</tr>
<tr>
<td>6.6</td>
<td>Renormalisation</td>
<td>98</td>
</tr>
<tr>
<td>6.6.1</td>
<td>Renormalisation factor</td>
<td>98</td>
</tr>
<tr>
<td>6.6.2</td>
<td>Anisotropic Cutoff</td>
<td>99</td>
</tr>
<tr>
<td>6.6.3</td>
<td>Truncated Momentum Space</td>
<td>100</td>
</tr>
<tr>
<td>6.6.4</td>
<td>Choice of Renormalisation Parameter</td>
<td>102</td>
</tr>
<tr>
<td>6.7</td>
<td>Density-Weighted Density in Terms of C-Fields</td>
<td>102</td>
</tr>
<tr>
<td>6.7.1</td>
<td>Wigner Ordering</td>
<td>102</td>
</tr>
<tr>
<td>6.7.2</td>
<td>Atom-Molecule Density-Weighted Density</td>
<td>103</td>
</tr>
<tr>
<td>6.7.3</td>
<td>Check with Initial State</td>
<td>104</td>
</tr>
<tr>
<td>7</td>
<td>Simulations of Bragg Scattering from $^{85}$Rb</td>
<td>107</td>
</tr>
<tr>
<td>7.1</td>
<td>Introduction</td>
<td>108</td>
</tr>
<tr>
<td>7.1.1</td>
<td>Properties of the Bragg Spectrum</td>
<td>108</td>
</tr>
<tr>
<td>7.1.2</td>
<td>Theoretical Predictions</td>
<td>109</td>
</tr>
<tr>
<td>7.1.3</td>
<td>Other work</td>
<td>111</td>
</tr>
<tr>
<td>7.1.4</td>
<td>Outline of Experiment</td>
<td>113</td>
</tr>
<tr>
<td>7.1.5</td>
<td>Experimental Results</td>
<td>114</td>
</tr>
<tr>
<td>7.1.6</td>
<td>Interpreting the Experiment</td>
<td>115</td>
</tr>
<tr>
<td>7.2</td>
<td>Simulation System Set-Up</td>
<td>117</td>
</tr>
<tr>
<td>7.2.1</td>
<td>Simulation Parameters</td>
<td>118</td>
</tr>
<tr>
<td>7.2.2</td>
<td>Initial State</td>
<td>119</td>
</tr>
<tr>
<td>7.2.3</td>
<td>Time Step</td>
<td>120</td>
</tr>
<tr>
<td>7.2.4</td>
<td>Bragg Pulse</td>
<td>121</td>
</tr>
<tr>
<td>7.2.5</td>
<td>Three-Body Loss Coefficient</td>
<td>123</td>
</tr>
<tr>
<td>7.3</td>
<td>Simulations of Structureless Atoms</td>
<td>123</td>
</tr>
<tr>
<td>7.4</td>
<td>Results of Simulations of the Mean-Field Equations</td>
<td>124</td>
</tr>
<tr>
<td>7.4.1</td>
<td>General Behaviour</td>
<td>124</td>
</tr>
<tr>
<td>7.4.2</td>
<td>Bragg Spectra and Line shift</td>
<td>126</td>
</tr>
<tr>
<td>7.5</td>
<td>Results of Full C-Field Simulations</td>
<td>128</td>
</tr>
<tr>
<td>7.5.1</td>
<td>Density-Weighted Density</td>
<td>130</td>
</tr>
<tr>
<td>7.5.2</td>
<td>Bragg Spectra from C-Field Simulations</td>
<td>132</td>
</tr>
<tr>
<td>8</td>
<td>Conclusion</td>
<td>135</td>
</tr>
<tr>
<td>8.1</td>
<td>Thesis Summary</td>
<td>135</td>
</tr>
<tr>
<td>8.1.1</td>
<td>Discussion</td>
<td>136</td>
</tr>
<tr>
<td>8.1.2</td>
<td>Relevance of C-field Formalism</td>
<td>137</td>
</tr>
<tr>
<td>8.2</td>
<td>Outlook</td>
<td>138</td>
</tr>
</tbody>
</table>
## Contents

8.2.1 Relating Theory to Experiment ................................................. 138
8.2.2 Directions for Future Work ...................................................... 139

A Interaction-Picture Integration Algorithm ..................................... 141
A.1 The RK4IP Algorithm ................................................................. 141
  A.1.1 Fourth-Order Runge–Kutta .................................................. 141
  A.1.2 Fourth-Order Runge–Kutta in the Interaction Picture ............... 142
  A.1.3 Projected Fourth-Order Runge–Kutta in the Interaction Picture .... 143
A.2 Atom-Molecule RK4IP-P ............................................................. 144
  A.2.1 Implementation ................................................................. 146
  A.2.2 Practical Experience ......................................................... 147

References ....................................................................................... 149
List of Figures

2.1 S-wave scattering length as a function of the magnetic field strength ........................................ 14
2.2 Two-channel model of a Feshbach resonance ................................................................................. 15
2.3 Experimental measurements of the normalised equilibration rate ............................................... 16
2.4 Experimental measurements of the molecule binding energy ....................................................... 17
2.5 Experimental data of the two- and three-body inelastic loss rates .................................................. 21
2.6 The three-body loss coefficient for $^{85}$Rb .................................................................................. 22
2.7 Schematic of Bragg scattering from a Bose–Einstein condensate .................................................... 23
2.8 Bragg spectrum from Bogoliubov theory ......................................................................................... 30
2.9 Line shift of Bragg spectra as function of the scattering length ....................................................... 30

4.1 Region of validity for the scattering amplitude .................................................................................. 51
4.2 Fractions of atom pairs and elementary molecules .......................................................................... 54
4.3 Coupling strength and detuning as functions of the scattering length ............................................. 58
4.4 $E_b/\epsilon$ and $\alpha$ as functions of the scattering length ..................................................................... 60
4.5 Ratio of the effective range expansion and the exact expression for $K\cot\delta$. ................................. 60

5.1 Detuning and coupling as functions of the inverse scattering length ............................................. 63
5.2 Thomas–Fermi profiles .................................................................................................................. 65
5.3 Radial density for atom-molecule system and structureless atom system ....................................... 66
5.4 Bogoliubov eigenvalues as functions of the momentum .................................................................. 72
5.5 Bogoliubov eigenvalues in instability region .................................................................................. 73
5.6 Bogoliubov eigenvector components ............................................................................................... 75
5.7 Bragg spectrum from atom-molecule Bogoliubov theory ............................................................... 78
5.8 Line shift of Bragg spectra as function of the scattering length ....................................................... 79

6.1 Comparison of the Thomas–Fermi profiles with the stationary solutions ....................................... 89
6.2 Projector in $xy$-plane ..................................................................................................................... 95
6.3 Number of particles in each momentum band as function of time ................................................. 98

7.1 Theoretical predictions for the shift of the peak of the Bragg spectrum ........................................... 110
7.2 Theoretical predictions for the shift of the peak of the Bragg spectrum . . . 112
7.3 Experimental measurements of the Bragg spectra . . . . . . . . . . . . . . 114
7.4 Experimental measurements of the Bragg line shift . . . . . . . . . . . . . . 115
7.5 Frequency scales in the JILA experiment . . . . . . . . . . . . . . . . . . . . . 118
7.6 Condensate coordinate space profiles . . . . . . . . . . . . . . . . . . . . . . 125
7.7 Momentum transfer as a function of time . . . . . . . . . . . . . . . . . . . . 127
7.8 Simulations of Bragg spectra . . . . . . . . . . . . . . . . . . . . . . . . . . . . 128
7.9 Bragg spectral line shift as a function of the scattering length . . . . . . . . 129
7.10 Phase plots of the condensate in the x-y-plane . . . . . . . . . . . . . . . . . 130
7.11 Time evolution of the density-weighted density during the Bragg pulse . . 132
7.12 Bragg spectrum from full c-field simulations . . . . . . . . . . . . . . . . . 133
List of Tables

7.1 Properties of $^{85}$Rb and the Feshbach resonance used in this simulation . . . 118
7.2 Initial scattering length and density-weighted densities . . . . . . . . . . . . . 120
7.3 Experimental average densities for different scattering lengths . . . . . . . 121
7.4 Pulse lengths for different scattering lengths . . . . . . . . . . . . . . . . . . . 122
7.5 Properties of the Bragg pulse for different scattering lengths . . . . . . . 122
7.6 Three-body loss parameters for different scattering lengths . . . . . . . 123
7.7 Three-body loss and density change during the Bragg pulse . . . . . . . 126
Chapter 1

Introduction

1.1 Background

1.1.1 Bose–Einstein Condensation

The last major contribution of Einstein to the field of quantum mechanics came around the same time as modern quantum theory was born. Inspired by de Broglie’s suggestion in 1924 that matter particles can exhibit wave properties, Einstein described his new theory in a letter to Ehrenfest the same year [91],

‘From a certain temperature on, the molecules “condense” without attractive forces, that is, they accumulate at zero velocity. The theory is pretty, but is there also some truth to it?’

The “pretty theory” that Einstein mentioned describes a phenomenon which is now referred to as Bose–Einstein condensation.

Einstein had used the work of Bose on the statistical properties of photons, and predicted that certain material particles would obey the same statistics. He showed that at zero temperature, the energy ground state of a dilute gas of identical bosons would become highly populated. That is, at low enough temperatures, a significant fraction of the particles will be in the ground state, creating a Bose–Einstein condensate. Unlike classical phase transitions, which are caused by thermal effects, Bose–Einstein condensation occurs only because of quantum statistical effects. These condensates are therefore excellent systems in which to study quantum mechanics, since the macroscopic population of the single quantum ground state means that it is possible to observe quantum effects on a macroscopic scale [73].

However, it was not only Einstein who had doubts about the existence of such a state of matter, and the usefulness of his predictions remained controversial until 1938
when the superfluidity of liquid helium was discovered. London \[75\] made the observation that the two phenomena, superfluidity and Bose–Einstein condensation, may be related, but nonetheless expressed his doubts on the existence of the latter:

‘[...] in the course of time the degeneracy of the Bose–Einstein gas has rather got the reputation of having only a purely imaginary existence.’

It was not until seventy years after Einstein’s prediction, in 1995, that the first Bose–Einstein condensates were experimentally realised \[2, 32, 21\]. This achievement earned Cornell, Wieman and Ketterle the Nobel Prize in Physics in 2001, and led to a massive growth in the field of ultra-cold atomic physics. Since this breakthrough, Bose–Einstein condensation has been achieved in a number of bosonic systems; Bose–Einstein condensates have been realised for all the stable alkali atoms \[2, 32, 20, 28, 81, 123, 117\], as well as for hydrogen \[46\], metastable helium \[103\], ytterbium \[119\], and most recently for photons \[64\].

Along with this progress in the experimental field of ultra-cold physics, a wealth of methods for describing their behaviour theoretically has been developed, both analytical and numerical. Because the analytical approaches are seldom exact and the numerical calculations are usually computationally demanding, much work has been made on developing accurate and efficient algorithms for simulating these systems and their dynamics.

1.1.2 JILA Experiment

The motivation for the work in this thesis comes from an experiment performed in 2008, in which Bragg scattering from a strongly interacting Bose–Einstein condensate was studied. The experiment was done by the group of Cornell and Wieman at JILA, Colorado, and is outlined in \[92\].

The first Bose–Einstein condensates of $^{85}$Rb were created by the JILA group in 2000, allowing the study of a condensate with widely tunable interaction strengths. The great advantage of studying $^{85}$Rb is the experimentally convenient magnetic Feshbach resonance near a magnetic field strength of 155 G.

The early experiments involving $^{85}$Rb by the JILA group included the investigation of the condensate shape and density at equilibrium for a range of different interaction strengths \[28\], observation of the condensate collapse for negative interactions \[105, 38\], and the observation of coherent atom-molecule oscillations \[37\].

Starting in 2001, the team at JILA prepared a new experimental set-up for making large, stable Bose–Einstein condensates of $^{85}$Rb for studying the condensate properties in the strongly interacting regime. The new set-up had much better optical access
1.2 This Work

In this thesis, we present a method for studying the system in the JILA experiment theoretically, using a c-field formalism and describing the effects of the increased scattering length in terms of a system of coupled atom-molecule fields.

Bose–Einstein condensates with weak interparticle interactions have been, in many cases, successfully described using a pseudo-potential formulation, in which just two parameters are involved: the density and the s-wave scattering length. Furthermore, in a large proportion of situations, mean-field theory can be used, leading to a description in terms of the Gross–Pitaevskii equation. Arising from this success, a quest for a tunable and possibly large interaction strength began, leading to the study of systems in which the scattering length was caused by a Feshbach resonance. These resonances enabled the inter-atomic interaction of a Bose–Einstein condensate to be tuned over a wide range.

Thus, using Feshbach resonances, it became possible to investigate condensates with strong interparticle interactions. This has been done both experimentally and theoretically with quite wide success, even though there are reasons to question the validity of the standard procedures at some of the interaction strengths used. The pseudo-potential and mean-field theory methods are the result of a perturbation treatment, which breaks down for sufficiently high interaction strengths and densities.
With this in mind, we introduce a more careful treatment of interactions mediated by weakly bound molecular states, such as those that arise in a Feshbach resonance. This is done by introducing a molecular field, whose interaction constants can be determined phenomenologically from scattering length and binding energy data. In our treatment, the interaction constants are relatively weak, but nevertheless reproduce many of the results of a simple pseudo-potential method, especially for static properties, such as the condensate shape, even at large scattering lengths. Also, we formulate a Bogoliubov description, and show that there are changes in the excitation spectrum at higher energies. Using this description, we find a modification in the Bragg scattering spectrum from a homogeneous infinite condensate very similar to that found experimentally by the JILA group.

This means that, by properly treating the dynamics behind the change in interaction strength, i.e. the dynamics of the Feshbach resonance, we find that a mean-field treatment of a strongly interacting system is still very much applicable.

1.2.1 Outline of Thesis

In Chap. 2, we present the general theoretical background for this thesis. We begin by introducing the concept of Bose–Einstein condensation and important parameters and standard theoretical models associated with this. We then briefly review the Bogoliubov theory for excitations in Bose–Einstein condensates. We also discuss the subject of interactions in condensates, with special emphasis on the concepts of Feshbach resonances and three-body recombination. Finally, we consider the phenomenon of Bragg scattering, and its application to Bose–Einstein condensates.

In Chap. 3, we review the c-field methodology that we use for the work in this thesis. C-field methods have become an indispensable tool in the quantitative description of many aspects of Bose–Einstein condensation physics [10]. They provide a description of the dynamics of highly degenerate bosonic gases, which incorporates quantum mechanics correctly, and is accurate provided the density of the Bose gas is sufficiently high.

In Chap. 4, we formulate a method for treating ultracold atoms close to a Feshbach resonance as a system of coupled atom and molecule fields. This method is applicable in the regime covered by the experiment in [92], and has been developed in such a way as to be directly applicable to a c-field description of a Bose–Einstein condensate in the vicinity of a Feshbach resonance.

The formalism outlined in Chap. 4 is implemented in Chap. 5 where we derive the expression for the Thomas–Fermi profiles for the atom-molecule system and compare them to those obtained from the Gross–Pitaevskii equation. We then go on to for-
mulate the Bogoliubov theory for excitations in a Bose–Einstein condensate close to a Feshbach resonance, described as a system of coupled atoms and molecules. We compare the resulting Bogoliubov spectrum to that obtained from a model of structureless atoms. Finally, we use Bogoliubov excitations to investigate the case of Bragg scattering from a uniform condensate, and compare the Bragg spectrum to that of the structureless atom model.

In Chap. 6, we describe the numerical techniques we use for the implementation of the formalism presented in Chap. 4. We outline a method for obtaining stationary solutions to the equations of motion, and present these equations in dimensionless form. We also describe the method for numerical integration of the projected Gross–Pitaevskii equation, and how this can be done for a set of disjoint bands in momentum space in the case of Bragg scattering.

In Chap. 7, we use the formalism of Chap. 4 to model the JILA experiment, using the methods described in Chap. 6. We outline the experimental procedure as well as the issues and difficulties that are associated with simulating this experiment accurately.

Lastly, a summary and conclusion is given in Chap. 8 in which we outline possible directions for future research.

### 1.2.2 Collaborations

The work presented in this thesis is the author's own. It was made under the supervision of Professor Crispin Gardiner, who has provided ideas and guidance throughout the project. Some of the calculations in Chap. 4, in particular those in Sect. 4.2.1 and parts of Sect. 4.2.3 were done together with Andrew Haines. The original idea for the project came from Professor Rob Ballagh and some of the MATLAB-code used for the numerical simulations is based on earlier code written by Associate Professor Blair Blakie.

### 1.2.3 Publications

Much of the work contained in this thesis has been submitted to *New Journal of Physics* in a series of three papers. The work on formulating a coupled atom-molecule theory within a c-field description, presented in Chap. 4 appears in [109]. The work presented in Chap. 5 on stationary solutions and Bogoliubov treatment of this system can be found in [110]. Finally, many parts of the work on simulating the JILA experiment, as discussed in Chap. 6 and Chap. 7 appear in [108].
Chapter 2

Background Theory

In this chapter, we review the theoretical background material relevant for the work in this thesis. In Sect. 2.1 we start by introducing some key concepts and presenting some of the standard approaches to treating Bose–Einstein condensates theoretically. Here we will focus on giving a brief overview of the areas of interest to the work presented in the following chapters. We refer the reader to one of the many extensive reviews in the area for further details (see for example [73, 31, 45, 96, 94]).

In Sect. 2.2, we go on to discuss the topic of Feshbach resonances, since the understanding of this phenomenon plays an important role for the work in this thesis. In Sect. 2.3 we review the subject of three-body recombination processes in ultra-cold Bose gases. Finally in Sect. 2.4 we discuss the topic of optical manipulation of Bose–Einstein condensates, with particular focus on Bragg scattering.

2.1 Bose–Einstein Condensation

At zero temperature, the behaviour of the condensate in many cases can be accurately described by the Gross–Pitaevskii equation. In this section we present this equation, the motivation behind it, and important parameters and approximations that are related to it.

2.1.1 The Gross–Pitaevskii Equation

The Hamiltonian for an ensemble of interacting bosons in an external trapping potential is given by

$$\hat{H} = \int \! dx \, \hat{\psi}^\dagger (x) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) \right) \hat{\psi} +$$

$$+ \frac{1}{2} \int \! dx \int \! dx' \, \hat{\psi}^\dagger (x) \hat{\psi}^\dagger (x') U_{\text{int}}(x-x') \hat{\psi}(x) \hat{\psi}(x'),$$  \hspace{1cm} (2.1)
where $\hat{\psi}^\dagger$ and $\hat{\psi}$ are the field creation and annihilation operators, respectively, which obey the usual Bose commutation relations,

\[
\left[ \hat{\psi}(x), \hat{\psi}^\dagger(x') \right] = \left[ \hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x') \right] = 0, \quad (2.2)
\]
\[
\left[ \hat{\psi}(x), \hat{\psi}^\dagger(x') \right] = \delta(x - x'). \quad (2.3)
\]

The external potential $V_{\text{ext}}$ describes the trapping of the condensate particles and the particle interactions are described by the two-body interaction potential $U_{\text{int}}$.

Bose–Einstein condensation occurs in one single mode of the field. We can therefore make a Bogoliubov separation, and decompose the field operator into a condensed part and a small perturbation,

\[
\hat{\psi}(x) = \psi(x) + \delta \hat{\psi}(x), \quad (2.4)
\]

where $\psi(x)$ is the condensate wavefunction, defined as the expectation value of the field operator,

\[
\psi(x) \equiv \langle \hat{\psi}(x) \rangle. \quad (2.5)
\]

Even at zero temperature, not all the atoms in the gas will be in the condensate. This is called quantum depletion and is caused by the interactions of the atoms. Although theoretically important, the corrections introduced by quantum depletion will in most practical situations be very small. In the case when they can be neglected, we can make the assumption $\delta \hat{\psi} = 0$, effectively replacing the field operator with the classical field, $\hat{\psi} \to \psi$.

### 2.1.2 Interaction Potential

The true inter-atomic potential supports bound states, which, as we shall see in Sect. 2.2 is relevant when tuning the interaction strength. These bound states of the potential make perturbative treatments of the condensate impossible [25]. Nevertheless, the mean-field approach which most Bose–Einstein condensation theory is based on requires perturbative treatments. Therefore it is necessary to approximate the true inter-atomic potential with one that allows perturbative treatments.

In the case of zero temperature, and where the bound states are unimportant for the behaviour of the system, the exact nature of the inter-atomic potential becomes irrelevant. In this case, the interaction potential term in the Hamiltonian (2.1) can be accurately described by only considering low-energy interactions [31], as is discussed further in Sect. 3.1. The interaction is then completely characterised by a single parameter, the $s$-wave scattering length, $a_s$. 

8
2.1. Bose–Einstein Condensation

The interaction potential is replaced by an effective contact potential \[ U_{\text{int}}(x - x') = U_0 \delta(x - x'), \] (2.6)

where the interaction strength \( U_0 \) is given by

\[ U_0 \equiv \frac{4\pi \hbar^2 a_s}{m}. \] (2.7)

The effective interaction term produces the same s-wave scattering length as the true potential, but does not have the complexity of the true potential. However, it is unphysical since particles with large relative momenta would scatter just as efficiently as particles with low momenta. As we shall see in Sect. 3.1.1, the unphysical properties of this potential can be avoided by limiting the number of modes through the introduction of an energy cut-off and renormalising the interaction.

Another approach is to replace the interaction potential with the pseudo-potential

\[ U_{\text{int}}(x - x') = U_0 \delta(x - x') \frac{\partial}{\partial (x - x')} (|x - x'| \psi(x - x')). \] (2.8)

This leads to a well defined two-body scattering problem, and is equivalent to a renormalised contact potential.

2.1.3 The Gross–Pitaevskii Equation

After making the effective contact potential approximation, using the Heisenberg equation of motion for the field operator and replacing the field operator with the classical field gives the time-dependent Gross–Pitaevskii equation,

\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) + U_0 |\psi(x, t)|^2 \right) \psi(x, t). \] (2.9)

For a stationary condensate the density is time-independent. The evolution of the condensate wavefunction can therefore be separated into spatial and temporal parts

\[ \psi(x, t) = \psi(x) e^{-i\mu t/\hbar}, \] (2.10)

where the phase factor \( \mu \) is the condensate eigenvalue. Applying this ansatz to the time-dependent Gross–Pitaevskii equation (2.9) we obtain the time-independent Gross–Pitaevskii equation,

\[ \mu \psi(x) = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) + U_0 |\psi(x)|^2 \right) \psi(x). \] (2.11)
The condensate eigenvalue $\mu$ corresponds to the energy required to add or remove a particle to the condensate, whilst conserving the correct normalisation condition. It is therefore usually identified as the condensate chemical potential, as is the case in statistical mechanics.

### 2.1.4 Validity of the Gross–Pitaevskii Equation

The Gross–Pitaevskii equation is valid for dilute and weakly interacting systems, or more specifically when the scattering length is much smaller than the average distance between atoms, $n^{-1/3}$, i.e. when $n|a_s|^3 \ll 1$, where $n$ is the condensate density [31].

When the scattering length or the density of the condensate is large, the Gross–Pitaevskii equation is expected to fail, and corrections to this description of the condensate may become important. The first-order correction to the chemical potential was calculated by Lee, Huang and Yang (LHY) [72, 71], and is given by

$$\mu_{\text{LHY}} = \mu \left(1 + \frac{32}{3\sqrt{\pi}} \sqrt{n a_s^3} \right).$$

(2.12)

Thus, the LHY corrections amounts to a perturbation about the mean-field result; the perturbation term is referred to as the LHY-correction.

### 2.1.5 Healing Length

The distance over which the condensate goes from zero density to its bulk density is called the healing length, or alternatively coherence length. The healing length can be estimated from the Gross–Pitaevskii equation, and is given by

$$\xi = \frac{\hbar}{\sqrt{2m n(x) U_0}}.$$  

(2.13)

where $n(x) = |\psi(x)|^2$ is the local density of the condensate [94]. For an inhomogeneous condensate the healing length has a spatial dependence; the peak density or the average density of the condensate is then used to obtain an order of magnitude estimate of the healing length [31].

### 2.1.6 Thomas–Fermi Approximation

In the limit where the kinetic energy term is much less than the nonlinear term, the kinetic term in the Gross–Pitaevskii equation can be neglected, and the time-independent equation (2.11) can be solved analytically. This is called the Thomas–Fermi approximation.
2.1. Bose–Einstein Condensation

and the wavefunction is then given by

\[
\psi_{\text{TF}}(x) = \sqrt{\frac{\mu_{\text{TF}} - V_{\text{ext}}(x)}{U_0}} \Theta(\mu_{\text{TF}} - V_{\text{ext}}(x)),
\]

(2.14)

where \( \Theta(x) \) denotes a Heaviside step function.

For the experimentally relevant case of 3D harmonic trapping, with external potential

\[
V_{\text{ext}}(x) = \frac{m}{2} \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right),
\]

(2.15)

the chemical potential of the condensate in the Thomas–Fermi limit, \( \mu_{\text{TF}} \), is

\[
\mu_{\text{TF}} = \frac{1}{2} \left( 15a_s \hbar^2 \sqrt{m \omega_x \omega_y \omega_z N_0} \right)^{2/5},
\]

(2.16)

where \( N_0 = \int dx |\psi_{\text{TF}}|^2 \) is the particle number in this approximation. The half-width of the condensate, known as the Thomas–Fermi radius, in the \( i \)th trap direction is found to be

\[
R_{\text{TF}}^i = \frac{1}{\omega_i} \sqrt{\frac{2\mu_{\text{TF}}}{m}}.
\]

(2.17)

If the particle number is large, the Thomas–Fermi wavefunction is usually a good approximation to the exact solution of the time-independent Gross–Pitaevskii equation. The only real difference between the two profiles is at the edge of the condensate, where the Thomas–Fermi wavefunction has a sharp cutoff, whereas the true Gross–Pitaevskii equation solution reduces smoothly to zero on the scale of the healing length.

2.1.7 Bogoliubov Excitations

By separating the field operator into a mean-field ground state and an operator part describing the excitations, we can investigate the excitations more easily. We expand the wavefunction in terms of a quasi-particle basis as

\[
\hat{\psi}(x, t) = \psi_0(x)e^{-i\mu t/\hbar} + e^{-i\mu t/\hbar} \sum_k \left( u_k(x) \hat{b}_k e^{-i\omega_k t} + v_k^*(x) \hat{b}_k^\dagger e^{i\omega_k t} \right),
\]

(2.18)

where the new operators obey the usual bosonic commutation relation

\[
[\hat{b}_k, \hat{b}_{k'}^\dagger] = \delta_{kk'}.
\]

(2.19)

By substituting this expansion into the time-dependent Gross–Pitaevskii equation (2.9), and collecting terms with the same phase, we find that the mode functions \( u_k(x) \), \( v_k(x) \)
satisfy the Bogoliubov–de Gennes equations

\[
\mathcal{L} \begin{pmatrix} u_k(x) \\ v_k(x) \end{pmatrix} = \hbar \omega_k \begin{pmatrix} u_k(x) \\ v_k(x) \end{pmatrix},
\]

which we have written here in terms of the matrix of operators

\[
\mathcal{L} \equiv \begin{pmatrix} -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) - \mu + 2U_0|\psi_0(x)|^2 & U_0\psi_0(x)^2 \\ -U_0\psi_0^*(x)^2 & \frac{\hbar^2 \nabla^2}{2m} - V_{\text{ext}}(x) + \mu - 2U_0|\psi_0(x)|^2 \end{pmatrix}.
\]

It is possible to show that the eigenstates with different energies obey the following orthogonality condition [94]

\[
\int dx \left( v_j(x)u_k(x) - u_j(x)v_k(x) \right) = 0.
\]

Furthermore, by requiring that \( \hat{b}_k \) satisfies the standard Bose commutation relations, we find that the quasi-particle modes are normalised, according to

\[
\int dx \left( u_j^*(x)u_k(x) - v_j^*(x)v_k(x) \right) = \delta_{jk}.
\]

### 2.1.8 Uniform Condensate

In the case of a uniform condensate, with density \( n \), we can find the exact eigenvalues and eigenvectors of the system; for details see [94]. We make the replacements

\[
\begin{align*}
u_k(x) & \rightarrow u_k e^{ik \cdot x / \sqrt{V}} \\
\psi_0(x) & \rightarrow \sqrt{n}
\end{align*}
\]

where \( V \) is the volume of the system. The mode functions \( u_k \) and \( v_k \) are then given by

\[
\begin{align*}
u_k^2 & = \frac{1}{2} \left( \frac{\hbar^2 k^2 / m + nU_0}{\hbar \omega_k} + 1 \right), \\
v_k^2 & = \frac{1}{2} \left( \frac{\hbar^2 k^2 / m + nU_0}{\hbar \omega_k} - 1 \right),
\end{align*}
\]

and the eigenvalues by

\[
\hbar \omega_k = \sqrt{\left( \frac{\hbar^2 k^2 / 2m + nU_0}{2m} \right)^2 - (nU_0)^2}.
\]
2.2 Interactions in Bose–Einstein Condensates

In all alkali vapour Bose–Einstein condensates, the repulsive interaction which enables the atoms to condense, and the associated positive s-wave scattering length is caused by the existence of a bound state just below the threshold in an attractive Lennard–Jones-like potential. The binding energy of the bound state is given by \( E_b = \frac{\hbar^2}{2ma_s^2} \), which leads to a binding frequency of \( f_b = \frac{E_b}{\hbar} \). The inter-atomic interaction strength \( U_0 \) can be related to the s-wave scattering length by the pseudo-potential \( \frac{2}{\pi} \), as long as the spatial extension of the condensate is much greater than the range of the interaction, and the phenomenon used to probe the condensate is much slower than the binding frequency \( f_b \).

It is possible to dramatically alter the inter-atomic interactions of the Bose–Einstein condensate by tuning an external magnetic field in the vicinity of a Feshbach resonance. For some species of alkali metals, such as \(^{85}\text{Rb}\), the existence of a Feshbach resonance is necessary for the experimental realisations of Bose–Einstein condensation. There is an extensive literature dealing with the theoretical description of Feshbach resonances, see for example \[82, 120, 53, 54, 67, 40, 41, 101, 49, 76, 66, 26\].

2.2.1 Feshbach Resonances

Close to a magnetic Feshbach resonance, the relationship between the s-wave scattering length, \( a_s \), and the external magnetic field, \( B \), is given by the expression \[82\]

\[
a_s(B) = a_{bg} \left( 1 - \frac{\Delta B}{B - B_0} \right),
\]

where \( a_{bg} \) is the background scattering length, that is, the scattering length in the absence of the external magnetic field. The parameter \( B_0 \) is the position of the Feshbach resonance, where the scattering length diverges, and \( \Delta B \) is the width of the resonance, defined as the difference in magnetic field between the resonance position and the point where the scattering length is zero. The most dramatic consequence of \( \text{(2.30)} \) is that even a small change in the magnetic field strength can lead to a change in sign of the interaction.

In Fig. 2.1, we show the s-wave scattering length as a function of the magnetic field for the case of \(^{85}\text{Rb}\) close to the Feshbach resonance at 155 G. In this case, the background scattering length is negative, but in a region of width \( \Delta B \) to the right of the resonance position \( B_0 \), the scattering length will assume positive values.

The scattering length changes close to the resonance because of the existence of a bound state just below the threshold energy of two free atoms. The theory behind this
Figure 2.1: S-wave scattering length, $a_s$, as a function of the magnetic field strength in the vicinity of a magnetic Feshbach resonance, located at $B_0$. Far from resonance the scattering length assumes the asymptotic value $a_{bg}$, indicated by the dashed line. The width of the resonance $\Delta B$ is the distance from the resonance position $B_0$ to the position where the scattering length is zero. The plot shows the Feshbach resonance for $^{85}$Rb, located at $B_0 = 155.04$ G. The background scattering length is in this case $a_{bg} = -443a_0$ and the width of the resonance is $\Delta B = 10.7$ G [26].

mechanism is well understood, see for example the reviews [120, 41, 66], although the explicit details are not relevant for the work in this thesis.

Consider a system of two atoms in an external homogeneous magnetic field. The inter-atomic potential experienced by the two atoms is shown schematically in Fig. 2.2. The open channel represents the usual inter-atomic potential for the two atoms in some hyperfine state, with the total energy of the two free atoms equal to $2\mu_a$. The closed channel is the inter-atomic potential for some other hyperfine state, which has a different energy due to the Zeeman shift. The open channel could support a bound state lower in energy than $2\mu_a$, but that bound state would not be accessible to the atoms without violating energy-momentum conservation.

There might, however, exist a bound state nearby in energy in the closed channel. This is the Feshbach state, and it has energy $\mu_{fb}$. The energy of the Feshbach state can be tuned via the magnetic field. The Feshbach state is coupled to the open channel bound state in such a way that if the energy of the Feshbach resonance is ramped down, then the open channel binding energy, $\mu_m$, increases. As $\mu_m$ approaches zero, strong
2.2. Interactions in Bose–Einstein Condensates

![Figure 2.2: Schematic of the two-channel model for a Feshbach resonance, showing the interatomic potential as a function of the atomic separation. The open channel is indicated by the black line (bottom curve), and the closed channel by the purple line (top curve).](image)

... 

coupling between the atomic and molecular states can be observed. It is this formation of atoms in bound pairs that creates the singularity in the s-wave scattering length.

Apart from these magnetically tunable resonances, there is also the possibility of achieving optical resonant coupling between unbound and bound states in optically tunable Feshbach resonances. These can be useful in the cases where magnetically tuned resonances are not present [26].

2.2.2 $^{85}$Rb Feshbach Resonance

In this work, we investigate the behaviour of $^{85}$Rb, so we shall present the properties of the $^{85}$Rb Feshbach resonance in greater detail.

In 1997, Vogels et al. [122] theoretically predicted the existence of several magnetically induced Feshbach resonances in $^{85}$Rb, based on experimentally measured bound state energies and continuum properties. One of these predictions was confirmed a year later, when Courteille et al. [30] observed an enhancement in the photoassociative loss in a thermal gas of $^{85}$Rb, indicating the presence of a Feshbach resonance. The
same year, Roberts et al. [104] confirmed the existence of this resonance by measuring the equilibration time constant $\tau_{eq}$ for several different temperatures of a thermal gas of $^{85}\text{Rb}$. The equilibration time constant is inversely proportional to the elastic collision rate, and therefore also to the s-wave scattering length. In this way, they were able to determine the position of the resonance to be at a magnetic field of 155 G, and its width to be 10 G. The results from these measurements are presented in Fig. 2.3 showing the normalised equilibration rate, $\Gamma_{\text{norm}} = \left(\overline{n \nu \tau_{eq}}\right)^{-1}$, where $n$ and $\nu$ are the density and velocity of the thermal gas and the bar indicates the average of several runs. The normalised equilibration rate is proportional to the average elastic cross section; in Fig. 2.3 the theoretical prediction of the cross section for two temperatures is plotted as a rough qualitative comparison to the data.

The first investigations of this Feshbach resonance using a Bose–Einstein condensate were performed by Claussen et al. [27] in 2003 using high-precision spectroscopy. The position and width of the resonance were determined within 20 mG to be $B_0 = 155.04$ G and $\Delta B = 10.7$ G, respectively (see Fig. 2.4). In the same experiment they also measured the binding energy of the bound state in the Feshbach resonance, as shown in Fig. 2.4.

---

**Figure 2.3:** Measurements of the normalised equilibration rate as a function of magnetic field for five different temperatures: 0.3 $\mu$K (▲), 0.5 $\mu$K (●), 1.0 $\mu$K (○), 3.5 $\mu$K (▼), and 9.0$\mu$K (■). The lines are calculations for the thermally averaged elastic cross sections for 0.5 $\mu$K (solid line) and 9.0 $\mu$K (dot-dashed line). The lines do not correspond to the equilibration rate, and are therefore not expected to fit the data points, but are intended to be used for rough qualitative comparison to the data. Figure adapted from [104].
2.3 Three-Body Recombination

Experimentally produced Bose–Einstein condensates from alkali gases have limited lifetimes. Due to the rapid increase in density that these systems exhibit below the critical condensation temperature, the process which most limits the lifetime of a condensate is that of three-body recombination \cite{32}.

Three-body recombination is a process in which a diatomic bound state — referred
to as a *molecule* — and an unbound atom are formed from three interacting atoms [14]. The resulting particles will gain kinetic energy from the negative binding energy of the molecule; if this energy is sufficiently large the particles will be energetic enough to escape the condensate. Thus, the three-body recombination process can lead to significant particle loss, especially when the scattering length and density are large.

For atoms with negative scattering length, the binding of two atoms will result in a deeply bound state. However, for atoms with positive scattering length, the binding will result in weakly bound dimers with binding energy $E_b = \hbar^2 / ma_s^2$ [14], and sizes much larger than the characteristic radius of the interaction [44]. In the following, we will assume that the scattering length is large and positive, and therefore only focus on the three-body recombination process into the shallow dimer state.

If three-body recombination is the only process causing particle loss from the system, the rate at which this occurs is described in terms of the three-body recombination rate constant, $K_3$. For a system of $N$ particles, and assuming that all three particles involved in the recombination process are lost from the system, the number loss is given by

\[
\frac{dN(t)}{dt} = -K_3 \int dx \, g^{(3)}(x)n(x, t)^3, \tag{2.31}
\]

where $n(x, t)$ is the number density and $g^{(3)}(x)$ is the third-order normalised equipartition correlation function [23]. The correlation function is a measure of the statistics of the system, taking the value 1 for a fully coherent system, and $3! = 6$ for a weakly interacting uncondensed gas [90].

### 2.3.1 Loss Rate Parameter

There is some inconsistency in the literature when dealing with the three-body recombination rate parameter, and whether it is referring to an *event rate* or to a *number rate*. In this work, we follow the notation of [15] and several other authors, and let $K_3$ denote the number rate, while the event rate is denoted by $\alpha_{\text{rec}}$. Since three particles are involved in each event, the three-body event rate is related to the three-body number rate as $3\alpha_{\text{rec}} = K_3$.

The three-body recombination rate is strongly dependent on the scattering length. For the shallow dimer of a wide resonance this is given by

\[
\alpha_{\text{rec}} = C \frac{\hbar a_s^4}{m}, \tag{2.32}
\]

for some coefficient $C$ [44]. Fedichev et al. [44] show how the $a_s^4$ dependence can be understood qualitatively, by considering three atoms of equal mass. In order for the
recombination process to occur, the binding energy must be

\[ E_b = \frac{3\hbar^2 k^2}{4m}, \]  

(2.33)

where \( k \sim 1/a_s \) is the final state momentum of the released atom relative to the centre of mass of the molecule. The number of recombination events per unit time and volume is \( \nu_{\text{rec}} = \alpha_{\text{rec}} n^3 \). This recombination rate can also be estimated as \( \nu_{\text{rec}} \sim n^2 \sigma \nu (n l^3) \), where \( n \) is the density, \( \nu \) is the velocity, \( \sigma \) is the cross section for pair collisions and \( n l^3 \) is the statistical weight associated with a third atom being inside a sphere of radius \( l \sim a_s \) around a colliding atom pair. By making the substitutions \( \nu \sim \hbar k/m \) and \( \sigma = 8\pi a_s^2 \), we therefore arrive at \( \alpha_{\text{rec}} \sim 8\pi \hbar a_s^4/m \).

Although the expression (2.32) is well established in the literature — as well as being verified in experiments [124] — the exact expression for the coefficient \( C \) is under current research. Fedichev et al. [44] found that the coefficient \( C \) has the universal value \( C = 3.9 \), however, the analysis used in this work has been questioned by later authors [14]. Indeed, several groups have independently shown that the coefficient \( C \) is not constant, but rather has a logarithmic periodic dependence on the scattering length \[ C \approx C_{\text{max}} \sin^2 \left[ s_0 \ln(a_s \kappa^* \Lambda^*) + \gamma \right], \]  

(2.34)

where \( \kappa^* \) is a parameter defined by the Efimov spectrum [14], \( \gamma \) is a phase constant, and \( C_{\text{max}} \) is the upper limit on the recombination coefficient. The parameter \( s_0 \) is a constant approximately equal to unity, \( s_0 \approx 1.00624 \) [14].

Thus, the value of \( C \) oscillates between zero and its maximum value, with more rapid oscillations closer to the Feshbach resonance. The maximum value of \( C \) is therefore of interest; Nielsen et al. [86] used hidden crossing theory to estimate the upper limit on the recombination coefficient to be \( C_{\text{max}} = 68.4 \), while Esry et al. [43] obtained a similar result by solving the three-body Schrödinger equation in hyperspherical coordinates.

Bedaque et al. [4] used the effective field theory methods of [5] to calculate \( C_{\text{max}} \) and \( \gamma \), as did Braaten et al. [13], with the result

\[ C \approx C_{\text{max}} \sin^2 \left[ s_0 \ln(a_s \Lambda^*) + 0.19 \right], \]  

(2.35)

where \( \Lambda^* \) is a renormalisation constant arising naturally from the effective field theory, with the relationship between \( \Lambda^* \) and \( \kappa^* \) given by [14] as

\[ s_0 \ln(a_s \Lambda^*) = s_0 \ln(a_s \kappa^*) + 0.97 \mod \pi. \]  

(2.36)
Petrov [35] showed that the constant $C$, in fact, can be given exactly by the analytical expression

$$C = \frac{C_{\text{max}}}{1 + \coth^2(\pi s_0) \tan^2[s_0 \ln(a\Lambda^\ast) + \delta]},$$

(2.37)

with the maximum value given by

$$C_{\text{max}} = \frac{(4\pi)^3 (8 - 6\sqrt{3}/\pi)}{\sinh^2(\pi s_0)} \approx 67.1177,$$

(2.38)

which is consistent with (2.35). Braaten et al. [15] simplified this expression, so that the three-body recombination constant is given by

$$\alpha_{\text{rec}} \approx 67.12 e^{-2\eta^\ast} \left[ \sin^2(s_0 \ln(a_s \Lambda^\ast)) + \sinh^2(\eta^\ast) \right] \frac{ha_s^4}{m},$$

(2.39)

where $\eta^\ast$ is a positive real parameter [16].

### 2.3.2 Experimental Evidence of Three-Body Loss

Experimentally, three-body recombination events can be observed by studying the increase in the inelastic loss rate close to a Feshbach resonance. The first such observations in alkali gases were made by tuning the scattering length of $^{23}\text{Na}$ in the vicinity of the Feshbach resonances at 907 G and 853 G [58].

For $^{85}\text{Rb}$, the inelastic collision rate was first studied by the JILA group [106]. They investigated the density and magnetic field dependence of the collision rate close to the 155 G resonance and were able to separate the contributions from two- and three-body processes. The loss rates are highly dependent on the magnetic field strength, changing by several orders of magnitude as the scattering length is tuned close to the resonance.

Experimental data by [106] of the two- and three-body inelastic rates for a range of magnetic fields are shown in Fig. 2.5. The arrows (↓) indicate points where only upper limits on the three-body rate were obtained. It is clear from the figures that the loss in the range 162–166 G is predominately two-body, whereas the loss above 175 G is predominately three-body; the open circles in both figures are determined by making the assumptions that the loss in the range 162–166 G is purely two-body and the loss above 175 G is purely three-body. The line in the plot for the two-body loss rate in Fig. 2.5 is a theoretical prediction from [79], and the line in the plot for the three-body loss rate is a theoretical prediction from [43].

In this thesis, we deal with a system in the region where the three-body loss is dominant, and we therefore focus on this process. In Fig. 2.6 the experimental data of
2.4 Atom Interactions with Light Fields

Light fields play an important role in ultra-cold atomic experiments, and are used for optical trapping of gases, as well as in the formation of optical lattices. Furthermore, optical manipulation of atomic gases in the form of Bragg scattering has proved a useful tool for a wide range of experiments \cite{35, 36, 59, 60, 69}. In particular, Bragg spectroscopy has been used to probe various properties of Bose–Einstein condensates, such as momentum width, excitation spectrum and chemical potential \cite{115, 118}.

Diffraction of atoms from a standing light wave was first demonstrated in 1983 \cite{84}, performed in the Raman–Nath regime where the interaction time between the atoms and the optical potential is short. The first experiment with clearly visible diffraction orders was conducted a few years later by Gould \textit{et al.} \cite{50}. The same group demonstrated the first Bragg scattering experiment in 1988 \cite{77}, with a specific momentum state being selectively occupied.

The first experimental realisation of Bragg scattering from a Bose–Einstein conden-
Figure 2.6: The three-body loss coefficient $K_3$ as a function of the magnetic field for $^{85}\text{Rb}$ near the Feshbach resonance at 155 G, indicated by the black dashed line. The dots ($\bullet$) indicate the measured values and the triangles (▼) indicate upper bounds of $K_3$ from [106], as in Fig. 2.5. The lines are the calculated values from (2.39) for $\kappa_\ast a_0 = 2$ and three different values of $\eta_\ast$. Figure adapted from [15].

sate was performed at NIST in 1999 [68]. In this experiment, they used two counter-propagating laser fields with a slight frequency difference, creating an optical potential that was moving relative to the condensate. By adjusting the frequency difference, they achieved Bragg scattering by up to six orders.

Bragg scattering from a Bose–Einstein condensate has been studied theoretically, for example by [8, 9, 7, 121]. Blakie et al. derived a Gross–Pitaevskii equation for describing the dynamics of a Bose–Einstein condensate interacting with a light grating. They investigated analytically the effects of scattering for the case of a non-interacting condensate. They also made a numerical study of the nonlinear case. Furthermore, they studied Bragg spectroscopy using Bogoliubov theory, and also compared the results from analytical calculations and simulations with the experimental results of [118, 115]. In the weakly interacting regime, the results of the simulations based on the Gross–Pitaevskii equation were similar to the experimental data [118], for the shift of the Bragg spectral peak [7]. However, the comparison between the experimental and theoretical result was only qualitative.

Tozzo et al. [121] built on the work of [8, 9], modelling the experimental work of [116], in which they investigated the effect of Bragg scattering from an elongated Bose–
2.4. Atom Interactions with Light Fields

Bragg scattering normally refers to the scattering of photons or neutrons from a crystal material. If we reverse the roles of matter and light as the providers of lattice and wave, the Bragg scattering process from a Bose–Einstein condensate can be seen as a Galilean transformation of the “normal” Bragg scattering case, with the diffraction light grating moving across the stationary matter wave.

Fig. 2.7 shows a schematic model of a Bose–Einstein condensate in an optical potential. Two laser beams with wave vectors $k_i$ and frequencies $\omega_i$, where $i = 1, 2$, intersect over the atom cloud. The laser beams are assumed to spatially extend much further than the condensate. The frequencies of the laser beams are similar, but with a small difference, $\omega = \omega_2 - \omega_1$, giving the temporal frequency of the resulting light grating. The wavevector of the light grating will similarly be given by $q = k_2 - k_1$.

Assuming that the electric fields have equal intensity, the total electric field is given by

$$E(x, t) = \frac{1}{2} E_0(t) \left( e^{i(k_1 \cdot x - \omega_1 t)} + e^{i(k_2 \cdot x - \omega_2 t)} + \text{c.c.} \right),$$

(2.40)

where $E_0(t)$ is the field amplitude. Blakie [7] shows how to derive an expression for the
effect of the laser fields on the condensate within a Gross–Pitaevskii equation description. This is done by modelling the atoms in the condensate as having two internal states: a ground state, \(|g\rangle\), and an excited state, \(|e\rangle\), with an electric dipole matrix element \(d = \langle e|\hat{d}|g\rangle\). The strength of the coupling between the two states is given by the Rabi frequency, \(\Omega_0 = dE_0(t)/\hbar\).

The dynamics of the ground and excited state wavefunctions, \(\psi\) and \(\psi_e\), can be described by Gross–Pitaevskii-like equations, according to

\[
\begin{align*}
\ih \frac{\partial \psi(x, t)}{\partial t} & = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) + U_{gg} |\psi(x, t)|^2 + U_{eg} |\psi_e(x, t)|^2 \right) \psi(x, t) \\
& \quad - \frac{1}{2} \hbar \Omega_0(t) \left( e^{i(k_1 \cdot x - \omega_1 t)} + e^{i(k_2 \cdot x - \omega_2 t)} + \text{c.c.} \right) \psi_e(x, t), \quad (2.41) \\
\ih \frac{\partial \psi_e(x, t)}{\partial t} & = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) + \hbar \omega_{eg} + U_{ee} |\psi_e(x, t)|^2 + U_{eg} |\psi(x, t)|^2 \right) \psi_e(x, t) \\
& \quad - \frac{1}{2} \hbar \Omega_0(t) \left( e^{i(k_1 \cdot x - \omega_1 t)} + e^{i(k_2 \cdot x - \omega_2 t)} + \text{c.c.} \right) \psi(x, t), \quad (2.42)
\end{align*}
\]

where \(\omega_{eg}\) is the Bohr frequency, \(U_{gg}\) and \(U_{ee}\) are the collisional interaction strengths between atoms in like states, and \(U_{eg}\) is the interaction between an atom in state \(|e\rangle\) and an atom in state \(|g\rangle\).

If the frequencies of the laser fields are sufficiently detuned from the \(|g\rangle \rightarrow |e\rangle\) transition, the field will not be significantly modified as it propagates through the condensate. We can also assume that effects from spontaneous emission processes are negligible. Blakie [7] shows how under this assumption, we can adiabatically eliminate the excited state from equations (2.41, 2.42). This gives a simplified equation for the dynamics of the condensate ground state under the influence of the laser fields:

\[
\ih \frac{\partial \psi(x, t)}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) + V_{\text{opt}}(x, t) + U_0 |\psi(x, t)|^2 \right) \psi(x, t), \quad (2.43)
\]

where we have \(U_0 \equiv U_{gg}\), and the optical potential is given by

\[
V_{\text{opt}}(x, t) = \hbar V_0(t) \cos(q \cdot x - \omega t). \quad (2.44)
\]

The magnitude of the optical potential is

\[
V_0(t) = \frac{|\Omega_0(t)|^2}{2\Delta}, \quad (2.45)
\]

where the detuning \(\Delta\) is given by

\[
\Delta = \omega_1 - \omega_{eg}. \quad (2.46)
\]
2.4.2 Scattering Regimes

The effect of the optical potential on the matter wave is mainly determined by two parameters, namely the maximum amplitude of the optical potential, \( V_0 \), and the duration of the atom-light interaction, \( T \). The scattering can be divided into three different scattering regimes, depending on the magnitude of these two parameters: Raman–Nath scattering, Bragg scattering, and channeling. In the following, we briefly discuss these different regions and the characteristics of the diffraction patterns obtained in them.

2.4.3 Raman–Nath Regime

If the interaction time between the atoms and the optical field is sufficiently short, Raman–Nath scattering is obtained \([102]\). On these short time scales, the optical potential simply imprints a phase on the wavefunction, which to some degree is washed out by the propagation of the potential. The atoms receive only discrete momentum kicks from the optical grating, so only certain momentum states are occupied. Unlike the diffraction pattern from Bragg scattering, the diffraction pattern from Raman–Nath scattering is characterised by symmetrically populated diffraction orders.

In order to be within the Raman–Nath regime, an upper limit on the duration of the optical pulse is given by

\[
T < \sqrt{\frac{1}{V_0 \omega_q}}, \tag{2.47}
\]

where \( V_0 \) is the amplitude of the optical potential, and

\[
\omega_q = \frac{\hbar q^2}{2m} \tag{2.48}
\]

is the atomic recoil frequency.

2.4.4 Bragg Regime

The Bragg regime is characterised by an asymmetric diffraction pattern where one momentum state, with momentum given by an integer multiple of the wave number of the optical potential, is significantly populated compared to the other momentum states.

For Bragg scattering to occur, the time during which the optical potential is exposed to the atoms must be long, so that the wavefunction is traversed by at least one wavelength of the moving optical potential \([7]\). This is obtained by setting a lower limit on
the duration of the optical pulse,

$$T > \frac{1}{\omega_q}.$$  \hfill (2.49)

As in the case of Bragg scattering from a crystal, it is important that the atoms can traverse the optical potential and interact with the many planes of the light grating. The Bragg regime is therefore characterised by shallow potentials, giving us an upper limit on the amplitude of the optical potential,

$$V_0 < \omega_q.$$  \hfill (2.50)

Unlike Raman–Nath scattering, Bragg scattering is a resonant process, since the optical potential is applied long enough to resolve the resonant frequency of the atoms.

### 2.4.5 Channeling Regime

In the regime where (2.49) holds, but (2.50) is violated, whereby the interaction time is long and at the same time the optical potential is high, the atoms are channelled along the potential valleys. The number of diffraction orders that can be populated this way depends on the potential height, but since this is large, the number of populated diffraction orders is usually large [61].

### 2.4.6 Bragg Excitation Spectrum

In this work, we are only interested in the Bragg region of scattering, and we will therefore focus solely on this in the following.

In the case of Bragg scattering of photons or neutrons from a crystalline material, the Bragg condition determines the parameters for which maximum positive interference will be obtained. In the case of atomic Bragg scattering, a similar condition for maximum positive interference can be obtained for the simple case of a non-interacting condensate. From a simple argument of energy-momentum conservation, the peak in the excitation spectrum must occur at

$$\hbar \omega = \frac{\hbar^2 q^2}{2m}.$$  \hfill (2.51)

Thus, in the absence of interactions, the energy of the excitation — or the energy to promote an atom out of the condensate — is simply equal to the kinetic energy.

A simple model for predicting the excitation energy in the case of an interacting condensate is given by considering a homogeneous condensate with density $n$ and chemical potential $\mu$. The energy to promote an atom out of the condensate is then
given by
\[ \hbar \omega = \frac{\hbar^2 q^2}{2m} + \mu. \] (2.52)

The shift in the Bragg line peak from the non-interacting case, which we shall denote \( \Delta \omega \), is therefore given by
\[ \Delta \omega = \mu = \frac{4\pi \hbar^2 a_s n}{m}. \] (2.53)

This expression is equal to the Bogoliubov eigenvalue (2.29) in the limit of large momentum.

As we discuss in greater detail in Sect. 7.1.1, the line shift prediction (2.53) has a very limited validity. However, it does offer a simple prediction for the line shift as long as the momentum is large, the scattering length is small, and the condensate is homogeneous. In the case of an inhomogeneous condensate, the homogeneous density has to be replaced with an appropriate estimate of the average density. In the JILA experiment, the homogeneous density is replaced with the space-averaged density of the inhomogeneous condensate; however, this is in general not uniquely determined and is therefore not an appropriate quantity to use. Stenger et al. [118] uses the density-weighted density instead, which can be motivated by using a local density description of the condensate. We discuss this issue further in Sect. 7.1.1.

### 2.4.7 Bogoliubov Excitations

The Bogoliubov quasi-particle description of the condensate wavefunction can be used to describe the excitation spectrum from Bragg scattering. Blakie [7, 9] shows how to derive an expression for the momentum transferred to the condensate under the influence of an optical potential.

As in the previous section, the equation of motion for the condensate subjected to a Bragg pulse is given by
\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) + V_{\text{opt}}(x, t) + U_0 |\psi(x, t)|^2 \right) \psi(x, t). \] (2.54)

Using the Bogoliubov expansion [2.18] and the Bogoliubov-de Gennes equations [2.20], we can simplify the equation of motion to
\[ i \sum_k \left( u_k \dot{b}_k e^{-i\omega_k t} + v^*_k \dot{b}^*_k e^{i\omega_k t} \right) = V_{\text{opt}} \psi, \] (2.55)

where we have suppressed the explicit spatial and temporal dependence for brevity. Morgan et al. [83] show how we can project out the quasi-particle derivatives \( \dot{b}_k \) from
CHAPTER 2. BACKGROUND THEORY

the above equation by using the orthogonality and normalisation relations (2.23, 2.22):

\[
\int dx \{ u^*_k V_{opt} \psi + v^*_k V_{opt} \psi^* \} = 
\int dx \sum_k \left\{ i u^*_k \left( u_k \hat{b}_k e^{-i\omega_k t} + v_k \hat{b}_k^* e^{i\omega_k t} \right) - i v^*_k \left( u_k^* \hat{b}_k^* e^{i\omega_k t} + v_k^* \hat{b}_k e^{-i\omega_k t} \right) \right\},
\]

(2.56)

\[
= i \sum_k \left\{ \int dx \left( u^*_k u_k - v^*_k v_k \right) \hat{b}_k e^{-i\omega_k t} + \int dx \left( u^*_k v_k^* - v^*_k u_k^* \right) \hat{b}_k^* e^{i\omega_k t} \right\},
\]

(2.57)

\[
= i \hat{b}'(t) e^{-i\omega_k t}.
\]

(2.58)

Therefore, we get

\[
\dot{b}_k(t) = -ie^{i\omega_k t} \int dx \left\{ u^*_k V_{opt} \psi + v^*_k V_{opt} \psi^* \right\}.
\]

(2.59)

Assuming \( \psi = \psi_0 \), with \( \psi_0 \) given as in (2.18), and integrating over time, we arrive at

\[
b_k(t) = b_k(0) - i \int_0^t dt' V_0 e^{i\omega k t'} \int dx (u^*_k + v^*_k) \cos(q \cdot x - \omega t') \psi_0.
\]

(2.60)

If we assume that \( b_k(0) = 0 \) and that we have the simplest type of optical potential, namely a square pulse with amplitude \( V_0 \) and duration \( T \), this equation can be simplified to

\[
b_k(T) = -ie^{i(\omega - \omega) T/2} \frac{\sin((\omega k - \omega) T/2)}{\omega k - \omega} \int dx (u^*_k + v^*_k) e^{i q x} \psi_0
\]

\[+ e^{i\omega T/2} \frac{\sin((\omega k + \omega) T/2)}{\omega k + \omega} \int dx (u^*_k + v^*_k) e^{-i q x} \psi_0].
\]

(2.61)

2.4.8 Uniform Condensate

For the ideal case of Bragg scattering from a uniform condensate, the quasi-particle amplitudes are given by (2.24, 2.25). The expression for \( b_p \) now simplifies to

\[
b_p(T) = -\frac{i V_0}{\sqrt{V}} e^{i\omega_p T/2} \int \sqrt{\bar{n}} (u^*_p + v^*_p) e^{ik x}
\]

\[\times \left[ e^{-i\omega T/2} \frac{\sin((\omega_p - \omega) T/2)}{\omega_p - \omega} e^{i q x} + e^{i\omega T/2} \frac{\sin((\omega_p + \omega) T/2)}{\omega_p + \omega} e^{-i q x} \right].
\]

(2.62)
2.4. Atom Interactions with Light Fields

Since the homogeneous excitations are plane waves, the spatial integral selects for excitation only the quasi-particles with wave vector \( k = \pm q \). We therefore get

\[
\hat{b}_p(T) = -iV_0 \sqrt{N} (u_p^* + v_p^*) \times \left[ e^{i(\omega_p - \omega)T/2} \frac{\sin((\omega_p - \omega)T/2)}{\omega_p - \omega} \delta_{p,-q} + e^{i(\omega_p + \omega)T/2} \frac{\sin((\omega_p + \omega)T/2)}{\omega_p + \omega} \delta_{p,q} \right],
\]

(2.63)

where \( N \) is the number of atoms.

The total momentum imparted to the condensate can now be evaluated using the Bogoliubov expansions (2.18), and the normalisation and orthogonality relations (2.23, 2.22),

\[
P(T) = \frac{\hbar}{2i} \int \text{d}x \psi^* \nabla \psi + \text{c.c.} \quad (2.64)
\]

\[
= \sum_p \hbar p |\hat{b}_p(T)|^2 \quad (2.65)
\]

\[
= \hbar q N V_0^2 |(u_q + v_q)|^2 \times \left[ \frac{\sin((\omega_q - \omega)T/2)}{\omega_q - \omega} \right]^2 - \left[ \frac{\sin((\omega_q + \omega)T/2)}{\omega_q + \omega} \right]^2. \quad (2.66)
\]

This expression will have its maximum values at the points where \( \omega = \pm \omega_q \), so that the peak in the momentum transfer will occur for the eigenfrequencies of the system, given by (2.29).

The proportion of scattered particles is given in terms of the momentum transfer as

\[
P_{\text{norm}}(T) = \frac{P(T)}{\hbar q N}. \quad (2.67)
\]

In Fig. 2.8 we plot the fraction of particles scattered out of the condensate during the Bragg pulse for three different scattering lengths for a system of \(^{85}\text{Rb}\). For this system, the momentum is \( q = 1.6 \times 10^7 \text{ m}^{-1} \), thus the resonance peak of a non-interacting gas would be located at \( 1/2\pi \times \hbar q^2 / 2m \approx 15.4 \text{ kHz} \). The resonance peaks of the Bragg spectra for the interacting systems are shifted from the free particle resonance, and the shifts increase as the scattering length is increased.

Fig. 2.9 shows how the shift of the Bragg resonance from the free particle resonance changes with the increase in scattering length. For comparison we have also plotted the result based on the simple model (2.53). The two models agree well for low scattering lengths, but differ dramatically for larger scattering lengths.
**CHAPTER 2. BACKGROUND THEORY**

Figure 2.8: Bragg spectrum showing the fraction of particles scattered out of the condensate as a function of the Bragg frequency for a uniform system of $^{85}$Rb with density $n = 10^{20} \text{ m}^{-3}$. Here we show the spectra for three different scattering lengths: $a_s = 100a_0$ (green dashed-dotted line), $a_s = 700a_0$ (red dashed line) and $a_s = 1000a_0$ (blue solid line). The duration of the Bragg pulse is $T = 0.1 \text{ ms}$, the momentum is $q = 1.6 \times 10^7 \text{ m}^{-1}$, and the intensity of the pulse is $V_0 = 2\pi \times 1 \text{ kHz}$.

Figure 2.9: The shift of the Bragg spectral peak from that of the non-interacting gas, plotted against the scattering length for a uniform system of $^{85}$Rb with density $n = 10^{20} \text{ m}^{-3}$. The black solid line is based on the resonance peak position calculated by the Bogoliubov eigenvalue (2.29), and the blue dashed line is calculated based on the simple model (2.53).
Chapter 3

C-field Theory

In this chapter, we present the \(c\)-field formalism that forms the basis of the work in this thesis. We begin by outlining an effective field method for Bose–Einstein condensates in Sect. 3.1, then go on to introduce the basic concepts behind the different \(c\)-field methods in Sect. 3.2. Finally, in Sect. 3.3, we briefly present the truncated Wigner formalism on which the \(c\)-field theory is based. We also discuss the properties of the truncated Wigner method, which is the particular \(c\)-field method used in this thesis.

Blakie et al. have summarised the \(c\)-field formalism in their recent review, [10]. In this chapter we briefly outline the most important concepts, and the reader is referred to this review for further details.

3.1 Effective Hamiltonian Method for Bose–Einstein Condensates

As mentioned in Sect. 2.1.2 it is normal when describing Bose–Einstein condensates to use an approximate Hamiltonian for the system of ultra-cold atoms which gives a good description of only the long-wavelength behaviour of the system, since this is all that is relevant for the observable physics. The relevant methods are called pseudo-potential methods or effective field theory methods, and there is a long history associated with the various formulations of these methods [22, 12, 56, 19]. In all of these formulations, the underlying philosophy is to find an approximate description of the physics of very low energy particles. The definition of “low energy” in practice is that the scattering amplitude for such energies does not differ significantly from its value at zero energy.

It is best to formulate the required concepts precisely, and in a form adapted to the study of a trapped ultra-cold gas. In such a system, all of the relevant physics involve particles with a finite small momentum — this means that we can restrict the descrip-
tion to particles with momentum less than a fixed cutoff value $\hbar \Lambda$. Consequently, the maximum relative momentum is $2\hbar \Lambda$, and for a given centre of mass momentum, $Q$, of any pair of colliding particles, the allowable values of relative momentum, $p$, satisfy $|p + \frac{1}{2}Q| \leq \hbar \Lambda$. Thus, the description of scattering of any pair of particles depends on their centre of mass momentum. If the possible values of $Q$ are themselves rather small in comparison with $\hbar \Lambda$, this dependence on the centre of mass momentum is not very strong, and it is normally ignored.

The appropriate quantum field theory description in the case that the centre of mass dependence can be neglected is essentially that of Braaten and Nieto [19], and can be characterised as:

1. The system of atoms is described by a quantum field operator $\hat{\psi}$, defined on the low energy subspace specified by a momentum space cutoff $\Lambda$,

$$\hat{\psi}(x) = \frac{1}{(2\pi)^{3/2}} \int_0^\Lambda dk \, a_k e^{ik \cdot x}. \quad (3.1)$$

2. The Hamiltonian for a trapped bosonic gas of interacting particles is given by

$$H = \int dx \left\{ \hat{\psi}^\dagger(x) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) \right) \hat{\psi}(x) + \frac{U_0}{2} \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}(x) \right\}, \quad (3.2)$$

where $V_a$ is the trapping potential.

3. The quantity $U_0$ is the inter-atomic scattering strength, and is related to the s-wave scattering length $a_s$ by

$$U_0 = \frac{4\pi \hbar^2 a_s}{m(1 - 2\Lambda a_s/\pi)}. \quad (3.3)$$

For the method to be useful it is necessary that $2\Lambda a_s/\pi \ll 1$, which will mean that the predictions of this Hamiltonian are independent of the cutoff, as long as this is not too big. In this case, at sufficiently low temperatures, the condensate wavefunction $\psi(x)$ is accurately described by the Gross–Pitaevskii equation,

$$i\hbar \frac{\partial \psi(x)}{\partial t} = -\frac{\hbar^2 \nabla^2}{2m} \psi(x) + V_{\text{ext}}(x) \psi(x) + \frac{4\pi \hbar^2 a_s}{m} |\psi(x)|^2 \psi(x). \quad (3.4)$$

Experimentally, this is a well-verified equation.

If $2\Lambda a_s/\pi$ is not sufficiently small, the simple relationship between the Hamiltonian and the Gross–Pitaevskii equation disappears. The derivation of the Gross–Pitaevskii equation from the Hamiltonian involves higher order terms in perturbation theory, which are implicitly summed by the choice of a sufficiently small $\Lambda$. 
3.1. Momentum Cutoff

The introduction of the momentum space cutoff is necessary for a number of reasons, as outlined in the following:

1. There are in principle an infinite number of modes in the field describing the Bose–Einstein condensate. However, for practical reasons it is not possible to describe a system with an infinite number of degrees of freedom in numerical computations; any numerical description of such a system must always be restricted to a finite number of modes. This restriction to the momentum space is naïvely provided by the finite spatial grid of the simulation, although implementing the restriction explicitly as a projector has other advantages; it has been shown \[33\, 87\] how a projector can be chosen so that the problem of aliasing of the wavefunction in simulation can be avoided.

The issue of aliasing is not so important for simple Gross–Pitaevskii equation simulations, since the occupations of modes at risk of being aliased are usually small. However, as we shall see in Sect.\[3.3.4\] in the truncated Wigner Gross–Pitaevskii method every mode has at least a half quantum of occupation, and aliasing is definitely an issue of concern.

2. As is discussed in Sect.\[3.3.4\] in the truncated Wigner Gross–Pitaevskii method, physics beyond mean-field theory arises because of vacuum noise corresponding to half a quantum per mode. The addition of these virtual particles mimics the role that vacuum fluctuations would have on the system, but if all physically allowed modes were included it would lead to ultra-violet divergencies \[10\]. The projection onto a small subspace of momentum space ensures that the contribution from the quantum noise to the stochastic average of the system is finite.

3. As in the Gross–Pitaevskii equation, the interactions between the condensed particles in the c-field formalism are represented by a localised contact potential. This pseudo-potential method implies the use of a cutoff, as has been argued by Braaten and Nieto \[19\], who introduced the requirement on the cutoff \(\Lambda\) and the inter-particle scattering length \(a_s\)

\[
\Lambda a_s \ll 1, \tag{3.5}
\]

for the validity of a pseudo-potential method. As implied by our use of the same notation, \(\Lambda\), the pseudo-potential cutoff and that required by the numerical sim-
ulations are in practice essentially identical.

In practice, the choice of cutoff that is mandated by the numerical algorithms used, fulfills this criterion with a satisfactory margin of safety; for example in the simulations done by Norrie et al. [88, 90, 89] the cutoff used satisfied $\Lambda a_s \approx 0.1$.

It is important to emphasise that, although $\Lambda$ is often called an “ultraviolet cutoff”, unlike such cutoffs in quantum electrodynamics, it has a finite value, and this value is small. Furthermore, in c-field methods, all states have at least half a quantum of occupation, so that all momenta up to $\hbar \Lambda$ participate in calculations, and the corrections discussed in Sect. 4.3 may be relevant.

### 3.2 C-field Methods

The c-field formalism was developed as an approach to one of the major problems associated with treating the dynamics of quantum mechanical systems; if treating the operator character of the fields explicitly, it is only possible to consider very simple systems. If, on the other hand, a classical approximation to the field operators is used, such as is used in the Gross–Pitaevskii equation, the quantum nature of the system is lost.

The way in which this is solved in the c-field approach is by mapping the quantum mechanical system to a classical analogue in such a way as to retain the quantum properties of the system. The density operator of the system is described in a coherent state basis using a distribution function that can be treated classically, but where the quantum behaviour is preserved. The great advantage of the c-field methods is in their ability to incorporate the quantum mechanical behaviour of the systems correctly, while at the same time being seemingly classical in their computational tractability — hence the name “c-field” from “classical-field”, which by no means should lead to the incorrect assumption that these methods are not quantum mechanical.

The c-field method is based on the use of a Wigner function representation, in which a truncation approximation is made, valid when the density of the Bose–Einstein condensate is large. The mathematical formulation of the c-field method which results from this is superficially very similar to that provided by the Gross–Pitaevskii equation. The principal feature in addition to the Gross–Pitaevskii equation is provided by the addition of a stochastic representation of quantum fluctuations in the initial conditions. In the high density limit, the method provides a treatment in which quantum and thermal phenomena are correctly accounted for. The predictions of c-field calculations can be dramatically different from those of the Gross–Pitaevskii equation, as

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1In principle there is a difference, discussed in the Sect. 6.6
was shown in the treatment of colliding condensates [88, 90, 89], in which the c-field method was first used to treat the effects of vacuum fluctuations in a realistic calculation.

### 3.2.1 Features of C-field Methods

The term “c-field” refers to three distinctly different theoretical methods for treating highly degenerate bosonic gases: the *Projected Gross–Pitaevskii* (PGPE), the *Truncated Wigner PGPE* and the *Stochastic PGPE*. Each one of these methods has a different range of applications and validity, but the underlying formalism is the same. In this thesis we use the truncated Wigner method, however, in this section we present all three methods. We will discuss the specific details of the truncated Wigner method in the next section.

One of the unifying features of the three c-field methods is the division of the momentum space into distinct regions. Firstly, as we described in the previous section, in order to use an effective field theory for the Bose–Einstein condensate, and in order for the pseudo-potential description of the condensate interactions to be valid, we have to restrict our theory to a low energy subspace of the full momentum space of the system. All states with energy above some cutoff value are therefore neglected. The remaining low energy region is itself divided into two regions: the c-field region and the incoherent region.

The c-field region contains all the modes below the c-field cutoff. It typically includes the condensate mode and all the other modes that either have a high population, or are important for the dynamics of the system. The c-field region can be simulated using fields that are seemingly classical, but that may include quantum effects in the form of stochastic terms.

The incoherent region consists of all the modes below the pseudo-potential cutoff, but above the c-field cutoff. These modes are therefore not directly important to the dynamics of the system. The incoherent region can in some cases contain a significant fraction of the total particle number, but the modes are sparsely populated. Because of the incoherent nature of the atoms in this region, they are treated as particle-like.

The most distinctive differences between the three different c-field methods are the way in which they treat these regions and the connection between them. We address how these methods differ in the following:

**Projected Gross–Pitaevskii Equation** In all the c-field methods, the evolution of the population in the c-field region is described by the *Projected Gross–Pitaevskii equation*, an equation identical to the Gross–Pitaevskii equation, with the sole
exception that the interaction terms that would generate population outside the
low energy subspace spanned by the c-field cutoff will be set to zero.

The Projected Gross–Pitaevskii method is valid for temperatures close to the con-
densation temperature, and the c-field cutoff is chosen such that all modes in
this region are highly occupied. The effects of quantum fluctuations will there-
fore be small, and can be neglected. The c-field region is treated as a micro-
canonical system, with fixed energy and particle number, and all couplings to
the incoherent region are neglected.

**Truncated Wigner Projected Gross–Pitaevskii Equation** If instead we are dealing with
temperatures far below the condensation temperature, there are modes in the c-
field region with low occupation. Therefore, the effects of quantum fluctuations
may be important, and need to be included in the model. This cannot be done
exactly, but can be approximated by adding stochastic samples of a Wigner dis-
tribution to the initial modes of the system. This method, which underlies all the
other c-field techniques, introduces spontaneous processes which are otherwise
absent in the Gross–Pitaevskii equation.

**Stochastic Projected Gross–Pitaevskii Equation** When dealing with a system in the
high temperature limit, but where scattering processes between the c-field re-
gion and the incoherent region are important, the exchange of particles and en-
ergy between these two regions need to be included. This is the case, for example,
when modelling evaporative cooling and vortex formation during Bose–Einstein
condensation.

### 3.3 Truncated Wigner Formalism

All the c-field techniques are based on the *truncated Wigner* method, in which a de-
terministic equation of motion can be seen as describing individual samplings of the
behaviour of the quantum mechanical system. In the following, we will briefly outline
the derivation of this equation, following the treatments in [47] [87] [10]. We will also
discuss the properties of the truncated Wigner methodology, which forms the basis for
the work in this thesis.

#### 3.3.1 The Wigner Distribution

A quantum mechanical system can be described by a quantum density operator $\hat{\rho}(t)$. The truncated Wigner method expresses the density operator on a basis of coherent
states using a classical probability distribution, the Wigner function. Thereby the quantum mechanical behaviour of the system is described by a classical stochastic process. The Wigner function was introduced by Wigner in 1932 and is defined as the Fourier transform of the symmetrically ordered quantum characteristic function.

Norrie [87] shows that for a multimode system with density operator $\hat{\rho}(t)$, the characteristic function $\chi_W(\{\lambda_i, \lambda_j^*\}, t)$ is given by

$$\chi_W(\{\lambda_i, \lambda_j^*\}, t) = \text{Tr} \left( \hat{\rho}(t) \prod_{j=1}^{M} \exp \left( \lambda_j \hat{a}_j^\dagger - \lambda_j^* \hat{a}_j \right) \right),$$

(3.6)

where $M$ is the number of modes. The operator $\hat{a}_j$ is the mode annihilation operator, annihilating a particle from the $j$-th mode. The corresponding coherent state eigenvalue is given by

$$\hat{a}_j |\alpha\rangle = \alpha |\alpha\rangle,$$

(3.7)

and the mode operators obey the usual Bose commutation relations

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}, \quad [\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0.$$  

(3.8)

The multimode Wigner function then takes the form

$$W(\{\alpha_i, \alpha_j^*\}, t) \equiv \frac{1}{\pi^2 M} \int d^2 \alpha_1 \ldots \int d^2 \alpha_M \prod_{j=1}^{M} \exp \left( \lambda_j \alpha_j^* - \lambda_j^* \alpha_j \right) \chi_W(\{\lambda_j, \lambda_j^*\}, t).$$

(3.9)

We decompose the field on the basis according to

$$\hat{\psi}(x) = \sum_j \psi_j(x) \hat{a}_j.$$  

(3.10)

The moments of the Wigner distribution give symmetrically ordered operator averages, so that, for example, the field density average is given by [10] as

$$\int d^2 \alpha_1 \ldots \int d^2 \alpha_M \prod_{j=1}^{M} \left| \psi(\alpha_j) \right|^2 W(\{\alpha_j, \alpha_j^*\}, t)$$

$$= \frac{1}{2} \left( \langle \hat{\psi}^\dagger(\alpha) \hat{\psi}(\alpha) + \hat{\psi}(\alpha) \hat{\psi}^\dagger(\alpha) \rangle \right)$$

$$= \langle \hat{\psi}^\dagger(\alpha) \hat{\psi}(\alpha) \rangle + \frac{1}{2} \delta(\alpha, \alpha),$$

(3.11)

where $\delta$ is the commutator,

$$\delta(\alpha, \alpha) = \left[ \hat{\psi}(\alpha), \hat{\psi}^\dagger(\alpha) \right].$$

(3.13)
We will discuss how to calculate these averages, in particular the average density, in greater detail in Sect. [5.7].

### 3.3.2 Operator Correspondences

As discussed previously, the advantage of the quasi-probability methods is the ability to transform the action of a quantum mechanical operator on the density operator, to that of a classical operator on the quasi-probability distribution. Every quantum mechanical operator can be written in terms of creation and destruction operators, for example the field operator is given by the decomposition (3.10).

The operator correspondences for the creation and destruction operators are reasonably straightforward, so by using these correspondences, the mapping for the whole system can be made. For the Wigner function, the operator correspondences for the actions of the creation and destruction operators are given by [47]

\[
\begin{align*}
\hat{a}_j \hat{\rho}(t) & \leftrightarrow \left( \alpha_j + \frac{1}{2} \frac{\partial}{\partial \alpha_j^*} \right) W\left\{ \{ \alpha_j, \alpha_j^* \}, t \right\}, \\
\hat{a}_j^\dagger \hat{\rho}(t) & \leftrightarrow \left( \alpha_j^* - \frac{1}{2} \frac{\partial}{\partial \alpha_j} \right) W\left\{ \{ \alpha_j, \alpha_j^* \}, t \right\}, \\
\hat{\rho}(t) \hat{a}_j & \leftrightarrow \left( \alpha_j - \frac{1}{2} \frac{\partial}{\partial \alpha_j^*} \right) W\left\{ \{ \alpha_j, \alpha_j^* \}, t \right\}, \\
\hat{\rho}(t) \hat{a}_j^\dagger & \leftrightarrow \left( \alpha_j^* + \frac{1}{2} \frac{\partial}{\partial \alpha_j} \right) W\left\{ \{ \alpha_j, \alpha_j^* \}, t \right\}.
\end{align*}
\]

(3.14a–3.14d)

Using these correspondences we can convert the equation of motion for the density operator into a classical partial-differential equation for the Wigner function.

### 3.3.3 Truncated Wigner Approximation

The dynamics of the c-field operator $\hat{\psi}$ are given by the Hamiltonian (3.2), so that the evolution of the density operator is given by the von Neumann equation,

\[
\frac{i\hbar}{\partial t} \delta \hat{\rho}(t) = \left[ \hat{H}(t), \hat{\rho}(t) \right].
\]

(3.15)

Norrie [87] shows in detail how we can obtain an equation for the time evolution of the Wigner function by using the operator correspondences (3.14a–3.14d) in the von Neumann equation (3.15). Applied to the Hamiltonian (3.2), the correspondences produce first-order derivatives, but also third-order derivatives, which cause problems when mapping the equation of motion to a stochastic representation.
3.3. Truncated Wigner Formalism

The evolution of the Wigner function can be mapped to a stochastic differential equation which can be seen as describing the trajectory that a single realisation of the system takes through phase-space. Summing over a large number of trajectories would then give an approximation of the Wigner function. There are no known practical techniques for performing the mapping for an equation with third-order derivatives, although this has been investigated in theory [97]. However, we can make the truncated Wigner approximation, by neglecting these higher order derivatives. Norrie [87] shows how the third-order derivatives are negligible as long as the particle density of the modes are sufficiently high, as discussed further in Sect. 3.3.5.

Polkovnikov [98] discusses a treatment which goes beyond the truncated Wigner approximation. Using perturbation theory on the full quantum mechanical system, Polkovnikov shows that the classical Gross–Pitaevskii equation can be recovered as the zeroth-order approximation, while the truncated Wigner can be obtained as the first-order approximation. However, the higher order corrections in this treatment would be intractable for a system as complex as the one we are treating in this thesis. Thus the method used by Polkovnikov would not be applicable here, and we shall therefore satisfy ourselves with the truncated Wigner approximation.

Applying the truncated Wigner approximation to the equation for the evolution of the Wigner function gives the truncated Wigner Fokker–Planck equation, which can be mapped to the stochastic differential equation for a single trajectory, known as the truncated Wigner projected Gross–Pitaevskii equation,

\[ i\hbar \frac{\partial \psi}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) \right) \psi + \mathcal{P} \left\{ U_0 \left( |\psi|^2 - \delta(x, x) \right) \psi \right\} . \] (3.16)

Blakie et al. [10] show how if we treat the Hamiltonian (3.2) classically, replacing the field operator with a classical field, we can obtain the projected Gross–Pitaevskii equation,

\[ i\hbar \frac{\partial \psi}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) \right) \psi + \mathcal{P} \left\{ U_0 |\Psi|^2 \psi \right\} . \] (3.17)

Obviously, this equation is equal to (3.16) in the classical limit, where in the absence of quantum noise the commutator term \( \delta \) can be neglected.

3.3.4 Sampling the Wigner Distribution

The evolution of the field according to the projected Gross–Pitaevskii equation is purely deterministic. However, in the truncated Wigner method, the stochastic properties of the field — corresponding to the quantum fluctuations — are included by adding a stochastic element to the initial state.
Blakie et al. [10] discusses in detail how the sampling of the Wigner distribution is done in order to recover the correct symmetrically ordered moments. In this thesis, we only treat systems in the zero-temperature limit, where the only fluctuations will be caused by quantum effects. In this case, the noise added to the initial mode amplitudes in order to correctly reproduce the Wigner function is given by [87] as

$$\alpha_j(0) \rightarrow \alpha_j(0) + \frac{1}{2} (A_j + iB_j),$$

(3.18)

where $A_j$ and $B_j$ are independent Gaussian random variables with zero mean and unit variance, such that

$$\langle A_j \rangle = \langle B_j \rangle = 0,$$

(3.19)

$$\langle A_i A_j \rangle = \langle B_i B_j \rangle = \delta_{ij},$$

(3.20)

$$\langle A_i B_j \rangle = 0.$$  

(3.21)

It is worth noting that although this method for sampling the Wigner distribution is accurate for the systems studied in this thesis, the more correct way would be to sample the Bogoliubov state, as is discussed in [10].

Physically, when modelling a system with $M$ modes, the method described in this section corresponds to adding an additional half quantum of noise per mode on average to the initial states. This introduces a total of $M/2$ virtual particles to the system, which should be subtracted in order to recover the correct atom number. The effects of the added virtual particles also need to be considered when recovering any other operator averages.

### 3.3.5 Validity of Truncated Wigner Method

The strict validity condition for the truncated Wigner approximation is that all modes are highly populated. However, for systems well below the condensation temperature, this condition is sometimes difficult to fulfill. Norrie [87] presents a less restrictive condition, namely that, in order to ensure the consistency of the short-term evolution of the field, it is sufficient that the system is highly populated in position space, so that the commutator $\delta$ is negligible in comparison to the field itself. In the homogeneous low-temperature case, this condition takes the form $N \gg M$, where $N$ is the number of particles in the field and $M$ is the number of modes. This condition is almost identical to that derived by Sinatra et al. [114],

$$N \gg \frac{M}{2}.$$  

(3.22)
3.3. Truncated Wigner Formalism

For an inhomogeneous system, the population of some regions may go to zero, making the truncation invalid in these areas. However, the application of the truncated Wigner approximation will still be valid, since the low population modes contribute the least to the evolution of the Wigner function [87].

The addition of the virtual particles to the initial modes as in Sect.3.3.4 can cause problems for the truncated Wigner formalism for simulations over long timescales. If the virtual particles thermalise, they may change the equilibrium properties of the system. Sinatra et al. [114] therefore propose an additional condition of validity for the truncated Wigner method, 

\[ |T - T_{\text{therm}}| \ll T, \]  

(3.23)

where \( T \) is the initial temperature of the system, and \( T_{\text{therm}} \) is the temperature once the virtual particles have thermalised. This condition is best met by ensuring that the number of modes is kept sufficiently low.

Both validity conditions are thus dependent on the value of the c-field cutoff, so the choice of projector is not arbitrary. If the cutoff is set too low, important modes for the physics of the system may be excluded from the c-field region. If, on the other hand, the cutoff is set too high, then many sparsely occupied modes will be included in the c-field region, which may invalidate the use of the truncated Wigner formalism. This issue is discussed further in Sect.6.5.
Chapter 4

Atom-Molecule Formalism

In this chapter, we present a model of a Bose-Einstein condensate close to a Feshbach resonance, using the c-field methods described in Chap. 3 as the basis of our formalism. The tunable scattering length of the atoms close to the Feshbach resonance is described using a system of coupled atom and molecule fields. The atom-molecule model gives a purely phenomenological description of the physics, and its parameters must therefore be determined to reproduce the correct experimentally measurable quantities. The two relevant parameters for the molecular field model are the binding energy of the weakly bound state, and the s-wave scattering length, which can be measured. The effective range, we will argue, is not a useful parameter for characterising the physics.

In Sect. 4.1, we present the Hamiltonian for the coupled atom-molecule model used here, and the parameters associated with it. In Sect. 4.2, we derive a Yamaguchi-like equation 126 for this Hamiltonian and show how it can be used to determine the scattering amplitude, binding energy and bound state wavefunction for our system. Then in Sect. 4.3, we discuss the corrections that would occur for non-zero momentum centre of mass. In Sect. 4.4, we derive expressions for the s-wave scattering length and binding energy within this formalism, and show how it is possible to accurately determine the phenomenological parameters in the Hamiltonian by relating these to the corresponding experimental parameters.

This chapter is based on the work presented in 109.

4.1 An Effective Field Method for Molecules

Apart from the solitary case of hydrogen condensates, in all Bose–Einstein condensate experiments the scattering length, $a_s$, used to describe the interactions arises because of the existence of a weakly bound state of two atoms. The use of Feshbach resonances
can give very large scattering lengths, consequently reducing the binding energy of this state to a very small value. This can introduce quite slow time scales, which make it wise to investigate the possible influence of molecular dynamics on Bose–Einstein condensation phenomena.

The c-field method cannot be directly applied to any exact description of the relevant molecular physics, since binding can only be described by an attractive potential, for which the Gross–Pitaevskii equation and similar c-field equations have no stable solutions, and certainly do not produce molecules. In this thesis, we want to combine the ideas of c-fields with those field theory methods which use an explicit “molecule field”, as originally introduced in \[59, 120, 53, 54, 40\]. These kinds of models are purely phenomenological descriptions of the physics, whose parameters must be determined to reproduce the correct experimentally measurable quantities.

### 4.1.1 The Molecular-Field Hamiltonian

Since the Gross–Pitaevskii equation cannot produce bound states, it is clear that in some sense these molecules must be introduced “by hand”. A method used by several other groups, as noted previously, is to add an additional field \(\hat{\phi}\) corresponding to a molecule state, giving the Hamiltonian:

\[
\hat{H} = \int dx \left\{ \psi^\dagger(x) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_a(x) \right) \psi(x) + \phi^\dagger(x) \left( -\frac{\hbar^2 \nabla^2}{4m} + V_m(x) + \varepsilon \right) \phi(x) + \frac{U_{aa}}{2} \psi^\dagger(x) \hat{\phi}^\dagger(x) \hat{\phi}(x) \hat{\phi}(x) \psi(x) + U_{am} \psi^\dagger(x) \phi^\dagger(x) \phi(x) \psi(x) + \frac{U_{mm}}{2} \phi^\dagger(x) \phi^\dagger(x) \phi(x) \phi(x) + \frac{g}{2} \left( \phi^\dagger(x) \psi(x) \phi(x) \psi(x) + \psi^\dagger(x) \phi^\dagger(x) \phi(x) \psi(x) \right) \right\}.
\]  

(4.1)

Here the parameters have the interpretations:

1. \(U_{aa}\) is the background atom interaction strength, leading to the concept of a background scattering length \(a_{bg} \equiv mU_{aa}/4\pi\hbar^2\). The details of the background scattering length and its connection to the Feshbach resonance is discussed in Sect. 2.2.

2. \(V_a\) and \(V_m\) are the external trapping potential for the atoms and the molecules, respectively. If the magnetic moment of the weakly bound molecule is twice that of the atom, then \(V_m = 2V_a\). However, this is not mandatory.

3. \(\varepsilon\) is an energy offset term, which allows for a finite binding energy of the molecule.

4. The coupling parameter, \(g\), describes the strength of coupling of the process by which a molecule is formed from two atoms.
5. The terms with factors $U_{am}$ and $U_{mm}$ correspond to atom-molecule and molecule-molecule scattering, respectively. Since the atom field is usually much larger than the molecule field in the situations we shall consider, these terms are in most cases negligible. Moreover, to the best of our knowledge, there is no information available on the values of these two parameters.

The model used in this work treats a system of an atomic and a molecular condensate, coupled together to allow for the formation of molecules from atoms and vice versa. However, it should be noted that this is a single channel system, and tuning the energy of the resonance results in sweeps in the single bound state channel. Thus, in this model, we are not including the detailed physics of the Feshbach resonance described in Sect. 2.2. Rather, we are using overall the mechanism of the Feshbach resonance — the existence of a bound state with tunable energy, coupled to the free atom state — to model its effect on the interaction strength.

4.1.2 Phenomenology

The Hamiltonian (4.1), it must be emphasised, provides only a phenomenological description of the physics. As mentioned previously, we are merely modelling the effect of the Feshbach resonance, instead of the full physics of this phenomenon, and the parameters in the Hamiltonian do not necessarily correspond to physical parameters. The coupling parameter $g$ gives an indication of the strength of a particular resonance, but $g$ need not be uniquely determined for that resonance. The energy offset, $\epsilon$, can be viewed as a representation of the effect of a Feshbach resonance on the scattering length and as such it is related to the binding energy of the molecule. However, the actual binding energy must be determined by solving the appropriate Schrödinger equation, and it will depend on the other parameters. Furthermore, for each value of $\epsilon$, the other parameters, and in particular $g$, may be different. Indeed, we will find that the values of $g$ and $\epsilon$ required to fit the measured scattering and binding properties are strongly inter-dependent. These dependencies, in practice, simply mean that when setting up a c-field simulation, one must choose the parameters appropriate to the experimental system under investigation.

In summary, the sole function of Hamiltonian (4.1) is to provide a practical method of implementing c-field theory for molecules in a way that is consistent with measured properties of the atom-molecule system. The basic theory to which it is an approximation is a Hamiltonian involving only atoms interacting through an appropriate inter-atomic potential $u(x - x')$. The molecular field method is only necessary in this thesis because the “exact” Hamiltonian cannot be represented inside a c-field theory. The
inter-dependence of the parameters $g$ and $\varepsilon$ in our model is something that, in general, would not be expected from a fundamental theory.

### 4.1.3 Momentum Cutoffs

In the case of a coupled atom-molecule model, there will be momentum cutoffs for both the molecular and the atomic fields. These can be expressed in terms of projectors $\mathcal{P}_a$ and $\mathcal{P}_m$ that project the wavefunctions onto the low energy subspace below the cutoff. Because a molecule is formed from two atoms, the interactions will only make sense if the molecule cutoff is twice that of the atom. Thus, if the atom cutoff is $\Lambda$, then the projectors can be defined as

$$
\mathcal{P}_a(k) = \Theta(\Lambda - |k|), \quad (4.2)
$$

$$
\mathcal{P}_m(k) = \Theta(2\Lambda - |k|), \quad (4.3)
$$

where $\Theta$ is the Heaviside step function.

In (4.2, 4.3) we have assumed isotropic cutoffs, but this is not necessarily the case for all systems. Indeed, as we shall see in Chap.7 in experimentally realistic systems the cutoff can be highly anisotropic. However, for the work in this chapter, the exact properties of the cutoff are not relevant, and we can therefore assume that it is isotropic.

### 4.2 Scattering Solutions

In order to determine the relationship of our theory to reality, the parameters and the fields have to be related to physically observable quantities. To do this, we need to compute:

1. The scattering amplitude,
2. The binding energy,
3. The bound state wavefunction.

We use standard techniques and concepts from scattering theory to investigate this; the reader is referred to [85] for further details.

#### 4.2.1 Schrödinger Equation in the 2-Atom : 1-Molecule Sector

If $|E\rangle$ is a state in the 2-atom : 1-molecule sector, i.e. a state that consists of either two atoms or one molecule, it has a two-component wavefunction, defined by the 2-atom
4.2. Scattering Solutions

amplitude

\[ \psi(x_1, x_2) \equiv \langle 0 | \hat{\psi}(x_1) \hat{\psi}(x_2) | E \rangle, \]  

(4.4)

and the 1-molecule amplitude

\[ \phi(x) \equiv \langle 0 | \hat{\phi}(x) | E \rangle. \]  

(4.5)

The normalisation of the wavefunctions is given by the condition

\[ \int |\psi(x_1, x_2)|^2 dx_1 dx_2 + 2 \int |\phi(x)|^2 dx = 1. \]  

(4.6)

Assuming that the system is homogeneous, we can set the trapping potentials in the Hamiltonian (4.1) to zero. The Schrödinger equation for the atom and molecule wavefunctions corresponding to (4.1) can then be written as

\[ E \psi(x_1, x_2) = -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) \psi(x_1, x_2) + \delta(x_1 - x_2) \left( U_{aa} \psi(x_1, x_2) + g \phi(x_1) \right), \]  

(4.7)

\[ E \phi(x) = -\frac{\hbar^2 \nabla^2}{4m} \phi(x) + \varepsilon \phi(x) + \frac{g}{2} \psi(x, x). \]  

(4.8)

The equivalent Schrödinger equations for the momentum space wavefunctions \( \tilde{\psi} \) and \( \tilde{\phi} \), after implementing the cutoff, take the form

\[ \left( E - \frac{\hbar^2}{2m} (p_1^2 + p_2^2) \right) \tilde{\psi}(p_1, p_2) = U_{aa} (2\pi)^3 \int_0^\Lambda dq_1 \int_0^\Lambda dq_2 \delta(q_1 + q_2 - p_1 - p_2) \tilde{\psi}(q_1, q_2) + g \tilde{\phi}(p_1 + p_2), \]  

(4.9)

\[ \left( E - \varepsilon - \frac{\hbar^2 p^2}{4m} \right) \tilde{\phi}(p) = \frac{g}{2(2\pi)^3} \int_0^\Lambda dq_1 \int_0^\Lambda dq_2 \delta(q_1 + q_2 - p) \tilde{\psi}(q_1, q_2). \]  

(4.10)

We transform the coordinate system to one of absolute and relative momenta by the substitutions \( P = (p_1 + p_2)/2, P' = (q_1 + q_2)/2, k = p_1 - p_2 \) and \( k' = q_1 - q_2 \). In the centre of mass frame where \( P = 0 \) the equations take the form

\[ \left( E - \frac{\hbar^2 k^2}{m} \right) \tilde{\psi}(k) = U_{aa} (2\pi)^3 \int_0^\Lambda dk' \tilde{\psi}(k') + g \tilde{\phi}(0), \]  

(4.11)

\[ (E - \varepsilon) \tilde{\phi}(0) = \frac{g}{2(2\pi)^3} \int_0^\Lambda dk' \tilde{\psi}(k'), \]  

(4.12)

where we have redefined \( \tilde{\psi} \) as the single-component momentum space wavefunction for the atomic field.
The projectors (4.2, 4.3) define a preferred frame; in a frame where $P \neq 0$, the range of the momentum integrals becomes $|k + \frac{1}{2} P| \leq \Lambda$. Since the most important interactions in a Bose–Einstein condensate correspond to very small centre of mass momentum (see Sect. 4.3), this is not a great problem.

### 4.2.2 The Yamaguchi Equation

Solving the molecule function (4.12) and substituting it into the atom equation (4.11), we obtain

$$\left(\frac{Em}{\hbar^2} - k^2\right)\tilde{\psi}(k) = \lambda(E) \int_0^\Lambda dk' \tilde{\psi}(k'),$$

where

$$\lambda(E) = m \frac{m}{{(2\pi)}^3 \hbar^2} \left(U_{aa} + \frac{g^2/2}{E - \varepsilon}\right).$$

Equation (4.13) is similar in form to Yamaguchi’s separable potential equation [126], with the important difference that our expression has an explicit dependence on the energy eigenvalue, $E$, in the $\lambda$-factor. However, the method of solution is essentially unaltered.

### 4.2.3 Scattering state solution

A scattering state will be characterised by a positive energy eigenvalue, so we make the substitution $E \rightarrow \hbar^2 K^2 / m$ in (4.13), which can now be written as

$$\tilde{\psi}(k) = \delta(K - k) + \frac{\lambda_K}{K^2 - k^2 + i\eta} \int_0^\Lambda dk' \tilde{\psi}(k'),$$

where we have defined $\lambda_K \equiv \lambda(\hbar^2 K^2 / m)$ and the infinitesimal number $\eta$ is introduced to remove the singularity at $K^2 = k^2$. Integrating over $k$ on both sides gives the result

$$\int_0^\Lambda dk \tilde{\psi}(k) = \left(1 - \lambda_K \int_0^\Lambda dk \frac{1}{K^2 - k^2 + i\eta}\right)^{-1}.$$  

**a) Small $K$ Approximation:** The integral on the right hand side can be evaluated exactly, and for $K \ll \Lambda$ approximated thus:

$$\int_0^\Lambda dk \frac{1}{K^2 - k^2 + i\eta} = -4\pi \Lambda - 2i\pi^2 K + 2\pi K \ln \left(\frac{\Lambda + K}{\Lambda - K}\right)$$
4.2. Scattering Solutions

\[ \approx -4\pi\Lambda - 2i\pi^2 K + 4\pi\frac{K^2}{\Lambda}. \]  

(4.17)

The atom wavefunction for the scattering state can therefore be written as

\[ \tilde{\psi}(k) = \delta(K - k) - \frac{1}{(-1/\lambda_K - 4\pi\Lambda - 2\pi^2 K + 4\pi K^2/\Lambda)} \frac{1}{(K^2 - k^2 + i\eta)}. \]  

(4.18)

Similarly, the solution for the molecular wavefunction is given by

\[ \tilde{\phi}(0) = \frac{g^2/2}{\hbar^2 K^2/m - \varepsilon} \int_0^\Lambda dK' \tilde{\psi}(k') = \frac{1}{(\hbar^2 K^2/m - \varepsilon) (-1 + \lambda_K (4\pi\Lambda + 2\pi^2 K - 4\pi K^2/\Lambda))}. \]  

(4.19)

b) Effective Range and Scattering Length: The scattering wavefunction \( \tilde{a}_K(k) \) for a particle of incident momentum \( K \) and final momentum \( k \) is

\[ \tilde{a}_K(k) = \delta(K - k) - \frac{f(k, K)}{2\pi^2 (K^2 - k^2 + i\eta)}. \]  

(4.20)

where \( f(k, K) \) is the scattering amplitude. Comparison with (4.15) and using (4.16) then gives

\[ f(k, K) = \frac{-2\pi^2 \lambda_K}{1 - \lambda_K} \frac{1}{\int_0^\Lambda dK' \frac{1}{K' - k^2 + i\eta}} = \left( -\frac{1}{2\pi^2 \lambda_K} - \frac{2}{\lambda - iK} + \frac{1}{\pi} K \ln \left( \frac{\Lambda + K}{\Lambda - K} \right) \right)^{-1}. \]  

(4.21)

The scattering amplitude for small incident momenta can be approximated by the effective range expansion [11],

\[ f(K) = \frac{1}{K \cot \delta - 1K} \approx \frac{1}{-1/\alpha_s - 1K + r_0 K^2/2}, \]  

(4.22)

where \( \delta \) is the phase shift, \( \alpha_s \) is the s-wave scattering length and \( r_0 \) is the effective range of the potential. Expanding the quantities \( \lambda_K \) and \( \ln \left( \frac{\Lambda + K}{\Lambda - K} \right) \) for small \( K \) gives

\[ \frac{1}{\lambda_K} \approx \frac{(2\pi)^3 \hbar^2}{m} \left( U_{aa} - \frac{g^2}{2\varepsilon} \right)^{-1} + \pi K^2 \left( \frac{4\pi \hbar^2}{m} \frac{g^2/2\varepsilon}{g(U_{aa} - g^2/2\varepsilon)} \right)^2, \]  

(4.23)

\[ \ln \left( \frac{\Lambda + K}{\Lambda - K} \right) \approx \frac{2K}{\Lambda}, \]  

(4.24)
where (4.24) is valid as long as
\[ K \ll \Lambda, \] (4.25)
and (4.23) is valid as long as
\[ \frac{\hbar^2 K^2}{m} \ll \frac{g^2}{2U_{aa}} - \varepsilon. \] (4.26)

We can then use equations (4.21) and (4.22) to identify
\[ a_s = \left[ \frac{4\pi \hbar^2}{m} \left( U_{aa} - \frac{g^2}{2\varepsilon} \right) + \frac{2\Lambda}{\pi} \right]^{-1}, \] (4.27)
\[ r_0 = \frac{4}{\pi \Lambda} - \frac{1}{\pi} \left( \frac{4\pi \hbar^2}{m} \frac{g^2/2\varepsilon}{g(U_{aa} - g^2/2\varepsilon)} \right)^2. \] (4.28)

c) Background Scattering Length: Setting \( g^2/\varepsilon \to 0 \) in (4.27) corresponds to the case when the effect of the Feshbach resonance is negligible; i.e., only the background scattering term is non-zero. This means that the background scattering length is
\[ a_{bg} = \left[ \frac{4\pi \hbar^2}{mU_{aa}} + \frac{2\Lambda}{\pi} \right]^{-1}. \] (4.29)

4.2.4 Nature of Effective Range Expansion

The effective range expansion of the scattering amplitude has a rather limited range of validity — the two conditions (4.25, 4.26) set an upper bound for \( K \), and for the expansion to be quantitatively valid, \( K \) must lie well inside the region defined by the intersection of the spaces determined by these bounds. The situation is illustrated in Fig. 4.1 for parameters appropriate to the problems we wish to study, for which the available \( K \)-space is limited by the bound determined by \( \Lambda \), that is, by the dashed circle.

However, the exact solution for the scattering amplitude, (4.21), possesses singularities at \( K = \pm \Lambda \), but is analytic for imaginary values of \( K \) with modulus very much greater than \( \Lambda \). In fact, the bound state solution to the scattering problem is given by the pole of (4.21) on the negative imaginary axis, and is well outside the region bounded by the dashed line. This pole cannot be obtained by making the effective range expansion (4.22) for the scattering amplitude. We will therefore interpret the available \( K \)-space region as the asymmetric region bound by the cutoff \( \Lambda \) on the real

\[ \text{In fact, in Sect. 4.2.5, we will find it more convenient to determine the bound state properties by direct solution of the scattering equation, rather than by direct evaluation of the position and residue of the pole, which is fully equivalent to determining the pole and its residue.} \]
Figure 4.1: The grey region shows the region of validity for the scattering amplitude (4.21) in the complex plane, as discussed in the text. The upper bounds given by (4.25, 4.26) for the individual expansions (4.23, 4.24) are given as the dashed and solid circles respectively. The region of validity for the effective range expansion is obviously situated within the smaller of these, while the bound state solution (black square) can be found far outside this area. The plot here is for a cutoff value of $\Lambda = 2.2 \times 10^6 \text{m}^{-1}$ and a scattering length of $a_s = 900 a_0$, but we get qualitatively similar results for the whole parameter range used in this thesis.

axis, but including the bound state on the imaginary axis, indicated by the shaded area in Fig. 4.1.

With the model we have chosen, it is not possible to simultaneously fit the binding energy, the scattering length and the effective range, since there are only two fitting parameters, $g$ and $\epsilon$. The scattering length and binding energy are the relevant measurable parameters for the kind of problem we wish to study, whereas the effective range does not play any direct role, and therefore we will determine $g$ and $\epsilon$ by fitting the measured values of scattering length and binding energy. In this thesis, we will not concern ourselves any further with the effective range parameter.
4.2.5 Bound state solution

In this model, a physical bound state will be a superposition of a state of two \( \psi \)-field “atoms”, defined by (4.4), and a state of one \( \phi \)-field “molecule”, defined by (4.5). A bound state solution is characterised by a negative energy eigenvalue, \( E \rightarrow -\frac{\hbar^2 \alpha^2}{m} \) in (4.13), where \( \alpha > 0 \). Equation (4.13) can now be written as

\[
\tilde{\psi}(k) = -\frac{\lambda_\alpha}{\alpha^2 + k^2} \int_0^\Lambda dk' \tilde{\psi}(k'),
\]

where we have defined \( \lambda_\alpha \) by setting \( E \rightarrow -\frac{\hbar^2 \alpha^2}{m} \) in (4.14). By taking the integral over \( k \) on both sides, we can remove the dependency on the wavefunction, to get

\[
1 = -4\pi \int_0^\Lambda \frac{\lambda_\alpha k^2}{\alpha^2 + k^2} dk = -4\pi \lambda_\alpha \left[ \Lambda - \alpha \arctan \left( \frac{\Lambda}{\alpha} \right) \right],
\]

so that \( \alpha \), and hence the binding energy, is determined by the solution of the equation

\[
\alpha \arctan \left( \frac{\Lambda}{\alpha} \right) = \left[ \frac{m^2}{2\pi^2 \hbar^2} \left( U_{aa} + \frac{g^2/2}{-\hbar^2 \alpha^2/m - \varepsilon} \right) \right]^{-1} + \Lambda.
\]

**a) Threshold of binding:** At the bound state threshold, where \( \alpha \rightarrow 0 \), we can solve (4.32) exactly in terms of \( \varepsilon \) to give

\[
\varepsilon_{\text{threshold}} = \frac{g^2}{2} \left[ U_{aa} + \frac{2\pi^2 \hbar^2}{m\Lambda} \right]^{-1},
\]

which is of course identical to the solution of the scattering length equation (4.27) when \( a_s = 0 \). Substituting from (4.29), this takes the form

\[
\varepsilon_{\text{threshold}} = \left( \frac{g^2}{2} \right) \left( \frac{m}{4\pi \hbar^2} \right) \frac{\pi/2\Lambda}{1 - 2\Lambda a_{bg}/\pi}.
\]

This is non-zero unless \( g^2 \rightarrow 0 \) at threshold.

**b) Weakly bound molecules:** For small values of \( \alpha \) we can expand the left hand side of (4.32) to give

\[
\alpha \left( \frac{\pi}{2} - \frac{\alpha}{\Lambda} \right) = \left[ \frac{m}{2\pi^2 \hbar^2} \left( U_{aa} + \frac{g^2/2}{-\hbar^2 \alpha^2/m - \varepsilon} \right) \right]^{-1} + \Lambda,
\]

so that we get for weakly bound molecules

\[
\alpha \approx \left( \frac{m}{4\pi \hbar^2} \left( U_{aa} + \frac{g^2/2}{-\varepsilon} \right) \right)^{-1} + \frac{2\Lambda}{\pi}.
\]
4.2. Scattering Solutions

It is clear that in the case of weakly bound molecules $\alpha \approx 1/a_s$, as expected from the relationship between the binding energy and the scattering length for sufficiently small binding energies \[26\]. However, it is also clear that in this regime, $\varepsilon$ is distinctly different from the binding energy $E_b = \hbar^2 \alpha^2 / m$, and must therefore not be interpreted as such, but rather as the energy detuning in the Feshbach resonance (see Sect. 2.2).

c) **Tightly bound molecules:** For large values of $\alpha$, expanding $\arctan(\Lambda/\alpha)$ in (4.32) yields

\[
\alpha \left( \frac{\Lambda}{\alpha} - \frac{\Lambda^3}{3\alpha^3} \right) \approx \left[ \frac{m}{2\pi^2\hbar^2} \left( U_{aa} - \frac{g^2/2}{\hbar^2 \alpha^2 / m + \varepsilon} \right) \right]^{-1} + \Lambda, \tag{4.37}
\]

so that we instead get

\[
\alpha^2 \approx -\frac{m \varepsilon \hbar^2}{2\pi^2\hbar^2} + \frac{\pi^2 \hbar^2 \Lambda^3 g^2}{3m} \left( \frac{2\pi^2 \Lambda^3 U_{aa}}{3} + \varepsilon \right)^{-1}. \tag{4.38}
\]

For sufficiently large values of $\varepsilon$ we have that $\alpha^2 \approx -m\varepsilon/\hbar^2$, which means that $\varepsilon$ is approximately equal to the binding energy $E_b = \hbar^2 \alpha^2 / m$ for large values of the detuning, as would be expected in this regime.

### 4.2.6 Atomic Fraction of the Bound State

The bound state solution for the atom wavefunction is

\[
\tilde{\psi}(k) = \frac{N}{\alpha^2 + k^2}, \tag{4.39}
\]

where, if the normalisation is chosen to be $\int d\k |\tilde{\psi}(k)|^2 = M$, the factor $N$ will be given by

\[
\frac{M}{N^2} = \int_0^\Lambda d\k \frac{1}{(\alpha^2 + k^2)^2} = 4\pi \int_0^\Lambda \frac{k^2}{(\alpha^2 + k^2)^2} \, d\k = 2\pi \left[ \frac{1}{\alpha} \arctan \left( \frac{\Lambda}{\alpha} \right) - \frac{\Lambda}{\Lambda^2 + \alpha^2} \right]. \tag{4.40}
\]

Similarly, the solution for the molecular state can be obtained by substituting (4.39) into (4.12), giving

\[
\tilde{\phi}(0) = -\frac{g}{2(\hbar^2 \alpha^2 / m + \varepsilon)} \int_0^\Lambda d\k' \tilde{\psi}(k'), \tag{4.41}
\]
Figure 4.2: The fractions of the atom pairs (dashed line) and elementary molecules (solid line). The values of the length parameters are in this case those for $^{85}\text{Rb}$; namely $l_{ug} \approx 10^{-7}$ m, $a_{bg} = -2.32 \times 10^{-8}$ m, and we have chosen $\Lambda = 2 \times 10^6$ m$^{-1}$.

$$\frac{P_{\text{mol}}}{P_{\text{atm}}} = \frac{|\phi(0)|^2}{\int d\mathbf{k} |\tilde{\psi}(\mathbf{k})|^2} = 8\pi \left( \frac{\alpha}{\Lambda} \right)^2 (l_{ug} \Lambda^2) \left( \frac{t(\alpha/\Lambda) - \pi/2a_{bg}}{t(\alpha/\Lambda) + \Lambda^2/(\Lambda^2 + \alpha^2)} \right)^2, \quad (4.44)$$

$$t(z) \equiv z \arctan(1/z) - 1, \quad (4.45)$$
$$l_{ug} \equiv \left( \frac{U_{aa}}{g} \right)^{2/3}. \quad (4.46)$$

The result depends on the four parameters which are all lengths, namely $l_{ug}$, $a_{bg}$, $\Lambda^{-1}$ and $\alpha^{-1}$. The parameter $l_{ug}$ is a measure of the coupling strength in terms of the interatomic interaction strength, but it has no straightforward physical interpretation. It is worth noting that while it is mandatory that $|K|/\Lambda$ be less than 1, the same is not true for $|\alpha|/\Lambda$, which does not necessarily have to be less than 1. On the contrary, in most experiments the binding energy is usually such that $|\alpha| \gg \Lambda$, for realistic values of the
4.3 Corrections for Non-Zero Centre of Mass Momentum

The parameter $\alpha^{-1}$ determines the spatial extent of the atom-pair part of the wavefunction of the bound state, and this can only be represented on the spatial grid corresponding to the cutoff $\Lambda$ if $\alpha / \Lambda \ll 1$. The crossover from the predominantly atom-pair wavefunction to the elementary molecule wavefunction corresponds to the molecular size becoming smaller than the size of the spatial grid. However, (4.44) shows that, as well as $\Lambda^{-1}$, there are the other lengths $a_{bg}$ and $l_{ug}$ which also come into play. This means that the intuitive idea that the crossover happens at $\alpha / \Lambda \approx 1$ is significantly modified, and in Fig. 4.2, which shows the fractions of the atom and the molecule states as functions of $\alpha / \Lambda$ for $^{85}$Rb, it can be seen that the crossover is closer to $\alpha / \Lambda \approx 0.01$.

The crossover is thus explicitly cutoff-dependent, but this is purely a technical issue. There is no fundamental physics in this crossover; it is determined simply by the technical need to have a cutoff. The cutoff has to be sufficiently large to represent the spatial features under investigation, and also has an upper bound determined by the requirement that $\Lambda a_s$ be much less than one. However, within this range it is arbitrary.

4.3 Corrections for Non-Zero Centre of Mass Momentum

In Sect. 4.2.1, we assume that the centre of mass momentum of the system is zero, and thus we solve the integral in (4.13) on the range $[0, \Lambda]$. In this section, we are investigating the corrections that occur when the centre of mass momentum is non-zero.

4.3.1 Scattering length

To find the corrections to the scattering length, we wish to evaluate the integral in (4.16)

$$I_s = \int_{\mathcal{R}_Q} \frac{1}{K^2 - q^2 + i\eta} \, dq,$$

where the range $\mathcal{R}_Q$ is now defined by

$$|Q \pm 2q| \leq 2\Lambda,$$  (4.48)

for the centre of mass momentum $\hbar Q \equiv p_1 + p_2 = p_3 + p_4$.

We change the integral to polar coordinates, so that the range $\mathcal{R}_Q$ is equivalent to

$$Q^2 + 4q^2 \pm 4qQ \cos \theta \leq 4\Lambda^2,$$  (4.49)

$$\Rightarrow |\cos \theta| \leq X \equiv \min \left(1, \frac{4\Lambda^2 - Q^2 - 4q^2}{4qQ}\right).$$  (4.50)
Thus, we can write

\[ J_s = 2\pi \int_0^{\sqrt{\Lambda^2 - Q^2/4}} \frac{q^2}{K^2 - q^2 + i\eta} \, dq \int_0^\pi 2d\cos \theta, \quad (4.51) \]

\[ = 4\pi \int_0^{\sqrt{\Lambda^2 - Q^2/4}} \frac{q^2}{K^2 - q^2 + i\eta} \, dq \min \left( 1, \frac{4\Lambda^2 - Q^2 - 4q^2}{4qQ} \right). \quad (4.52) \]

Noting that the point at which \( (4\Lambda^2 - Q^2 - 4q^2) / 4mqQ = 1 \) is when \( q = 2\Lambda - Q \), we can write

\[ J_s = 4\pi \int_{\Lambda - Q/2}^{\sqrt{\Lambda^2 - Q^2/4}} \frac{q^2}{K^2 - q^2 + i\eta} \, dq \frac{4\Lambda^2 - Q^2 - 4q^2}{4qQ} \, dq \]

\[ + 4\pi \int_0^{\Lambda - Q/2} \frac{q^2}{K^2 - q^2 + i\eta} \, dq, \quad (4.53) \]

\[ = 4\pi \left( \frac{\Lambda - Q}{2} + \frac{\Lambda^2 - Q^2/4 - K^2/2}{2Q} \ln \left| \frac{K^2 - (\Lambda - Q/2)^2}{K^2 - \Lambda^2 + Q^2/4} \right| \right) \]

\[ + 4\pi \left( -\Lambda + \frac{Q}{2} - \frac{i\pi}{2} K + \frac{K}{2} \ln \left| \frac{K + \Lambda - Q/2}{K - \Lambda + Q/2} \right| \right), \quad (4.54) \]

\[ - 2\pi \Lambda + \pi Q - 2i\pi K + 2\pi \frac{\Lambda^2 - Q^2/4 - K^2/2}{Q} \ln \left| \frac{K^2 - (\Lambda - Q/2)^2}{K^2 - \Lambda^2 + Q^2/4} \right| \]

\[ + 2\pi K \ln \left| \frac{K + \Lambda - Q/2}{K - \Lambda + Q/2} \right|. \quad (4.55) \]

In the case when \( K \ll \Lambda \), we can set \( K \to 0 \) in (4.55) and the expression for the scattering amplitude becomes

\[ f = -\frac{2\pi^2 \Lambda K}{1 - \lambda K J_s} \left( - \frac{1}{2\pi^2 \lambda K} - \frac{\Lambda}{2\pi} + \frac{Q}{2\pi} + \frac{1}{\pi} \frac{\Lambda^2 - Q^2/4}{Q} \ln \left| \frac{\Lambda - Q/2}{\lambda + Q/2} \right| \right)^{-1}, \quad (4.56) \]

which gives the expression for the scattering length,

\[ a_s = \left[ \frac{4\pi \hbar^2}{m} \left( U_{aa} - \frac{g^2}{2\epsilon} \right) \right]^{-1} \left( \frac{\Lambda}{\pi} - \frac{Q}{2\pi} + \frac{1}{\pi} \frac{\Lambda^2 - Q^2/4}{Q} \ln \left| \frac{\Lambda - Q/2}{\lambda + Q/2} \right| \right)^{-1}. \quad (4.57) \]

For \( Q \ll 2\Lambda \), this can be approximated by

\[ a_s \approx \left[ \frac{4\pi \hbar^2}{m} \left( U_{aa} - \frac{g^2}{2\epsilon} \right) \right]^{-1} + \frac{2}{\pi} \Lambda - \frac{Q}{2\pi} - \frac{Q^2}{6\pi \Lambda} \left| \lambda + Q/2 \right|^{-1}. \quad (4.58) \]

Thus, the consequence of a non-zero centre of mass momentum is a reduction in the effective value of the cutoff, \( \Lambda \). However, this reduction will have very little impact on
the value of the scattering length, since in practice $\lambda$ must be chosen to reduce any such effects.

### 4.3.2 Binding Energy

To find the correction to the binding energy, we wish to solve the integral in \((4.31)\),

\[
J_b = \int_{\mathcal{R}_Q} dq \frac{1}{\alpha^2 + q^2},
\]

where the range $\mathcal{R}_Q$ is now defined by

\[
|Q \pm 2q| \leq 2\Lambda,
\]

for the centre of mass momentum $\hbar Q \equiv p_1 + p_2 = p_3 + p_4$.

Following the same method as above, we can write the integral as

\[
J_b = 4\pi \int_{\Lambda - Q/2}^{\sqrt{\frac{\Lambda^2 - Q^2}{4}}} \frac{q^2}{\alpha^2 + q^2} dq + 4\pi \int_0^{\Lambda - Q/2} \frac{q^2}{\alpha^2 + q^2} dq, \tag{4.61}
\]

\[
= \pi Q - 2\pi \Lambda + \pi \frac{4\Lambda^2 - Q^2 + 4\alpha^2}{2Q} \ln \left( \frac{\alpha^2 + \Lambda^2 - Q^2/4}{\alpha^2 + (\Lambda - Q/2)^2} \right) + 4\pi \Lambda - 2\pi Q - 4\pi \arctan \left( \frac{\Lambda - Q/2}{\alpha} \right), \tag{4.62}
\]

\[
\approx -4\pi \arctan \left( \frac{\Lambda - Q/2}{\alpha} \right) + 4\pi (\Lambda - Q/2) + \frac{\pi Q}{\alpha^2 + \Lambda^2} (\Lambda - Q/2)^2 + ..., \tag{4.63}
\]

where the expansion on the last line is valid as long as $Q^2 \ll 4\alpha^2 + 4\Lambda^2$. This is a reasonable approximation, since $Q < 2\Lambda$ always, and $\alpha \gg \Lambda$ usually holds. The expression for the binding energy corresponding to \((4.32)\) then becomes

\[
\alpha \arctan \left( \frac{\Lambda - Q/2}{\alpha} \right) \approx \left[ \frac{m}{2\pi^2 \hbar^2} \left( U_{aa} + \frac{g^2/2}{-\hbar^2 \alpha^2 / m - \epsilon} \right) \right]^{-1} (+\Lambda - Q/2) \left( 1 + \frac{Q(\Lambda - Q/2)}{4(\alpha^2 + \Lambda^2)} \right). \tag{4.64}
\]

The assumed condition $Q^2 \ll 4\alpha^2 + 4\Lambda^2$ means that the final term on the right hand side is very little different from $\Lambda - Q/2$, so that the effect of non-zero $Q$ is to replace $\Lambda$ in the binding energy condition \((4.32)\) by $\Lambda - Q/2 < \Lambda$. This reduction of $\Lambda$ will have very little effect on the binding energy, as can be seen in Fig. 4.4.
4.4 Results

4.4.1 Determination of Parameters

Of the parameters in the Hamiltonian (4.1) necessary for our modelling, $g$, $\epsilon$ and $U_{aa}$, it is only the last that can be directly determined experimentally, since the background scattering length, $a_{bg}$, is given by (4.29). The coupling, $g$, and the energy detuning, $\epsilon$, however, need to be derived using other physically measurable quantities.

The s-wave scattering length, $a_s$, is well known for most condensate systems, and for $^{85}$Rb the molecular binding energy $E_b \equiv \hbar^2 \alpha^2 / m$ has been measured for a range of magnetic fields which covers that used to vary the scattering length by means of a Feshbach resonance. Thus, $\alpha$ exists for a range of corresponding experimental values of $a_s$. By matching these to the expressions (4.27) and (4.32), it is possible to determine the necessary sets of values of $g$ and $\epsilon$ for a chosen value of the cutoff $\Lambda$. These have
4.4. Results

In Fig. 4.3 we show the Hamiltonian parameters as functions of the s-wave scattering length calculated in this way, with the binding energy taken from [27], for two different values of the cutoff $\Lambda$. In order to investigate the effect that the choice of $\Lambda$ has on the simulation parameters, we chose to use one value that is roughly on the same order as those used in a typical simulation (as in Chap. 7), and one value that is significantly higher for comparison. As can be seen in Fig. 4.3, the dependence on $\Lambda$ is quite weak.

Fig. 4.3 also shows that the parameter $g$ is essentially a linear function of $a_s^{-1}$, while the energy offset, $\epsilon$, has an inversely quadratic behaviour, similar to that of the binding energy, $E_b$. Looking at Fig. 4.4 it can be seen that $E_b$ and $\epsilon$ are essentially equal except for the very small binding energies which occur at large $a_s$. In fact, since the data show that $g$ is unlikely to be zero at the threshold of binding, where $a_s^{-1} \to 0$, it can be seen from (4.33) that $\epsilon_{\text{threshold}} \neq 0$, and given that for $^{85}\text{Rb}$ the background scattering length is negative, the threshold value of $\epsilon$ is in fact positive.

In panel b) of Fig. 4.4, it can also be seen that $a_s^{-1}$ and $\alpha$ become very close, but when equality approaches at weak binding, the mean field effect of the Bose–Einstein condensate used in the experimental measurement obscures the equality, which was also noted in [27].

4.4.2 Validity of the Effective Range Expansion

Using (4.65) and (4.66) we can now estimate the validity of the effective range expansion in Sect. 4.2.3(b). In Fig. 4.5 we plot the ratio of the effective range expansion, 

$$K \cot \delta \approx 1/a_s + r_0 K^2/2$$

and the exact expression for $K \cot \delta$, given by the inverse of the real part of the right hand side of (4.21). We can easily see that the effective range expansion is only valid up to $K \approx 0.6 \Lambda$.

---

Note: The In applications to c-field calculations, the cutoff is related to the size of the simulation grid and it is important to choose the grid such that $a_s$ and $E_b$ depend only weakly on the value of $\Lambda$. The results of such calculations should not depend on the choice of $\Lambda$; indeed, in all the simulations we have run, we have never seen any indication that they would. However, a full investigation to prove that the results are completely independent of the value of $\Lambda$ is outside of the scope of the work in this thesis.
CHAPTER 4. Atom-Molecule Formalism

Figure 4.4: a) The ratio $E_b/\epsilon$ plotted for cutoff values $\Lambda = 2.2 \times 10^6 \text{ m}^{-1}$ (hollow black circles) and $\Lambda = 1 \times 10^7 \text{ m}^{-1}$ (solid red circles). This ratio is seen to be very close to 1, deviating only at scattering lengths of more than about $5 \times 10^{-8} \text{ m} \approx 1000 a_0$. The deviation at larger scattering lengths depends strongly on the choice of cutoff $\Lambda$, and is also affected by mean field effects; b) Plot of $\alpha$ as a function of $a_s^{-1}$; the value of $\alpha$ must approach $a_s^{-1}$ for sufficiently small $\alpha$. However, the data used for these plots is measured in a Bose–Einstein condensate, and the four points corresponding to $a_s^{-1} < 1 \times 10^7 \text{ m}^{-1}$ deviate from this law because of mean field effects specific to that situation. In both plots the parameters are calculated using data of the binding energy and scattering length taken from [27].

Figure 4.5: Ratio of the effective range expansion and the exact expression for $K \cot \delta$. The dash-dotted purple line corresponds to $\Lambda = 10^7 \text{ m}^{-1}$ and the blue solid line corresponds to $\Lambda = 2.2 \times 10^6 \text{ m}^{-1}$. The scattering length is set to $a_s = 900 a_0$ and the effective range is given by equation (4.28).
Chapter 5

Stationary Solutions and Bogoliubov Excitations in Atom-Molecule Systems

In this chapter, we formulate some simple mean-field theory results for a Bose-Einstein condensate close to a Feshbach resonance, described as a coupled atom-molecule system. We use the formalism developed in Chap. 4 and investigate the stationary solutions and the Bogoliubov spectrum for this atom-molecule model.

In Sect. 5.1 we derive the expression for the Thomas–Fermi profiles for the atom-molecule system and compare them to those obtained from the Gross–Pitaevskii equation. In Sect. 5.2 we derive the Bogoliubov–de Gennes equation for our atom-molecule system. In Sect. 5.3 we investigate the excitation spectrum for the simple case of a uniform condensate and compare this with that obtained from a model of structureless atoms. In Sect. 5.4 we apply this formalism to the special case of Bragg scattering from a uniform condensate, and find that for moderate and large scattering lengths, there is a dramatic difference in the shift of the peak of the Bragg spectra, compared to that based on a structureless atom model.

By deriving the Bragg spectrum from Bogoliubov theory, we obtain a benchmark comparison of the behaviour of a Feshbach molecule treatment with that of the structureless atom models, avoiding the numerous complexities which necessarily arise in experiment. We thus can isolate the effects which arise only from the dynamics of the molecular basis of the Feshbach resonance from those which are forced on us by the practicalities of experimental procedure. This chapter is a precursor to Chap. 7 in which full c-field computations of Bragg scattering will be performed, in a way which is directly comparable with experiment of [92].

This chapter is based on the work presented in [110].
5.1 Formalism

The formalism used here is outlined in Chap. 4 and is based on the c-field methods described in Chap. 3.

5.1.1 Phenomenological Hamiltonian for Atom-Molecule System

As introduced in Sect. 4.1, the Hamiltonian of a coupled atom-molecule system is given by

$$\hat{H} = \int dx \left\{ \hat{\psi}^\dagger(x) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_a(x) \right) \hat{\psi}(x) + \hat{\phi}^\dagger(x) \left( -\frac{\hbar^2 \nabla^2}{4m} + V_m(x) + \varepsilon \right) \hat{\phi}(x) \right. $$

$$+ \frac{U_{aa}}{2} \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}(x) + U_{am} \hat{\psi}^\dagger(x) \hat{\phi}^\dagger(x) \hat{\phi}(x) \hat{\psi}(x) $$

$$+ \frac{U_{mm}}{2} \hat{\phi}^\dagger(x) \hat{\phi}^\dagger(x) \hat{\phi}(x) \hat{\phi}(x) + \frac{g}{2} \left( \hat{\phi}^\dagger(x) \hat{\psi}(x) \hat{\psi}(x) + \hat{\psi}^\dagger(x) \hat{\phi}^\dagger(x) \hat{\phi}(x) \right) \right\},$$

(5.1)

where $U_{aa} = 4\pi\hbar^2 a_{bg} / m$ is the background interaction strength, and $V_a$ and $V_m$ are the external trapping potentials for the atoms and molecules, respectively. The terms with factors $U_{am}$ and $U_{mm}$ correspond to atom-molecule and molecule-molecule scattering. However, in the systems considered here, the molecule field arises only during collisions, and is very small, making these terms negligible.

5.1.2 Values of Parameters

The parameters $g$ and $\varepsilon$ are the coupling strength and detuning in the Feshbach resonance, respectively. These are derived in Chap. 4. In our formalism they are given in terms of the experimentally measurable binding energy and s-wave scattering length by

$$g^2 = \frac{8\pi\hbar^4 a_s^2}{m^2} \frac{(\alpha_{bg}(\pi - 2\Lambda a_s) - \pi a_s)(1 - 2\Lambda a_{bg} t(\frac{\pi}{\Lambda})/\pi)}{2\Lambda a_s(1 + t(\frac{\alpha}{\Lambda})) - \pi},$$

(5.2)

$$\varepsilon = \frac{\hbar^2 a_s^2}{2m} \frac{(\pi - 2\Lambda a_s)(1 - 2\Lambda a_{bg} t(\frac{\pi}{\Lambda})/\pi)}{\Lambda a_s(1 + t(\frac{\alpha}{\Lambda})) - \pi},$$

(5.3)

where $t(x) = x - \arctan 1/x$, $\hbar^2 a_s^2 / m$ is the molecule binding energy for a certain value of the s-wave scattering length, $a_s$, and $\Lambda$ is the momentum space cutoff. It is important to note that, in this phenomenological model, the parameters $g$ and $\varepsilon$ take on different values, depending on the proximity to the Feshbach resonance.
5.1. Formalism

Figure 5.1: The Feshbach resonance detuning $\epsilon$, and coupling parameter $g$, as functions of the inverse scattering length. The black circles indicate the values calculated using the experimental data from [27] and equations (5.2) and (5.3). The black lines are fits to these calculated values. The shaded blue areas indicate the range of scattering lengths of interest in the experiment of [92], as well as in the later sections of this chapter. The momentum cutoff is here chosen to be of the same order as that used in a typical simulation in Chap. 7, $\Lambda = 10^6$ m$^{-1}$. Note that the $x$-axis range and value of $\Lambda$ used in these plots are different to those in Fig. 4.3, leading to a difference in appearance of the curves compared to those in that figure.

In this and the following chapters, we will consider a Bose–Einstein condensate of $^{85}$Rb, for which there is experimental data of the binding energy close to the Feshbach resonance at 155 G [27]. For a given momentum cutoff $\Lambda$, we can then calculate the values of the coupling $g$, and detuning $\epsilon$, for each value of the scattering length, using (5.2, 5.3). We fit curves to the values calculated from the experimental data in order to extrapolate to other values of the scattering length. The data, obtained using (5.3, 5.2) are well fitted by a linear relationship between $g$ and $a_s^{-1}$, and a quadratic relationship between $\epsilon$ and $a_s^{-1}$. We show the data and fits in Fig. 5.1.

It is important to note that the most significant points on the fit curve are those for moderate to large scattering lengths, which lie to the left in the plots in Fig. 5.1. This region is important because this is where the dynamics behind the change in scattering length is expected to be significant. These points are not extrapolated, but rather interpolated, since there are data points on both sides of them, and we can easily see that they lie on the fitted curve. The points which are the least interesting, are those for low scattering lengths; these are the ones that are extrapolated in Fig. 5.1. Any change in the fitting technique, would therefore have very little effect on the results discussed in Chap. 7.
CHAPTER 5. STATIONARY SOLUTIONS AND BOGOLIUBOV EXCITATIONS

5.1.3 C-Field Equations

Since the atom field is usually much larger than the molecule field in the situations we shall consider, we can set \( U_{am} \) and \( U_{mm} \) equal to zero and the c-field equations of motion corresponding to the Hamiltonian (5.1) become

\[
\begin{align*}
\frac{i\hbar}{\partial t} \psi(x) & = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_a(x) \right) \psi(x) + U_{aa} |\psi(x)|^2 \psi(x) + g \psi(x)^* \phi(x), \\
\frac{i\hbar}{\partial t} \phi(x) & = \left( -\frac{\hbar^2 \nabla^2}{4m} + \epsilon + V_m(x) \right) \phi(x) + \frac{g^2}{2} \psi^2(x).
\end{align*}
\]

(5.4) (5.5)

In practice, when solving these equations numerically, it is necessary to explicitly use a projector in order to restrict the wavefunctions to the momentum subspace below the cutoff \( \Lambda \), as described in Chap. 4 and implemented in Chap. 7.

The value of the momentum space cutoff \( \Lambda \) will, in the case of numerical simulation, arise from the simulation grid; any such computation is restricted to a finite number of momentum space modes. It is also necessary to introduce a projector in order to avoid effects from aliasing [10]. Furthermore, a momentum cutoff is necessary in order for the pseudo-potential approximation to be valid [14]. However, as we showed in Chap. 4 the actual choice of the cutoff has only a very small effect on the values of the phenomenological Hamiltonian parameters.

5.1.4 Thomas–Fermi Solutions

Stationary solutions to the equations of motion (5.4, 5.5) can be obtained by letting the time evolution of the wavefunctions be

\[
\begin{align*}
\psi(x, t) & = \psi(x) e^{-i\mu_a t/\hbar}, \\
\phi(x, t) & = \phi(x) e^{-i\mu_m t/\hbar}.
\end{align*}
\]

(5.6) (5.7)

It is clear that \( \mu_m = 2\mu_a \) in order for the coupling terms to be time-independent, so we get

\[
\begin{align*}
\mu_a \psi(x) & = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_a(x) \right) \psi(x) + U_{aa} |\psi(x)|^2 \psi(x) + g \psi(x)^* \phi(x), \\
2\mu_a \phi(x) & = \left( -\frac{\hbar^2 \nabla^2}{4m} + \epsilon + V_m(x) \right) \phi(x) + \frac{g^2}{2} \psi^2(x).
\end{align*}
\]

(5.8) (5.9)

As discussed in Sect. 2.1.6 the Thomas–Fermi limit is characterised by the kinetic energy of the system being negligible in comparison to the interaction energy. The kinetic term, given by the Laplacian, can therefore be neglected. Taking the Thomas–Fermi
5.1. Formalism

Figure 5.2: Thomas–Fermi profiles for a spherically symmetric condensate of $^{85}$Rb for two different scattering lengths: $a_s = 856a_0$ (left panel) and $a_s = 2133a_0$ (right panel). The trapping frequency is $\omega_r = 2\pi \times 17.5$ Hz, and the total particle number — counting each molecule as two atoms — is $10^5$. The blue solid lines are the atom Thomas–Fermi profiles from (5.10), the green solid lines are the molecule profiles given by (5.11), and the black dashed lines are the Thomas–Fermi profiles obtained from the Gross–Pitaevskii equation (GPE) for structureless atoms. The parameter $r_0$ is the length scale associated with the trap, given by $r_0 = \sqrt{\hbar/2m\omega_r}$ (see Sect. 6.2).

limit and solving for $\psi$ and $\phi$ gives the Thomas–Fermi solutions:

$$|\psi_s(x)| = \sqrt{\frac{\mu_a - V_a(x)}{U_{aa} + \frac{g^2}{2(2\mu_a - \epsilon - V_m(x))} \psi^2(x)}}$$

(5.10)

$$\phi_s(x) = \frac{g}{2(2\mu_a - \epsilon - V_m(x))^{1/2}}$$

(5.11)

Fig. 5.2 shows the Thomas–Fermi wavefunctions for a spherically symmetric condensate of $10^5$ atoms of $^{85}$Rb. The Thomas–Fermi solution for the atom wavefunction is similar to that for the structureless model for the same atom number and scattering length (also shown in the figure), with the important difference that the denominator has a spatial dependence. As long as the scattering length is moderate (left panel of Fig. 5.2), the detuning, $\epsilon$, will be large and the molecular trapping potential will be negligible in comparison, making the atom-molecule Thomas–Fermi solution indistinguishable from the standard Thomas–Fermi solution. However, for very large scattering lengths (right panel of Fig. 5.2), the detuning $\epsilon$ will be small enough for the molecular trapping potential to be significant, making the atom-molecule Thomas–Fermi profile different from that of the structureless atom model.

Also, note that in equation (5.10), since the potential $V_m(x)$ is normally negligible
Figure 5.3: Radial density for a spherically symmetric condensate of $^{85}$Rb for two different scattering lengths: $a_s = 856a_0$ (left panel) and $a_s = 2133a_0$ (right panel). The system is the same as that in Fig. 5.2. For this system, the portion of atoms in the form of molecules is approximately 0.6% for $a_s = 856a_0$ and 4.5% for $a_s = 2133a_0$. (Note: At first glance, it appears that the solution $\psi_{GPE}$ (dashed line) has fewer atoms, than that given by the atom-molecule model, but, as can be seen in the right hand figure, the discrepancy in the centre is compensated by the wings, where the extra factor of $4\pi r^2$ becomes more significant.)

compared to $2\mu_a - \epsilon$, the Thomas–Fermi solution for the atomic field is essentially of the same form as that for the Gross–Pitaevskii equation at the same chemical potential. However, for the same total number of atoms — counting each molecule as two atoms — the chemical potential for the Gross–Pitaevskii equation is slightly different from that found in this model. As well as this, the molecule field corresponds to the number of elementary molecules, and each physical molecule is a superposition of an elementary molecule and an atom pair, as discussed in Chap. 4. Closer to the Feshbach resonance, the proportion of atom pairs can become more than 50%, although in the systems we study here, these effects will be so small that they can be neglected.

The atom density of the condensate in the Thomas–Fermi limit is given by

\[ n(x) = |\psi_s(x)|^2 + 2|\phi_s(x)|^2. \]  

Fig. 5.3 shows the radial density profile for a spherically symmetric condensate of $10^5$ atoms of $^{85}$Rb in the Thomas–Fermi limit. For comparison we have also plotted the Thomas–Fermi density profile obtained from a structureless atom model for the same scattering length and atom number.
5.2 Quasiparticle Excitations

As discussed in Sect. 2.1.7, in the Bogoliubov approximation, the field operator can be separated into a mean-field ground state and an operator part describing the excitations. In our coupled system, we expand the atom and molecule fields in terms of quasi-particle bases as

\[
\begin{pmatrix}
\psi(x,t) \\
\phi(x,t)
\end{pmatrix} = \begin{pmatrix}
\psi_0(x) \\
\phi_0(x)
\end{pmatrix} + \sum_p \begin{pmatrix}
u_p^*(x) \\
sp_p^*(x)
\end{pmatrix} \hat{b}_p e^{-i\omega_p t} + \begin{pmatrix}u_p(x) \\
r_p(x)
\end{pmatrix} \hat{b}_p e^{i\omega_p t},
\]

(5.13)

where the first terms are the condensate atom and molecule ground state wavefunctions, and \(\hat{b}_p\) and \(\hat{b}_p^\dagger\) are the quasi-particle destruction and creation operators respectively. Unlike the standard Bogoliubov expansion of Sect. 2.1.7, where the only mixture is between the atom creation and destruction terms, in this case it is also necessary to include the molecule creation and destruction terms. The quasi-particle operators in this expansion thus have both atom and molecule components.

5.2.1 Two-Component Bogoliubov–de Gennes Equations

Making these substitutions to the equations of motion (5.4, 5.5) gives, after collecting terms with the same phase, the two-component Bogoliubov–de Gennes equations

\[
\mathcal{L} U_p + \mathcal{M} V_p = \hbar \omega_p U_p,
\]

(5.14)

\[
\mathcal{L} V_p + \mathcal{M}^\dagger U_p = -\hbar \omega_p V_p,
\]

(5.15)

where \(U_p = (u_p(x), r_p(x))^T\) and \(V_p = (v_p(x), s_p(x))^T\). Here \(\mathcal{L}\) is Hermitian, but \(\mathcal{M}\) need not be Hermitian. In our case they are given by

\[
\mathcal{L} = \begin{pmatrix}
-\frac{\hbar^2 c^2}{2m} + V_a(x) - \mu_a + 2 U_{a0}|\psi_0(x)|^2 & g \psi_0(x) \\
g \psi_0^*(x) & -\frac{\hbar^2 c^2}{4m} + \varepsilon + V_m(x) - 2\mu_a
\end{pmatrix},
\]

(5.16)

\[
\mathcal{M} = \begin{pmatrix}
U_{a0}|\psi_0(x)|^2 + g \phi_0(x) & 0 \\
0 & 0
\end{pmatrix}.
\]

(5.17)

When \(\psi_0\) and \(\phi_0\) are chosen to be real, both \(\mathcal{L}\) and \(\mathcal{M}\) are Hermitian; in fact they are also symmetric. The multi-component equations (5.14, 5.15) are strikingly similar to the single-component ones. Indeed, if we let \(g \rightarrow 0\) in these equations, the upper components obey the standard Bogoliubov–de Gennes equation for a single atom field.
5.2.2 Orthogonality and Normalisation Conditions

The normalisation and orthogonality conditions of the quasi-particle amplitudes can be derived by using the symmetry properties of $L$ and $M$. The orthogonality conditions of the quasi-particle amplitudes can be derived by writing

$$\hbar \omega_p \int dx \left( U_{p'}^\dagger U_p - V_{p'}^\dagger V_p \right) = \int dx U_{p'}^\dagger \left( L U_p + M V_p \right)$$
\hspace{1cm} + \int dx V_{p'}^\dagger \left( L V_p + M^\dagger U_p \right), \quad (5.18)$$

$$\hbar \omega_{p'} \int dx \left( U_{p}^\dagger U_{p'} - V_{p}^\dagger V_{p'} \right) = \int dx \left( U_{p'}^\dagger L + V_{p'}^\dagger M^\dagger \right) U_p$$
\hspace{1cm} + \int dx \left( V_{p}^\dagger L^\dagger + U_{p}^\dagger M \right) V_{p'} \label{eq:5.19}.$$ (5.19)

The Hermitian nature of $L$ means that the two right hand sides are equal so that, for an appropriate normalisation, we can write

$$\int dx \left( U_{p'}^\dagger U_p - V_{p'}^\dagger V_p \right) = \delta_{p,p'} \label{eq:5.20}.$$ (5.20)

Since both $L$ and $M$ are symmetric, we can then write

$$\hbar \omega_{p'} \int dx \left( V_p^T U_{p'} - U_p^T V_{p'} \right) = \int dx V_p^T \left( L U_{p'} + M V_{p'} \right)$$
\hspace{1cm} + \left( U_p^T L^\dagger + M^\dagger U_p \right), \quad (5.21)$$

$$\hbar \omega_p \int dx \left( V_{p'}^T U_p - U_{p'}^T V_p \right) = -\int dx \left( V_{p'}^T L + U_{p'}^T M^\ast \right) U_p$$
\hspace{1cm} - \left( U_p^T L + V_p M \right) V_{p'}, \quad (5.22)$$

so that, assuming $\omega_p \neq -\omega_{p'}$, we can say

$$\int dx \left( V_{p'}^T U_p - U_{p'}^T V_p \right) = 0. \quad (5.23)$$

We can also find normalisation conditions using the Bose commutation relations for the components of $\psi = (\psi, \phi)^T$:

$$\delta_{\alpha,\beta} \delta(x - x') = \left[ \psi_\alpha(x), \psi_\beta^\dagger(x') \right]$$
\hspace{1cm} = \sum_{p,p'} \left\{ U_{\alpha,p}(x) U_{\beta,p'}^*(x') \left[ \hat{b}_p(x), \hat{b}_p^\dagger(x') \right] \right.$$\hspace{1cm} + $V_{\alpha,p}(x) V_{\beta,p'}^*(x') \left[ \hat{b}_p(x), \hat{b}_p^\dagger(x') \right]$
\hspace{1cm} + $U_{\alpha,p}(x) V_{\beta,p'}(x') \left[ \hat{b}_p(x), \hat{b}_p(x') \right]$. \hspace{1cm}
\[ + V_{\alpha,p}(x) U_{\beta,p'}(x') \left\{ \hat{b}_p(x), \hat{b}_{p'}^+(x') \right\}, \quad (5.24) \]

from which, assuming that the quasi-particle operators \( \hat{b}_p \) obey the usual Bose commutation relations, we obtain the normalisation condition of the amplitudes,

\[ \sum_p \left( U_{\alpha,p} U_{\beta,p}^* - V_{\alpha,p} V_{\beta,p}^* \right) = \delta_{\alpha\beta}. \quad (5.25) \]

Similarly, the other commutation relation,

\[ 0 = \left[ \psi_\alpha(x), \psi_\beta(x') \right] \]

\[ = \sum_{p,p'} \left\{ U_{\alpha,p}(x) U_{\beta,p'}(x') \left[ \hat{b}_p(x), \hat{b}_{p'}(x') \right] + V_{\alpha,p}(x) V_{\beta,p'}^*(x') \left[ \hat{b}_p^+(x), \hat{b}_{p'}^+(x') \right] + U_{\alpha,p}(x) V_{\beta,p'}^*(x') \left[ \hat{b}_p^+(x), \hat{b}_{p'}^+(x') \right] + V_{\alpha,p}(x) U_{\beta,p'}(x') \left[ \hat{b}_p^+(x), \hat{b}_{p'}(x') \right] \right\}, \quad (5.26) \]

gives the condition

\[ \sum_p \left( U_{\alpha,p} V_{\beta,p}^* - V_{\alpha,p}^* U_{\beta,p} \right) = 0. \quad (5.27) \]

The four conditions (5.20, 5.23, 5.25, 5.27) are related; indeed (5.25) and (5.27) can be derived from (5.20) and (5.23).

### 5.3 Uniform Condensate

For the case of a uniform condensate, the Thomas–Fermi solutions (5.10, 5.11) are constant and give

\[ \psi_0 = \sqrt{\frac{\mu_a}{\mu_a + g^2/2(2\mu_a - \epsilon)}} \equiv \sqrt{n_a}, \quad (5.28) \]

\[ \phi_0 = \frac{g}{2(2\mu_a - \epsilon)} \psi_0^2 \equiv \sqrt{n_m}, \quad (5.29) \]

where we have chosen \( \psi_0 \) to be real and positive. The quasi-particle amplitudes can be expressed as plane waves, according to

\[ u_{k,l}(x) \rightarrow \frac{u_{k,l}e^{i k \cdot x}}{\sqrt{V}}, \quad (5.30) \]

\[ v_{k,l}^*(x) \rightarrow \frac{v_{k,l}^*e^{-i k \cdot x}}{\sqrt{V}}, \quad (5.31) \]
Section 5.3.1 Eigenvalues of the Bogoliubov–de Gennes Equations

The eigenvalues of the Bogoliubov–de Gennes equations are now given by solving the linear system (5.14, 5.15), using the uniform expressions of $L$ and $M$ given by (5.34, 5.35).

In order to express the solutions explicitly in a simple form, we follow a somewhat intricate procedure:

**A:** Define the quantities

\[
\mathcal{R} = \mathcal{L}_{11}^2 - \mathcal{M}_{11}^2 + \mathcal{L}_{22}^2, \\
S = (\mathcal{L}_{11}^2 - \mathcal{M}_{11}^2 - \mathcal{L}_{22}^2)^2 + 4\mathcal{L}_{12}^2 ((\mathcal{L}_{11} + \mathcal{L}_{22})^2 - \mathcal{M}_{11}^2). \tag{5.36, 5.37}
\]

**B:** Define the quantities $K^l$ and $K^h$ as the smallest and largest positive values of $|\mathbf{k}|$ for which $S = 0$. 

**Equations:**

\[
\begin{align*}
    r_{k,l}(x) & \rightarrow \frac{r_{k,l}e^{ikx}}{\sqrt{V}}, \\
    s_{k,l}^*(x) & \rightarrow \frac{s_{k,l}^*e^{-ikx}}{\sqrt{V}},
\end{align*}
\]  

where $V$ is the volume of the system and $l$ can take on two discrete values, as discussed below.

In this case, we can express $L$ and $M$ as

\[
L = \begin{pmatrix}
\frac{\hbar^2 k^2}{2m} & -\mu_a + 2U_{aa}n_a \\
g\sqrt{n_a} & \frac{\hbar^2 k^2}{4m} + \epsilon - 2\mu_a
\end{pmatrix}, \tag{5.34}
\]

\[
M = \begin{pmatrix}
U_{aa}n_a + g\sqrt{n_m} & 0 \\
0 & 0
\end{pmatrix}. \tag{5.35}
\]
C: For the range of values of $|k|$ given by $0 \leq |k| \leq K^l$, 

$$\omega_{k,A} = \frac{1}{\sqrt{2}} \sqrt{\mathcal{R} - \sqrt{\mathcal{S}}}, \quad (5.38)$$

$$\omega_{k,M} = -\frac{1}{\sqrt{2}} \sqrt{\mathcal{R} + \sqrt{\mathcal{S}}}. \quad (5.39)$$

D: For the range of values of $|k|$ given by $K^l \leq |k| \leq K^h$, 

$$\omega_{k,A} = \frac{1}{\sqrt{2}} \sqrt{\mathcal{R} - i\sqrt{|\mathcal{S}|}}, \quad (5.40)$$

$$\omega_{k,M} = -\frac{1}{\sqrt{2}} \sqrt{\mathcal{R} + i\sqrt{|\mathcal{S}|}}. \quad (5.41)$$

E: For the range of values of $|k|$ given by $K^h \leq |k|$, 

$$\omega_{k,A} = \frac{1}{\sqrt{2}} \sqrt{\mathcal{R} + \sqrt{\mathcal{S}}}, \quad (5.42)$$

$$\omega_{k,M} = -\frac{1}{\sqrt{2}} \sqrt{\mathcal{R} - \sqrt{\mathcal{S}}}. \quad (5.43)$$

Fig. 5.4 shows the eigenvalues calculated using this procedure for a uniform condensate of $^{85}\text{Rb}$ with a total density of $n \equiv n_A + 2n_m = 10^{20} \text{ m}^{-3}$ at a scattering length of $900a_0$. Here, we use the experimental values of the binding energy taken from [27] to determine $\epsilon$ and $g$, using (5.3, 5.2). The momentum is measured in units of the momentum $q$ of the Bragg pulse in the experiment of Papp et al. [92], where $q = 1.6 \times 10^7 \text{ m}^{-1}$. The following points should be noted:

1. As can be seen clearly in the figure, the atomic eigenvalue, $\omega_{k,A}$, is similar to that obtained from the Gross–Pitaevskii equation, but is slightly shifted from this, due to the coupling between the atoms and the molecules. This shift is not dramatic, but is still measurable, for example by using Bragg scattering, as in the experiment of [92].

2. The atomic eigenvalue, $\omega_{k,A}$, belongs to the atom-dominated state. The energy to create an atom-dominated quasi-particle is thus $\hbar \omega_{k,A}$.

3. Similarly, the energy to create a molecule-dominated quasi-particle is given by $\hbar \omega_{k,M}$. Since $\omega_{k,M}$ is related to the binding energy of the molecules, and $\epsilon$ is negative, $\omega_{k,M}$ is also negative. Thus, the energy to create a molecule-dominated
Figure 5.4: Real part of eigenvalues $\omega_{k,A}$ (blue solid line) and $\omega_{k,M}$ (green solid line) as functions of the momentum, $k$, for $^{85}$Rb at 900$a_0$. The atom-dominated eigenvalue is similar to that obtained from the Gross–Pitaevskii equation (grey solid line), whereas the molecule-dominated eigenvalue is related to the molecule field detuning, $\varepsilon$, (grey dash-dotted line). The shaded area is the region given by $K^l < k < K^h$, in which the eigenvalues have a non-zero imaginary part. The total density of the condensate is here $10^{20}$ m$^{-3}$ and $q$ is $1.6 \times 10^7$ m$^{-1}$.

quasi-particle is *negative*, and increases with $|k|$, which is expected for a bound state.

4. The eigenvalue $\omega_{k,M}$ has the same general behaviour as $\omega_{k,A}$, but since it is related to the binding energy of the molecules, it is shifted downwards. As $k \to 0$, and as long as the density is moderate, $\omega_{k,M}$ can be approximated by

$$\hbar \omega_{0,M} \approx \varepsilon + 2U_{aa} n - 4\mu_a,$$

(5.44)

and as $n \to 0$, it will approach the value of the molecule field detuning $\varepsilon$.

### 5.3.2 High Momentum Instability

As can be seen in Fig. 5.4, there is a crossover which occurs when $\omega_{k,A} + \omega_{k,M} = 0$, where the energy to simultaneously create a molecular-dominated quasi-particle and an atom-dominated quasi-particle is zero. As one proceeds through the crossover, the eigenvalue formula is determined successively by the procedures C, D and E, as given
5.3. Uniform Condensate

The midpoint of the crossover region is at the momentum
\[ \frac{\hbar^2 k^2}{2m} = 2\mu_a - \frac{2}{3} (2U_{aa} n + \epsilon). \]  

Fig. 5.4 shows the behaviour of the eigenvalues in the crossover region, where each eigenvalue has an imaginary part. The maximum amplitude of the imaginary parts of the eigenvalues is approximately 1.5 kHz. For this system, we would therefore expect a relatively fast instability to occur — on a time scale of approximately 0.07 ms — with atom-molecule pairs being created and destroyed.

The instability arises because the energy to create a molecular quasi-particle of momentum \( k \) becomes equal to the energy to destroy an atomic quasi-particle of momentum \( -k \). In this model, this is a natural instability to expect; it provides a mechanism for the condensate, which is metastable when the underlying interaction is attractive, to achieve the true ground state of the model, a condensate of molecules. The relatively high value of the momentum required would make this a very much less important phenomenon in a trapped condensate, since the wavefunctions of high energy quasi-particles are largely located outside of the condensate. Since the transformation can only take place where there is a condensate, this would significantly decrease the size of the imaginary part.
5.3.3 Eigenvectors of the Bogoliubov–de Gennes Equations

Using the normalisation condition \(5.25\), we can find a unique set of eigenvectors of the Bogoliubov–de Gennes equations corresponding to the eigenvalues \(5.38–5.43\):\[
\begin{align*}
\text{For } l = A, M, \\
u_{k,l} &= A_{k,l} u_{k,l}, \\
r_{k,l} &= B_{k,l} u_{k,l}, \\
s_{k,l} &= C_{k,l} v_{k,l},
\end{align*}
\]
where
\[
\begin{align*}
A_{k,l} &= \frac{1}{N_{11}} \left( -\mathcal{L}_{11} + \hbar \omega_{k,l} - \frac{\mathcal{L}_{12}^2}{\hbar \omega_{k,l} - \mathcal{L}_{22}} \right), \\
B_{k,l} &= \frac{\mathcal{L}_{12}}{\hbar \omega_{k,l} - \mathcal{L}_{22}}, \\
C_{k,l} &= -\frac{\mathcal{L}_{12}}{\hbar \omega_{k,l} + \mathcal{L}_{22}}.
\end{align*}
\]

The components of the eigenvectors for the same system as that in Fig. 5.4 are plotted in Fig. 5.6 as a function of the scattering length, for low momentum (Fig. 5.6(a)) and moderate momentum (Fig. 5.6(b)). At low scattering lengths, the eigenvector corresponding to the low eigenvalue \(\omega_{k,A}\) is dominated by the atom components \(u_{k,A}\) and \(v_{k,A}\), with the molecule components \(r_{k,A}\) and \(s_{k,A}\) becoming more significant the larger the scattering length. For larger scattering lengths, the amplitude of the molecule destruction operator is clearly significant compared to the atom one, and there is a large portion of molecules in the atom state.

For the higher eigenvalue \(\omega_{k,M}\), the situation is reversed with the dominating eigenvector component being the one associated with the molecule destruction operator. Here, we also see increased mixing between the two states as the scattering length is increased.
5.4. Application to Bragg Scattering

The quasi-particle description of the excitations in our atom-molecule system can be used to describe the excitation spectrum from Bragg scattering. Following the procedure of [9] and [121], we derive the momentum transferred onto the condensate from a Bragg pulse, and compare the results we obtain here to those in [9].

The equations of motion for the coupled atom and molecule fields subject to a
Bragg pulse are given by
\[
\begin{align*}
\frac{i\hbar}{\partial t} \frac{\partial \psi(x)}{\partial t} &= \left( -\frac{\hbar^2 \nabla^2}{2m} + V_a(x) \right) \psi(x) + U_{aa}|\psi(x)|^2 \psi(x) + \hbar V_{opt} \psi(x) + g\psi(x)^* \phi(x), \\
\frac{i\hbar}{\partial t} \frac{\partial \phi(x)}{\partial t} &= \left( -\frac{\hbar^2 \nabla^2}{4m} + \epsilon + V_m(x) \right) \phi(x) + 2\hbar V_{opt} \phi(x) + \frac{g}{2} \psi^2(x),
\end{align*}
\]
(5.54)
(5.55)
where
\[
V_{opt} = V_0(t) \cos(q \cdot x - \omega t),
\]
(5.56)
and \(V_0, q\) and \(\omega\) are the intensity, the momentum and the frequency of the Bragg pulse, respectively [8].

### 5.4.1 Quasiparticle Evolution

Using the expansion (5.13) and the Bogoliubov–de Gennes equations (5.14, 5.15), we can write the equations of motion
\[
\begin{align*}
\sum_p \left( U_{p'}^* \hat{b}_p e^{-i\omega_p t} + V_{p'}^* \hat{b}_p^* e^{i\omega_p t} \right) = V_{opt}\psi,
\end{align*}
\]
(5.57)
where
\[
V_{opt} = V_{opt} \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix},
\]
(5.58)
and \(\psi = (\psi, \phi)^T\). Similarly to the method in [83], we can project out \(b_p\) from the above equation by writing
\[
\int dx \left\{ \left( U_{p'}^* V_{opt} \psi + V_{p'}^* V_{opt} \psi^* \right) \right\} = \int dx \sum_p \left\{ iU_{p'}^* \left( U_{p'} \hat{b}_p e^{-i\omega_p t} + V_{p'}^* \hat{b}_p^* e^{i\omega_p t} \right) - iV_{p'}^* \left( U_{p'}^* \hat{b}_p e^{i\omega_p t} + V_{p'} \hat{b}_p^* e^{-i\omega_p t} \right) \right\},
\]
(5.59)
\[
= i \sum_p \int dx \left( U_{p'}^* U_p - V_{p'}^* V_p \right) \hat{b}_p e^{-i\omega_p t} + \int dx \left( U_{p'}^* \psi^* - V_{p'}^* U_p^* \right) \hat{b}_p^* e^{i\omega_p t} \right\},
\]
(5.60)
\[
= i \hat{b}_{p'}(t) e^{-i\omega_{p'} t},
\]
(5.61)
where on the last line we have used the normalisation and orthogonality conditions (5.20, 5.23). We therefore have
\[
\hat{b}_{p'}(t) = -ie^{i\omega_{p'} t} \int dx \left\{ \left( U_{p'}^* V_{opt} \psi + V_{p'}^* V_{opt} \psi^* \right) \right\}.
\]
(5.62)
(5.63)
Setting $\psi = (\psi_0, \phi_0)^T$, we obtain

$$b_p(t) = -i \int_0^t e^{i\omega_p t'} dt' \int dx \left\{ V_{opt} \left( \psi_0(u_p^* + v_p^*) + 2\phi_0(r_p^* + s_p^*) \right) \right\}. \quad (5.64)$$

Assuming that the Bragg pulse is square, with amplitude $V_0$ and duration $T$, we obtain

$$b_p(T) = -i V_0 \int dx \left( \psi_0(u_p^* + v_p^*) + 2\phi_0(r_p^* + s_p^*) \right)$$

$$\times \int_0^T dt' e^{i\omega_p t'} \left( e^{i(q \cdot x - \omega t')} + e^{-i(q \cdot x - \omega t')} \right), \quad (5.65)$$

which is equal to

$$b_p(T) = -i V_0 e^{i\omega_p T/2} \int dx \left( \psi_0(u_p^* + v_p^*) + 2\phi_0(r_p^* + s_p^*) \right)$$

$$\times \left[ e^{-i\omega T/2} e^{i q \cdot x} \frac{\sin((\omega_p - \omega) T/2)}{\omega_p - \omega} \right.$$

$$\left. + e^{i\omega T/2} e^{-i q \cdot x} \frac{\sin((\omega_p + \omega) T/2)}{\omega_p + \omega} \right]. \quad (5.66)$$

### 5.4.2 Momentum Transfer from Uniform Condensate

For the ideal case of Bragg scattering from a uniform condensate, the quasi-particle amplitudes are given by (5.46–5.50), and the ground state is given by (5.10, 5.11). The expression for $b_p$ now simplifies to

$$b_p(T) = -i V_0 e^{i\omega_p T/2} \int dx \left( \sqrt{N_a}(u_p^* + v_p^*) + 2\sqrt{N_m}(r_p^* + s_p^*) \right) e^{i k \cdot x}$$

$$\times \left[ e^{-i\omega T/2} \frac{\sin((\omega_p - \omega) T/2)}{\omega_p - \omega} e^{i q \cdot x} + e^{i\omega T/2} \frac{\sin((\omega_p + \omega) T/2)}{\omega_p + \omega} e^{-i q \cdot x} \right], \quad (5.67)$$

$$= -i V_0 \left( \sqrt{N_a}(u_p^* + v_p^*) + 2\sqrt{N_m}(r_p^* + s_p^*) \right)$$

$$\times \left[ e^{i(\omega_p - \omega) T/2} \frac{\sin((\omega_p - \omega) T/2)}{\omega_p - \omega} \delta_{p,-q} + e^{i(\omega_p + \omega) T/2} \frac{\sin((\omega_p + \omega) T/2)}{\omega_p + \omega} \delta_{p,q} \right], \quad (5.68)$$

where $N_a$ and $N_m$ are the number of atoms and molecules, respectively.

The total momentum imparted to the condensate can now be evaluated using the Bogoliubov expansions (5.13), and the normalisation and orthogonality relations (5.20, 5.23, 5.25),

$$P(T) = \frac{\hbar}{2i} \int dx \left\{ \psi^* \nabla \psi + \frac{1}{2} \phi^* \nabla \phi \right\} + \text{c.c.}$$
Figure 5.7: Bragg spectrum showing the momentum transfer of the condensate as a function of the Bragg frequency for a uniform system of 40,000 $^{85}\text{Rb}$ atoms. Here, we show the spectra for three different scattering lengths: $a_s = 100a_0$ (green dashed-dotted line), $a_s = 700a_0$ (red dashed line) and $a_s = 1000a_0$ (blue solid line). The grey dotted line indicates the free particle resonance position $\omega_0$. The duration of the Bragg pulse is $T = 0.1\text{ms}$, and the intensity of the pulse is $V_0 = 2\pi \times 1\text{ kHz}$.

Figure 5.7 shows the fraction of particles being scattered out of the condensate during the Bragg pulse for three different scattering lengths. The portion of scattered particles is related to the momentum transfer as $P/\hbar q N$, where $N \equiv N_a + 2N_m$ is the total num-

\[
\begin{align*}
\sum_p \hbar p \left( |b_p(T)|^2 + \frac{1}{2} |b_p(T)|^2 \right) &= 3\hbar q V_0^2 \sum_l \left[ \left( \frac{\sin((\omega_{q,l} - \omega)T/2)}{\omega_{q,l} - \omega} \right)^2 - \left( \frac{\sin((\omega_{q,l} + \omega)T/2)}{\omega_{q,l} + \omega} \right)^2 \right] \\
&\times \left| \sqrt{N_a (u_q + v_q)} + 2 \sqrt{N_m (r_q + s_q)} \right|^2, \quad (5.69)
\end{align*}
\]

where, as previously, the subscript $l = A, M$ denotes the two different eigenvalues. This expression will have its maximum values at the points where $\omega = \pm \omega_{q,l}$, and if the atom field is much larger than the molecular field — as is the case for the system studied here — then the only significant maximum will be at the lower eigenvalue $\omega_{k,A}$. Consequently, the Bragg resonance peak will occur at the eigenvalue of the atom state ($\omega_{k,A}$ in Fig. 5.4), corresponding to the momentum of the Bragg pulse.
5.4. Application to Bragg Scattering

Scattering length $a_s$\[a_0\]

Figure 5.8: The shift of the peak of the Bragg spectra from that of the non-interacting gas, plotted against the scattering length, $a_s$. The blue solid line is based on the peak position calculated by (5.69), and the black dashed line is the equivalent calculation based on the model of structureless atoms, as in [9]. The black triangles mark the values of the scattering length for which Claussen et al. [27] give experimental data for the binding energy.

Fig. 5.8 shows how the shift of the Bragg resonance from the free particle resonance changes with the increase in the scattering length. This can easily be calculated, since we see from (5.69) that the peak of the Bragg spectrum will be located at $\omega_A$. The shift is therefore given by $\Delta \omega = \omega_A - \omega_0$, where $\omega_0$ is the free particle resonance. For comparison, in Fig. 5.8, we have also plotted the result based on the model of a condensate of structureless atoms with increased scattering length, as shown in Sect. 2.4.7. The two models agree well for low scattering lengths, but differ dramatically for larger scattering lengths. In the figure we have also marked the scattering lengths for which there is available data of the binding energy, as in [27]. The values outside of these are calculated by the method described in Sect. 5.1.

The Bragg peak shift obtained from our model of a coupled atom-molecule condensate is significantly different from that obtained by a model of structureless atoms. Even though it describes the ideal case of Bragg scattering from a uniform condensate
and is therefore not directly comparable to that obtained in the experiment of Papp et al. [92], it is still qualitatively similar to the experimental result. Most importantly, unlike other approaches to this problem, for example that by Kinnunen et al. [63], the line shift in Fig. 5.8 shows a clear downward behaviour for large scattering lengths, just like the one reported in [92]. This will be discussed in greater detail in Sect. 7.1.
Chapter 6

Numerical Methods

In this chapter, we outline the methods that we use to numerically implement the formalism which is presented in Chap. 4. In Sect. 6.1, we briefly review the formalism that is being implemented and present the equations of motion that describe the dynamics of our system. In Sect. 6.2, we go on to discuss the reformulation of the equations of motion in terms of dimensionless quantities, which is necessary for the implementation. In Sect. 6.3, we outline a method for obtaining the stationary solutions to the equations of motion, which we use as the initial states in the simulations.

In Sect. 6.4, we describe the method we use for the numerical integration of the projected Gross–Pitaevskii equation. We also discuss how to choose the simulation parameters for our system. Then in Sect. 6.5, we show how to divide the simulation into disjoint bands in momentum space, as is necessary for the case of Bragg scattering.

In Sect. 6.6, we go on to demonstrate how to relate the renormalisation constant used in our formalism to the cutoff arising from the simulation grid. Finally, in Sect. 6.7, we show how to calculate observable averages from a set of c-field trajectories.

The results of the simulations are presented in Chap. 7.

6.1 Formalism

As described in Chap. 4, in order to model the Feshbach resonance bound state, we add an additional field, corresponding to a bound atom pair (referred to as a “molecule”), to the usual Hamiltonian for a trapped system of interacting bosons. The equations of motion for the atom $\psi$ and molecule $\phi$ fields in the resulting c-field model are given by

$$i\hbar \frac{\partial \psi(x)}{\partial t} = -\frac{\hbar^2 \nabla^2}{2m} \psi(x) + \mathcal{P}_a \{ V_a(x) \psi(x) + U_{a\alpha} |\psi(x)|^2 \psi(x) + g \psi^*(x) \phi(x)$$

$$-i\gamma \left( |\psi(x)|^2 + 2|\phi(x)|^2 \right) \psi(x) \},$$

(6.1)
\[ i\hbar \frac{\partial \phi(x)}{\partial t} = -\frac{\hbar^2 \nabla^2}{4m} \phi(x) + \mathcal{P}_m \left\{ (\epsilon + V_m(x)) \phi(x) + \frac{g}{2} \psi^2(x) \right\}, \]  

(6.2)

where \( U_{aa} = 4\pi \hbar^2 a_{bg} / m \) is the background interaction strength, and \( V_a \) and \( V_m \) are the external trapping potential for the atoms and molecules respectively. The last term in (6.1) is added to account for losses from the condensate due to three-body recombination events [90]; we discuss this more extensively in Sect. 7.2.5.

### 6.1.1 Parameters

The parameters \( g \) and \( \epsilon \) are the coupling strength and detuning in the Feshbach resonance, respectively. As is shown in Chap. 4, they are in our formalism given by

\[
\epsilon = \frac{\hbar^2 a^2 \left( \pi - 2\Lambda a_s \right) \left( 1 - \frac{2\Lambda a_{bg}}{\pi} t\left(\frac{\alpha}{\Lambda}\right) \right)}{2m \left( \Lambda a_s (1 + t\left(\frac{\alpha}{\Lambda}\right)) - \pi \right)}, \quad (6.3)
\]

\[
g^2 = \frac{8\pi \hbar^4 a^2 \left( a_{bg} (\pi - 2\Lambda a_s) - \pi a_s \right) \left( 1 - \frac{2\Lambda a_{bg}}{\pi} t\left(\frac{\alpha}{\Lambda}\right) \right)}{2\Lambda a_s (1 + t\left(\frac{\alpha}{\Lambda}\right)) - \pi}. \quad (6.4)
\]

where \( t(x) = x - \arctan \frac{1}{x} \), and \( h^2 a^2 / m \) is the molecule binding energy for a certain value of the s-wave scattering length \( a_s \). The parameter \( \Lambda \) is the renormalisation factor, determined by the momentum space cutoffs, as we shall show in Sect. 6.6.

As is shown in Sect. 2.4, the effect of the Bragg field on the condensate is included by making the following substitutions in the equations of motion:

\[
V_a \rightarrow V_a + V_{\text{opt}} \quad (6.5)
\]

\[
V_m \rightarrow V_m + 2V_{\text{opt}} \quad (6.6)
\]

where

\[
V_{\text{opt}} = V_0 \cos (x \cdot q - \omega t), \quad (6.7)
\]

and \( V_0, q \) and \( \omega \) are the intensity, the momentum and the frequency of the Bragg pulse respectively [8].

### 6.1.2 Three-Body Loss in the Gross–Pitaevskii Equation

The way in which to include three-body loss in a c-field formalism was originally developed by Norrie et al. [90], who modelled the three-body recombination process by adding loss terms to the Gross–Pitaevskii equation according to

\[
\frac{i\hbar}{\partial t} \psi(x, t) = \left( \frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(x) + U_0 |\psi(x, t)|^2 \right) \psi(x, t)
\]
6.1. Formalism

\begin{equation}
-\frac{1}{2}K_3 |\psi(x, t)|^4 \psi(x, t) + \sqrt{\frac{3K_3}{2}} |\psi(x, t)|^2 \xi(x, t),
\end{equation}

where $K_3$ is the number loss rate constant, as in Sect. 2.3, and $\xi(x, t)$ is a stochastic function; if we let $\xi(x, t) \, dt \to dW(x, t)$, the functions $dW(x, t)$ are complex Wiener processes, which obey

\begin{align}
\langle dW(x, t) \rangle &= 0, \quad (6.9) \\
\langle dW(x, t) \, dW(x', t) \rangle &= 0, \quad (6.10) \\
\langle dW(x, t) \, dW^*(x', t) \rangle &= \delta(x - x') \, dt. \quad (6.11)
\end{align}

The number loss rate $K_3$ can easily be related to the event loss rate $\alpha_{rec}$, treated in Sect. 2.3, as $3\alpha_{rec} = K_3$. However, as is discussed in Sect. 2.3, it is important to note that our notation of the recombination constants follows that of Braaten et al. [15], which is different from that used by Norrie et al. [90]. To avoid this confusion, as well as to simplify the notation, in the remainder of this thesis we use the notation $\gamma$ for the three-body loss term coefficient, which we define as

\begin{equation}
\gamma \equiv \frac{K_3}{2} = \frac{\alpha_{rec}}{6}. \quad (6.12)
\end{equation}

This treatment includes a stochastic term in the equations of motion, but Norrie et al. [90] show that this term can in most cases be neglected to a good order of approximation. In (6.1), we have used this approximate form, and have extended it phenomenologically to include the molecule population as well. This extension is quite simple-minded; we include all of the losses in the equation for the atomic field, and use the total density of atoms plus molecules in the loss term as the object that corresponds most logically to the measurable density of atoms. Since the atomic field is very much larger than the molecular field in the situations we are considering, this kind of model should be a reasonably accurate approximation.

In principle, the formulation of the theory in terms of atoms and molecules provides an opportunity to give a model of three-body loss which would incorporate the actual mechanism of three-body loss as arising from inelastic collisions between atoms and molecules. In such a collision, both the atom and the molecule would normally be transferred to untrapped states, and be lost from the system — equivalent to a loss of three atoms. We hope to develop this kind of model in future work.
6.2 Dimensionless Implementation

6.2.1 Computational Units

Typical parameters when describing quantum-mechanical systems are very small in SI units. Therefore, in order to numerically implement the projected Gross–Pitaevskii equation, it is necessary to reformulate it using dimensionless quantities. By choosing an appropriate basis for our computational units, we can ensure that the numerical quantities in the calculations are of a reasonable magnitude, and thus minimise round-off errors. Working with dimensionless quantities is also favourable since it often reduces the number of parameters on which the system depends.

The systems of interest in this thesis all have a harmonic trap, thus we follow the work of [7], and define our dimensionless parameters in terms of the trapping frequency. More specifically, since we treat systems in a cigar-shaped geometry, we use the radial trapping frequency \( \omega_r \) of the trap as the base for our units. This way we define a length scale \( r_0 \) as

\[
    r_0 = \sqrt{\frac{\hbar}{2m\omega_r}},
\]

and a time scale \( t_0 \) as

\[
    t_0 = \frac{1}{\omega_r},
\]

where \( m \) is the mass of an atom.

Using these we can define a corresponding energy unit \( \epsilon_0 \), defined as

\[
    \epsilon_0 = \hbar \omega_r,
\]

and a wavenumber unit \( k_0 \) as

\[
    k_0 = \frac{1}{r_0}.
\]

6.2.2 Dimensionless Parameters

Dimensionless time \( \tilde{t} \) and position \( \tilde{x} \) can now be defined as

\[
    \tilde{t} = \frac{t}{t_0}, \quad \tilde{x} = \frac{x}{r_0}.
\]

The wavefunction is in units of \([\text{length}]^{-D/2}\), where \( D \) is the dimension of the system. Therefore, for our three dimensional system, a dimensionless wavefunction can
be defined as
\[ \tilde{\psi}(\tilde{x}, \tilde{t}) = \frac{\psi(x, t)}{r_0^{-3/2}}. \] (6.18)

Similarly, the dimensionless atom-atom interaction \( \tilde{U}_{aa} \), atom-molecule coupling parameter \( \tilde{g} \) and three-body loss parameter \( \tilde{\gamma} \) will be given by
\[ \tilde{U}_{aa} = \frac{U_{aa}}{\hbar \omega r_0^3}, \] (6.19)
\[ \tilde{g} = \frac{g}{\hbar \omega r_0^{3/2}}, \] (6.20)
\[ \tilde{\gamma} = \frac{\gamma}{\hbar \omega r_0^6}, \] (6.21)
respectively.

In terms of the dimensionless time and position, the trapping potential and optical potential can be expressed as
\[ V_a(x, t) = \frac{m \omega^2}{2}(\tilde{x}^2 + \tilde{y}^2 + \lambda^2 \tilde{z}^2) = \frac{\hbar \omega}{4}(\tilde{x}^2 + \tilde{y}^2 + \lambda^2 \tilde{z}^2), \] (6.22)
\[ V_{opt}(x, t) = V_0 \cos(\tilde{\omega} t - \tilde{\omega} \tilde{t} - \tilde{x} \tilde{r}_0) = V_0 \cos(\tilde{\omega} \tilde{x} - \tilde{\omega} \tilde{t}), \] (6.23)
respectively. These are both in units of energy, so the dimensionless trapping potential \( \tilde{V}_a \) and optical potential \( \tilde{V}_{opt} \) are given by
\[ \tilde{V}_a(\tilde{x}, \tilde{t}) = \frac{V_a(x, t)}{\hbar \omega r} = \frac{1}{4}(\tilde{x}^2 + \tilde{y}^2 + \lambda^2 \tilde{z}^2), \] (6.24)
\[ \tilde{V}_{opt}(\tilde{x}, \tilde{t}) = \frac{V_0}{\hbar \omega r} \cos(\tilde{\rho} \cdot \tilde{x} - \tilde{\omega} \tilde{t}). \] (6.25)

### 6.2.3 Dimensionless Equations

Inserting the dimensionless parameters from the previous subsection into the equations of motion for the atom and molecule field, (6.1) and (6.2), gives
\[
\begin{align*}
\hbar \frac{\partial \tilde{\psi}_0^{-3/2}}{\partial \tilde{t} \tilde{t}_0} &= -\frac{\hbar^2 \tilde{\psi}^2}{2 m r_0^2} \tilde{\psi} r_0^{-3/2} + \frac{\hbar \omega}{4}(\tilde{x}^2 + \tilde{y}^2 + \lambda^2 \tilde{z}^2) \tilde{\psi} r_0^{-3/2} + \\
&+ \tilde{V}_0 \hbar \omega r_0^{-3/2} \tilde{\psi} r_0^{-3/2} + \tilde{U}_{aa} \hbar \omega r_0^3 |\tilde{\psi} r_0^{-3/2}|^2 \tilde{\psi} r_0^{-3/2} + \\
&+ \tilde{g} \hbar \omega r_0^{3/2} \tilde{\psi} r_0^{-3/2} - i \tilde{\gamma} \hbar \omega r_0^6 (|\tilde{\psi} r_0^{-3/2}|^2 + 2 |\tilde{\phi} r_0^{-3/2}|^2) \tilde{\psi} r_0^{-3/2},
\end{align*}
\] (6.26)
where we have suppressed the \( \tilde{x}_0 \) and \( \tilde{t}_0 \) dependency. This simplifies to

\[
{i \hbar \omega_r} \frac{\partial \psi}{\partial \tilde{t}} = -{\hbar \omega_r} \vec{\nabla}^2 \tilde{\psi} + \frac{\hbar \omega_r}{4} (\tilde{x}^2 + \tilde{y}^2 + \lambda^2 \tilde{z}^2) \tilde{\psi} + \tilde{V}_0 \hbar \omega_r \cos (\tilde{q} \cdot \tilde{x} - \tilde{\omega} \tilde{t}) \tilde{\psi} + \tilde{U}_{aa} \hbar \omega_r |\tilde{\psi}|^2 \tilde{\psi} + \tilde{g} \hbar \omega_r \tilde{\psi}^* \tilde{\phi} - i \tilde{\gamma} \hbar \omega_r (|\tilde{\psi}|^2 + 2|\tilde{\phi}|^2)^2 \tilde{\psi},
\]

(6.29)

which is equivalent to

\[
\frac{1}{i} \frac{\partial \psi}{\partial \tilde{t}} = -\vec{\nabla}^2 \tilde{\psi} + \frac{1}{4} (\tilde{x}^2 + \tilde{y}^2 + \lambda^2 \tilde{z}^2) \tilde{\psi} + \tilde{V}_0 \cos (\tilde{q} \cdot \tilde{x} - \tilde{\omega} \tilde{t}) \tilde{\psi} + \tilde{U}_{aa} |\tilde{\psi}|^2 \tilde{\psi} + \tilde{g} \tilde{\psi}^* \tilde{\phi} - i \tilde{\gamma} (|\tilde{\psi}|^2 + 2|\tilde{\phi}|^2)^2 \tilde{\psi},
\]

(6.30)

In the remainder of this chapter we will suppress the explicit tilde-notation (\( \tilde{\cdot} \)), but, unless stated otherwise, we will refer to the dimensionless parameters.

### 6.3 Initial State

We simulate the atom-molecule system by solving the equations of motion numerically. This is done using MATLAB, and the set-up for the simulations is discussed in Sect. 6.4.2 In the present section, we describe the methods we use for finding stationary solutions to the equations of motion, to be used as initial states in the simulations.

In order to implement our analytical system in MATLAB, we need to transform it to a computationally describable system and discretise the continuous time as well as position and momentum space, as will be described in Sect. 6.4.2. In this section and the next, we will express the discretisation of our parameters explicitly. However, in the remainder of the thesis, we will use a continuous notation, in which the discretisation needed for implementation is implied.

86
6.3. Initial State

6.3.1 Thomas–Fermi Solutions

The Thomas–Fermi solutions of the equations (6.1, 6.2) are given in Sect. 5.1.4, and take on the discrete form

\[ |\psi_s(x_{ijk})| = \sqrt{\frac{\mu_a - V_a(x_{ijk})}{U_{aa} + g^2/2(2\mu_a - \epsilon - V_m(x_{ijk}))}}, \]  

(6.32)

\[ \phi_s(x_{ijk}) = \frac{g}{2(2\mu_a - \epsilon - V_m(x_{ijk}))} \psi^2(x_{ijk}), \]  

(6.33)

where \(x_{ijk}\) denotes a point on the spatial grid. The total number of atoms in the two fields is given by

\[ N = \sum_i \sum_j \sum_k dV \left( |\psi_s(x_{ijk})|^2 + 2|\phi_s(x_{ijk})|^2 \right), \]  

(6.34)

where \(dV\) is the spatial volume element (see Sect. 6.4.2).

For a given value of the scattering length, \(g\) and \(\epsilon\) are given by (6.3) and (6.4), respectively. However, the chemical potential \(\theta_a\) is not known. In order to determine the chemical potential, we choose a fixed total number of atoms \(N_{\text{fix}}\) and find the value of \(\theta_a\) which solves the expression

\[ \sum_i \sum_j \sum_k dV \left( |\psi_s(x_{ijk})|^2 + 2|\phi_s(x_{ijk})|^2 \right) = N_{\text{fix}}, \]  

(6.35)

with \(\psi_s\) and \(\phi_s\) given by (6.32) and (6.33), respectively. This is done using the MATLAB function \texttt{fsolve} [78], which solves the system using a nonlinear least-squares algorithm. The starting guess used by the solver is set to \(\mu_a = 1\).

6.3.2 Optimisation

As an initial state for our simulations, we wish to find the stationary solutions to the equations of motion (6.1, 6.2), with \(\gamma = 0\). The discretised, time-independent versions of these equations are given by

\[ \left( -\nabla^2 + V_a(x_{ijk}) + U_{aa} |\psi(x_{ijk})|^2 \right) \psi(x_{ijk}) + g \psi^*(x_{ijk}) \phi(x_{ijk}) = \mu_a \psi(x_{ijk}), \]  

(6.36)

\[ \left( -\frac{\nabla^2}{2} + \frac{\epsilon}{2} + V_m(x_{ijk}) \right) \phi(x_{ijk}) + \frac{g}{2} \psi^2(x_{ijk}) = 2\mu_a \phi(x_{ijk}). \]  

(6.37)

For a given value of the scattering length, the Feshbach parameters \(g\) and \(\epsilon\) are given by (6.3) and (6.4), and for a fixed value of the particle number, the chemical potential, \(\mu_a\), can be determined as described in the previous section. Using the Thomas–Fermi profiles (6.32, 6.33) as an initial guess, we optimise the time-independent equa-
tions by finding the \( \psi \) and \( \phi \) which solve the coupled expressions (6.36, 6.37), setting the boundary conditions \( \psi = \phi = 0 \) on the edges of the spatial grid. Again, this optimisation is done by using the `fsolve` function in MATLAB [78].

Solving this kind of optimisation problem in three dimensions is computationally demanding. Fortunately, the systems we study in this thesis are all cylindrically symmetric, and we can therefore reduce them to a two-dimensional system by expressing them in cylindrical coordinates. The equations of motion then become

\[
\begin{align*}
-\left( r_i \frac{\partial^2}{\partial r^2} + 2 \frac{\partial}{\partial r} + 2 \frac{\partial^2}{\partial \zeta^2} \right) + r_i \left( V_a + U_{aa} |\psi|^2 - \theta_a \right) \psi + g r_i \psi^* \phi &= 0, \\
- \frac{1}{2} \left( r_i \frac{\partial^2}{\partial r^2} + 2 \frac{\partial}{\partial r} + r_i \frac{\partial^2}{\partial \zeta^2} \right) + r_i \left( \epsilon + V_m - 2 \mu_a \right) \phi + \frac{g}{2} r_i \psi^2 &= 0,
\end{align*}
\]

where \( r \) is the radial coordinate, and \( \zeta \) is the axial coordinate. Here we have multiplied both sides with \( r_i \) in order to avoid the singularity at \( r_i = 0 \), and we have suppressed the spatial dependence for brevity.

The derivatives are evaluated using a finite difference approximation, so that the \( m \)-th derivative at \( r_i \) is given by

\[
\frac{\partial^m \psi}{\partial r^m} \approx \frac{1}{(\Delta r)^m} \sum_{l=-\lfloor (M-1)/2 \rfloor}^{\lfloor (M-1)/2 \rfloor} c_l \psi(r_i + l\Delta r),
\]

where \( M \) is the number of points used to calculate the derivative, \( \Delta r \) is the grid spacing, and \( c_l \) is an element of the finite difference stencil; for details see for example [7]. For the work in this thesis we use a stencil with \( M = 5 \).

Fig. 6.1 shows the stationary solutions obtained in this way. For comparison, we have also plotted the corresponding Thomas–Fermi profiles (6.32, 6.33). It is clear from the figure that the Thomas–Fermi solutions are good approximations of the condensate profiles, except on the edges of the condensate. There is also a small discrepancy between the two solutions in the middle of the profile, around \( r = 0 \), although this is hard to tell from direct observation of Fig. 6.1. This discrepancy is hardly surprising since the true stationary solution and the Thomas–Fermi solution have the same number of particles. The true solution has more particles located on the edge of the condensate, and the Thomas–Fermi solution must consequently have more particles in the middle of the profile.

Not surprisingly, we find that this optimisation routine is faster the more even in

---

1 When performing the full simulation, this is no longer possible, since we add stochastic terms to the initial state in order to simulate the effects of vacuum noise. However, before the noise is added, the systems are symmetric, and the optimisation routine for determining the stationary solutions can therefore be performed in two dimensions.
6.3. Initial State

The atom wavefunction in the radial direction is shown in the left panel and the molecule wavefunction in the right panel. The total number of atoms — counting one molecule as two atoms — is $10^4$, of which approximately 400 are atoms in the form of molecules. The parameter $r_0$ is the length scale associated with the radial direction of the trap, given by $r_0 = \sqrt{\hbar/2m\omega_r} \approx 1.84 \times 10^{-6} \, \text{m}$ (see Sect. 5.2), and the renormalisation parameter is here given by $\Lambda = 2 \times 10^6 \, \text{m}^{-1}$.

After finding a solution to the cylindrical equations of motion, we translate this solution from a two-dimensional cylindrical grid to a three-dimensional cartesian grid. This is done by generating the cartesian grid and then at each grid point, calculating the approximate value of the wavefunction, using an interpolation routine.

Using these methods we do not obtain perfect stationary solutions to our equations of motion, due to the coarseness of the grids used and the difficulties in translating the solution from one grid to another. However, this does not cause any problems, since we do not require perfectly stationary initial states in order to simulate the experiment of [92]. On the contrary, the ramping of the scattering length before the addition of the Bragg pulse (as discussed in Sect. 7.2.2), and the addition of the noise terms (as discussed in the next section), will cause far more disruption to the stationary solution than the translation from the two- to the three-dimensional grid.

6.3.3 Initial Noise

As described in Sect. 3.3.4, we mimic the effects of quantum fluctuations on the system by adding on average a half quantum of Gaussian random noise per mode of the initial momentum state. In practice this means that for each atom and molecule mode, $\psi_k$
and $\phi_k$, we make the substitutions

$$
\psi_k \rightarrow \psi_k + \frac{1}{2} (A_k + iB_k),
$$

(6.41)

$$
\phi_k \rightarrow \phi_k + \frac{1}{2} (C_k + iD_k),
$$

(6.42)

where $A_k$, $B_k$, $C_k$ and $D_k$ are independent Gaussian random variables with zero mean and unit variance, such that

$$
\langle A_k \rangle = \langle B_k \rangle = \langle C_k \rangle = \langle D_k \rangle = 0,
$$

(6.43)

$$
\langle A_j A_k \rangle = \langle B_j B_k \rangle = \langle C_j C_k \rangle = \langle D_j D_k \rangle = \delta_{jk},
$$

(6.44)

$$
\langle A_j B_k \rangle = \langle A_j C_k \rangle = \langle A_j D_k \rangle = \langle B_j C_k \rangle = \langle B_j D_k \rangle = \langle C_j D_k \rangle = 0.
$$

(6.45)

By adding these noise terms to the initial modes, we introduce a total of $M/2$ virtual particles to the system, where $M$ is the number of modes. In order to recover the correct operator averages we must therefore subtract these from the field. The way in which to do this for the complicated case of the density-weighted density is described later in this chapter, in Sect. 6.7.

As noted in Sect. 3.3.4, the more correct way of including the effects of quantum fluctuations would be to use samplings of the Bogoliubov state. However, the initial state used in the simulations in Chap. 7 is, as we will discuss in Sect. 7.2.2, far from an equilibrium state, and there is no knowledge of what state it actually is. Sampling the Bogoliubov state would therefore hardly be worthwhile and the method described above is a good approximation.

### 6.4 MATLAB Implementation

#### 6.4.1 Propagation Algorithm

The equations of motion (6.1, 6.2) are evolved in MATLAB using a version of the fourth-order Runge–Kutta algorithm. The original method, the fourth order Runge–Kutta in the interaction picture (RK4IP), was developed by Ballagh [3] and Davis [33] in order to efficiently simulate the Gross–Pitaevskii equation. Norrie [87] modified this method and introduced a projector description of the modes in momentum space, the Projected Runge–Kutta Fourth-order Interaction Picture method (P-RK4IP). The version of two coupled fields that we make use of in this work was first described by Dempsey [34]. We outline these methods, as well as the explicit algorithm that we use for the temporal integration of the equations of motion, in Appendix A.
6.4.2 Discretised Grids

The propagation algorithm contains terms that can be evaluated using MATLAB's Fast Fourier transforms (FFTs). These are most efficient on a grid where the number of grid points, \( N_x \), \( N_y \) and \( N_z \), are numbers with small prime factors. The best choice is therefore \( N_{x,y,z} = 2^n \), where \( n \) is some positive integer.

We define our system on some three-dimensional coordinate space with dimensions \( L_x \times L_y \times L_z \), which are divided into \( N_x \times N_y \times N_z \) grid points. The total volume of the grid is given by \( V = L_x L_y L_z \) and the total number of grid points is \( N = N_x N_y N_z \).

The dimension of a single grid element is \( dx \times dy \times dz \), where

\[
\frac{dx}{N_x} = \frac{L_x}{N_x}, \quad \frac{dy}{N_y} = \frac{L_y}{N_y}, \quad \frac{dz}{N_z} = \frac{L_z}{N_z}.
\]  

(6.46)

The volume of a grid element is thus

\[
dV = dx dy dz = \frac{V}{N}.
\]  

(6.47)

If the origin of the position space is situated in the centre of the grid, then the grid references can be expressed as

\[
x = \frac{L_x}{N_x} \left[ -\frac{N_x}{2}, -\frac{N_x}{2} + 1, ..., \frac{N_x}{2} - 1 \right],
\]  

(6.48)

\[
y = \frac{L_y}{N_y} \left[ -\frac{N_y}{2}, -\frac{N_y}{2} + 1, ..., \frac{N_y}{2} - 1 \right],
\]  

(6.49)

\[
z = \frac{L_z}{N_z} \left[ -\frac{N_z}{2}, -\frac{N_z}{2} + 1, ..., \frac{N_z}{2} - 1 \right].
\]  

(6.50)

For this coordinate space, there exists a corresponding momentum space with dimensions \( K_x \times K_y \times K_z \), described by

\[
k_x = \frac{2\pi}{L_x} \left[ -\frac{N_x}{2}, -\frac{N_x}{2} + 1, ..., \frac{N_x}{2} - 1 \right],
\]  

(6.51)

\[
k_y = \frac{2\pi}{L_y} \left[ -\frac{N_y}{2}, -\frac{N_y}{2} + 1, ..., \frac{N_y}{2} - 1 \right],
\]  

(6.52)

\[
k_z = \frac{2\pi}{L_z} \left[ -\frac{N_z}{2}, -\frac{N_z}{2} + 1, ..., \frac{N_z}{2} - 1 \right].
\]  

(6.53)

The dimension of a single momentum space grid element is \( dk_x \times dk_y \times dk_z \), where

\[
dk_x = \frac{2\pi}{L_x}, \quad dk_y = \frac{2\pi}{L_y}, \quad dk_z = \frac{2\pi}{L_z}.
\]  

(6.54)
and the volume is
\[ \text{d}k = \text{d}k_x \text{d}k_y \text{d}k_z = \frac{(2\pi^3)}{V}. \quad (6.55) \]

### 6.4.3 Projectors

The functions \( \mathcal{P}_a \) and \( \mathcal{P}_m \) are the atom and molecule projectors that restrict the wavefunctions to the low energy subspace below the momentum cutoff,

\[
\mathcal{P}_a = \Theta \left( \left( \frac{k_x^2}{k_{x,\text{cut}}^2} + \frac{k_y^2}{k_{y,\text{cut}}^2} + \frac{k_z^2}{k_{z,\text{cut}}^2} \right) - 1 \right), \quad (6.56)
\]

\[
\mathcal{P}_m = \Theta \left( \frac{1}{4} \left( \frac{k_x^2}{k_{x,\text{cut}}^2} + \frac{k_y^2}{k_{y,\text{cut}}^2} + \frac{k_z^2}{k_{z,\text{cut}}^2} \right) - 1 \right), \quad (6.57)
\]

where the momentum space cutoff in the \( j \)-th direction is given by

\[ k_{j,\text{cut}} = \frac{\max (k_j)}{2}. \quad (6.58) \]

These projectors arise from the simulation grid, and they are defined in order to avoid aliasing in our simulations [10]. However, as discussed in Chap. 2, it is necessary to include the momentum space cutoff for two other reasons: in order for a pseudopotential treatment of the interaction to be valid, and in order to avoid excessive quantities of noise being added in the c-field method.

The projected region corresponds to a region centered around the origin of momentum space containing all low-energy modes, i.e. all modes below the cut-off value. Effectively, the projector represents a discretised zero-padded momentum space mask, which, when multiplied elementwise with derivatives of the mode amplitudes, will prevent population from entering the high-energy modes. This technical description should, however, not be interpreted as the projector introducing any particle loss from the system; the projector simply suppresses all interactions where the outcome would occupy modes larger than the cut-off value.

### 6.4.4 Aliasing

Davis [33] and Norrie [87] treat the problem of Fourier aliasing. Aliasing can occur because of the use of Fourier transforms in the propagation algorithm. It amounts to modes outside the cut-off being mapped on to modes within the projection region. Norrie shows that in order to avoid aliasing, we must choose \( k_{j,\text{cut}} \) according to

\[ 2k_{j,\text{cut}} \leq \min(K_x, K_y, K_z). \quad (6.59) \]
For simplicity, we choose our cut-off to be

\[ k_{j,\text{cut}} = \frac{1}{2} K_j. \] (6.60)

A molecule that has been created from two atoms will have the added momentum of the two atoms, so if the atoms are initially in the same mode, the resulting molecule will be in the mode with twice the momentum of a single atom. Therefore, the region in momentum space that is available for the molecule has to have a radius that is twice that of the atoms, and thus the molecule cut-off is twice that of the atoms. Since the molecule equation of motion does not contain any nonlinear terms in the molecule field, this will not cause any problems with aliasing.

### 6.4.5 Discretised Time

The propagation algorithm evolves the atom and molecule fields from a time \( t_0 = 0 \) to a time \( t_{\text{final}} \) over a set of evenly spaced discrete time steps \( N_{\text{steps}} \). The size of each step \( \Delta t \) is chosen such that the effective computation time is as low as possible, while at the same time the differential equations converge. This is done by using a method of trial and error, propagating the equations of motion with the three-body loss parameter \( \gamma \) set to zero. We use the total number of atoms, \( N = N_a + 2 N_m \), as a criterium of accuracy; a simulation is discarded if the final atom number differs by more than 0.01\% from the initial atom number. This is discussed further in Sect. 7.2.3.

The fewer the molecules, the more unstable the coupled equations appear to be, and thus for smaller scattering lengths the number of time steps has to be significantly increased compared to that for larger scattering lengths. The approximate time step sizes used in our simulations are given in Sect. 7.2.3.

### 6.5 Momentum Space Truncation

#### 6.5.1 General method

Assuming the Bragg pulse is only applied in the \( x \)-direction, we can write the optical potential as

\[ V_{\text{opt}} = V_0 \cos (Q x - \omega t) = \frac{V_0}{2}(e^{i(Q x - \omega t)} + e^{-i(Q x - \omega t)}), \] (6.61)

where \( Q = |q| \). To include all the physics that we are interested in, the momentum space needs to include at least the first few orders of Bragg momentum, at \( |k| = nQ \), where \( n \) is an integer. To fulfill this condition, as well as the condition that \( N_x = 2^n \) for some positive integer \( n \), the number of grid points in the \( x \)-direction is chosen to be
2048. The \( y \)- and \( z \)-directional grids are chosen to have \( N_y = N_z = 64 \), since these directions are of less importance, making the total number of grid points \( 2 \times 2048 \times 64 \times 64 \). Including this many modes would not only make the simulations very computationally difficult, but also, since in the c-field formalism we will have on average half a quasi-particle of noise per mode in the initial state, we would get many more noise than condensate particles. According to the validity condition for the c-field methods [89], this would make our simulations invalid.

To get around this problem, but still include all the momentum space of relevance, we neglect the parts of momentum space where the population in excess of noise will be insignificant, and include only those modes that are initially populated, or where we can expect to get significant population from scattering. Because the interest here is Bragg scattering with a Bragg pulse applied in the positive \( x \)-direction, we divide momentum space into bands in this direction, each centered around \( nQ \) for some integer \( n \), where \( Q \) is the momentum of the pulse. We can thus write the wavefunctions \( \psi \) and \( \phi \) as

\[
\psi(x) = \sum_n \psi_n(x)e^{inQx}, \quad (6.62)
\]
\[
\phi(x) = \sum_n \phi_n(x)e^{inQx}, \quad (6.63)
\]

where \( \psi_n \) and \( \phi_n \) are the Fourier transforms of the momentum space wavefunction in the band centred around \( nQ \).

The projectors \( P_a \) and \( P_m \) which act on \( \psi_n \) and \( \phi_n \) for each band are given by

\[
P_a = \Theta\left(\frac{k_x^2}{k_x^2,\text{cut}} + \frac{k_y^2}{k_y^2,\text{cut}} + \frac{k_z^2}{k_z^2,\text{cut}}\right) - 1, \quad (6.64)
\]
\[
P_m = \Theta\left(\frac{1}{4}\left(\frac{k_x}{k_x^2,\text{cut}} + \frac{k_y}{k_y^2,\text{cut}} + \frac{k_z}{k_z^2,\text{cut}}\right)\right) - 1, \quad (6.65)
\]

with the \( x \)-directional cutoff now given by

\[
k_{x,\text{cut}} = \frac{\Delta k}{4}, \quad (6.66)
\]

where \( \Delta k \) is the width of each momentum space band. The projectors are the same for all the wavefunctions \( \psi_n \) and \( \phi_n \); for each band the projectors are ellipsoids centered around the midpoint at \( y = z = 0 \) and \( x = nQ \). The full wavefunctions, \( \psi \) and \( \phi \), are thus projected onto four disjoint regions in momentum space (see Fig. 6.2). The band width \( \Delta k \) is chosen as a compromise between two factors: it needs to be large enough to include as much as possible of the momentum space wavefunction, but at the same
Figure 6.2: Atom field projector (top panel) and molecule field projector (bottom panel) in the $xy$-plane for the case of four bands in momentum space being significantly populated. The width of each band is $\Delta k$. The blue areas indicate the regions of momentum space that the wavefunctions are projected into, determined by the parameters $k_{x,\text{cut}}$ and $k_{y,\text{cut}}$. The parameter $r_0$ is the length scale associated with the radial direction of the trap, given by $r_0 = \sqrt{\hbar/2m\omega r} \approx 6.665 \times 10^{-7}$ m. Here $\Delta k = 3 \times 10^6$ m$^{-1}$, $k_{x,\text{cut}} = 7.5 \times 10^5$ m$^{-1}$, and $k_{y,\text{cut}} = 8.2 \times 10^6$ m$^{-1}$.

time small enough to not include too much of the initial noise.

6.5.2 Four Significant Bands

We find that only the four momentum bands corresponding to the orders $n = -1, 0, 1, 2$ acquire sufficient population to affect the simulation — the asymmetry of the population around $x = 0$ is due to the Bragg pulse being directed in the positive $x$-direction. Thus, we can write

$$\psi(x) = \psi_{-1}(x)e^{-iQx} + \psi_0(x) + \psi_1(x)e^{iQx} + \psi_2(x)e^{2iQx}, \quad (6.67)$$

$$\phi(x) = \phi_{-1}(x)e^{-iQx} + \phi_0(x) + \phi_1(x)e^{iQx} + \phi_2(x)e^{2iQx}. \quad (6.68)$$

Fig. 6.2 shows the projector in the $xy$-plane for the full wavefunctions resulting from this procedure. We have also indicated the width, $\Delta k$, of each band and the momentum space cutoffs $k_{x,\text{cut}}$ and $k_{y,\text{cut}}$. 

95
This gives us the following expression for the squared norm of $\psi$

$$|\psi(x)|^2 = A_{-3}(x)e^{-3iQx} + A_{-2}(x)e^{-2iQx} + A_{-1}(x)e^{-iQx} +$$
$$+ A_0(x) + A_1(x)e^{iQx} + A_2(x)e^{2iQx} + A_3(x)e^{3iQx}, \quad (6.69)$$

where

$$A_0 = |\psi_{-1}|^2 + |\psi_0|^2 + |\psi_1|^2 + |\psi_2|^2, \quad (6.70a)$$
$$A_1 = \psi_{-1}^*\psi_0 + \psi_0^*\psi_1 + \psi_1^*\psi_2 = A_{-1}^*, \quad (6.70b)$$
$$A_2 = \psi_{-1}^*\psi_1 + \psi_0^*\psi_2 = A_{-2}^*, \quad (6.70c)$$
$$A_3 = \psi_{-1}^*\psi_2 = A_{-3}^*. \quad (6.70d)$$

Similarly for the squared norm of $\phi$ we have

$$|\phi(x)|^2 = B_{-3}(x)e^{-3iQx} + B_{-2}(x)e^{-2iQx} + B_{-1}(x)e^{-iQx} +$$
$$+ B_0(x) + B_1(x)e^{iQx} + B_2(x)e^{2iQx} + B_3(x)e^{3iQx}, \quad (6.71)$$

where

$$B_0 = |\phi_{-1}|^2 + |\phi_0|^2 + |\phi_1|^2 + |\phi_2|^2, \quad (6.72a)$$
$$B_1 = \phi_{-1}^*\phi_0 + \phi_0^*\phi_1 + \phi_1^*\phi_2 = B_{-1}^*, \quad (6.72b)$$
$$B_2 = \phi_{-1}^*\phi_1 + \phi_0^*\phi_2 = B_{-2}^*, \quad (6.72c)$$
$$B_3 = \phi_{-1}^*\phi_2 = B_{-3}^*. \quad (6.72d)$$

The density squared now becomes

$$\left(|\psi(x)|^2 + 2|\phi(x)|^2\right)^2 = C_{-3}(x)e^{-3iQx} + C_{-2}(x)e^{-2iQx} + C_{-1}(x)e^{-iQx} +$$
$$+ C_0(x) + C_1(x)e^{iQx} + C_2(x)e^{2iQx} + C_3(x)e^{3iQx}, \quad (6.73)$$

where

$$C_0 = (A_0 + 2B_0)^2 + 2|A_1 + 2B_1|^2 + 2|A_2 + 2B_2|^2 + 2|A_3 + 2B_3|^2, \quad (6.74a)$$
$$C_1 = 2(A_0 + 2B_0)(A_1 + 2B_1) + 2(A_{-1} + 2B_{-1})(A_2 + 2B_2) +$$
$$+ 2(A_{-2} + 2B_{-2})(A_3 + 2B_3) = C_{-1}^*, \quad (6.74b)$$
$$C_2 = (A_1 + 2B_1)^2 + 2(A_0 + 2B_0)(A_2 + 2B_2) +$$
$$+ 2(A_{-1} + 2B_{-1})(A_3 + 2B_3) = C_{-2}^*, \quad (6.74c)$$
$$C_3 = 2(A_0 + 2B_0)(A_3 + 2B_3) + 2(A_1 + 2B_1)(A_2 + 2B_2) = C_{-3}^*, \quad (6.74d)$$

96
and terms with \( n < -3 \) or \( n > 3 \) have been neglected.

These expressions, together with the expressions for \( \psi \) and \( \phi \) are substituted into the equation of motion for the atom wave function \((6.1)\). Dropping all terms with a factor of \( e^{i n Q x} \) with \( n \neq -1, 0, 1, 2 \), and collecting terms corresponding to the same band together, we get

\[
\begin{align*}
\frac{i}{\partial t} \psi_{-1} &= -\frac{\tilde{V}^2}{2} \psi_{-1} + Q_a \left\{ V_a \psi_{-1} + \frac{V_0}{2} \psi_0 e^{i \omega t} + U_{aa} \left( A_0 \psi_{-1} + A_1 \psi_0 + A_2 \psi_1 + A_3 \psi_2 \right) \right. \\
& \quad \left. + g \left( \psi_0^* \phi_{-1} + \psi_1^* \phi_0 + \psi_2^* \phi_1 \right) - i \gamma \left( C_0 \psi_{-1} + C_1 \psi_0 + C_2 \psi_1 + C_3 \psi_2 \right) \right\}, \quad (6.75a) \\
\frac{i}{\partial t} \psi_0 &= -\frac{\tilde{V}^2}{2} \psi_0 + Q_a \left\{ V_a \psi_0 + \frac{V_0}{2} \left( \psi_{-1} e^{-i \omega t} + \psi_1 e^{i \omega t} \right) \right. \\
& \quad \left. + U_{aa} \left( A_1 \psi_{-1} + A_2 \psi_0 + A_3 \psi_1 + A_4 \psi_2 \right) + g \left( \psi_{-1}^* \phi_0 + \psi_0^* \phi_{-1} + \psi_1^* \phi_1 + \psi_2^* \phi_2 \right) - i \gamma \left( C_1 \psi_{-1} + C_2 \psi_0 + C_3 \psi_1 + C_4 \psi_2 \right) \right\}, \quad (6.75b) \\
\frac{i}{\partial t} \psi_1 &= -\frac{\tilde{V}^2}{2} \psi_1 + Q_a \left\{ V_a \psi_1 + \frac{V_0}{2} \left( \psi_{-1} e^{-i \omega t} + \psi_2 e^{i \omega t} \right) \right. \\
& \quad \left. + U_{aa} \left( A_2 \psi_{-1} + A_3 \psi_0 + A_4 \psi_1 + A_5 \psi_2 \right) + g \left( \psi_{-1}^* \phi_2 + \psi_0^* \phi_1 + \psi_1^* \phi_0 \right) - i \gamma \left( C_2 \psi_{-1} + C_3 \psi_0 + C_4 \psi_1 + C_5 \psi_2 \right) \right\}, \quad (6.75c) \\
\frac{i}{\partial t} \psi_2 &= -\frac{\tilde{V}^2}{2} \psi_2 + Q_a \left\{ V_a \psi_2 + \frac{V_0}{2} \psi_1 e^{-i \omega t} + U_{aa} \left( A_3 \psi_{-1} + A_4 \psi_0 + A_5 \psi_1 + A_6 \psi_2 \right) \right. \\
& \quad \left. + g \left( \psi_{-1}^* \phi_2 + \psi_0^* \phi_1 + \psi_1^* \phi_0 \right) - i \gamma \left( C_3 \psi_{-1} + C_4 \psi_0 + C_5 \psi_1 + C_6 \psi_2 \right) \right\}, \quad (6.75d)
\end{align*}
\]

where

\[
\tilde{V}^2 = V^2 + i 2n \frac{\partial}{\partial x} - n^2 Q^2.
\]

Similarly, the equations of motion for the bands of the molecule wavefunction \((6.2)\), become

\[
\begin{align*}
\frac{i}{\partial t} \phi_{-1} &= -\frac{\tilde{V}^2}{4} \phi_{-1} + P_m \left\{ V_m \phi_{-1} + V_0 \phi_0 e^{i \omega t} + g \psi_{-1} \psi_0 \right\}, \quad (6.77a) \\
\frac{i}{\partial t} \phi_0 &= -\frac{\tilde{V}^2}{4} \phi_0 + P_m \left\{ V_m \phi_0 + V_0 \left( \phi_{-1} e^{-i \omega t} + \phi_1 e^{i \omega t} \right) \right. \\
& \quad \left. + \frac{g}{2} \left( 2 \psi_{-1} \psi_1 + \psi_{-1} \psi_1^* \right) \right\}, \quad (6.77b) \\
\frac{i}{\partial t} \phi_1 &= -\frac{\tilde{V}^2}{4} \phi_1 + P_m \left\{ V_m \phi_1 + V_0 \left( \phi_0 e^{-i \omega t} + \phi_2 e^{i \omega t} \right) \right. \\
& \quad \left. + g \left( \psi_{-1} \psi_2 + \psi_0 \psi_1 \right) \right\}, \quad (6.77c)
\end{align*}
\]
Figure 6.3: Total number of particles — counting each molecule as two atoms — for each momentum space band as a function of time for the truncated simulation (blue solid line) and the full simulation (red dashed line). The simulations are based on the system described and the parameters listed in Chap. 7 for the scattering length $890a_0$. The initial noise terms have been omitted for clarity.

$$i \frac{\partial \phi_2}{\partial t} = -\tilde{\nabla}_C^2 \phi_2 + \mathcal{P}_m \left\{ V_m \phi_2 + V_0 \phi_1 e^{-i\omega t} + \frac{g}{2} (2\psi_0 \psi_2 + \psi_1^2) \right\}.$$  (6.77d)

### 6.5.3 Validity of Band Truncation

Fig. 6.3 shows the number of particles in each of the bands as a function of time for a typical simulation with the momentum space truncated into bands. For comparison, we have also plotted the corresponding result for the full simulation.

### 6.6 Renormalisation

#### 6.6.1 Renormalisation factor

We tend to refer to the parameter $\Lambda$ as the momentum space cutoff. However, in reality this is only true in the special case of isotropic cutoffs. The relationship between the renormalisation constant, $\Lambda$, and the momentum space cutoffs, $k_{x,\text{cut}}$, $k_{y,\text{cut}}$ and $k_{z,\text{cut}}$, is given by

$$4\pi \Lambda = \int_V \frac{dk}{k^2}.$$  (6.78)
where $V$ is the ellipsoidal volume spanned by the momentum space vectors, corresponding to the projectors (6.56) [6.57].

In the simplest case, the momentum space cutoff is the same in all directions, and the volume of the populated low energy subspace is spherical so that evaluating (6.78) gives

$$\Lambda = k_{R,\text{cut}},$$

(6.79)

where $k_{R,\text{cut}}$ is the value of the isotropic cutoff.

### 6.6.2 Anisotropic Cutoff

In the case of an anisotropic cutoff, as the one used for the numerical calculations in this thesis, the exact value of $\Lambda$ needs to be evaluated using equation (6.78). In the following we will treat the two cases that are relevant for our work here.

Firstly we consider the case when the truncation, as described in Sect.5.5, has not been performed, and we are thus considering the full momentum space. The momentum space below the cutoff can be described by an ellipsoid of volume $V$, with radii $R_x$ and $R_{yz}$. Because of the cylindrical symmetry of the volume we can simplify the problem by changing to polar coordinates to obtain

$$I = \int_{-R_x}^{R_x} \int_{0}^{\rho_{\text{max}}(\zeta)} \frac{2\pi \rho}{\rho^2 + \zeta^2} d\rho d\zeta$$

(6.80)

$$= 2\pi \int_{0}^{R_x} \left( \ln(\rho^{2\max}(\zeta) + \zeta^2) - \ln(\zeta^2) \right) d\zeta,$$

(6.81)

where $\rho_{\text{max}}$ is given by

$$\rho^{2\max}(\zeta) = R_{yz}^2 \left( 1 - \frac{\zeta^2}{R_x^2} \right).$$

(6.82)

If the volume $V$ is a proper ellipsoid and not a sphere, we have that $R_{yz}^2 \neq R_x^2$ and therefore we can write

$$I = 2\pi \int_{0}^{R_x} \left( \ln \left( \zeta^2 + \frac{R_{yz}^2}{1 - R_{yz}^2 / R_x^2} \right) + \ln \left( 1 - \frac{R_{yz}^2}{R_x^2} \right) - 2\ln(\zeta) \right) d\zeta.$$

(6.83)

If the volume is cigar shaped, then $R_{yz}^2 < R_x^2$ and the integral can be solved as

$$I_{\text{cigar}} = 2\pi \left[ \zeta \ln \left( \zeta^2 + \frac{R_{yz}^2}{1 - R_{yz}^2 / R_x^2} \right) - 2\zeta \right.$$

$$+ \frac{2R_{yz}}{\sqrt{1 - R_{yz}^2 / R_x^2}} \arctan \left( \frac{\zeta \sqrt{1 - R_{yz}^2 / R_x^2}}{R_{yz}} \right) \left. \right].$$
\begin{align}
+\zeta \ln \left( 1 - \frac{R_{yz}^2}{R_x^2} \right) - 2\zeta \ln(\zeta) + 2\zeta \right|_0^{R_x} = \\
= \frac{4\pi R_{\text{max}}}{\sqrt{1 - R_{\text{max}}^2/x_{\text{max}}^2}} \arctan \left( \frac{x_{\text{max}} \sqrt{1 - R_{\text{max}}^2/x_{\text{max}}^2}}{R_{\text{max}}} \right). 
\end{align}

(6.84)

If instead the volume is pancake shaped, $R_{yz}^2 > R_x^2$ and the solution is

\begin{align}
J_{\text{pancake}} &= 2\pi \left[ \zeta \ln \left( \zeta^2 - \frac{R_{yz}^2}{R_x^2} \right) - 2\zeta \\
&\quad + \frac{2R_{yz}}{\sqrt{1 - R_{yz}^2/R_x^2}} \ln \left( \frac{\zeta + R_{yz}/\sqrt{1 - R_{yz}^2/R_x^2}}{\zeta - R_{yz}/\sqrt{1 - R_{yz}^2/R_x^2}} \right) \\
&\quad + \zeta \ln \left( \frac{R_{yz}^2}{R_x^2} - 1 \right) - 2\zeta \ln(\zeta) + 2\zeta \right|_0^{R_x} \\
&= \frac{2\pi R_{yz}}{\sqrt{R_{yz}^2/R_x^2} - 1} \ln \left( \frac{R_x + R_{yz}/\sqrt{1 - R_{yz}^2/R_x^2}}{R_x - R_{yz}/\sqrt{1 - R_{yz}^2/R_x^2}} \right). 
\end{align}

(6.86)

(6.87)

In the limit where $R_x^2 \to R_{yz}^2$, both the solutions approach the spherical case

\begin{align}
J_{\text{cigar}} \to 4\pi R_{yz} \quad \text{and} \quad J_{\text{pancake}} \to 4\pi R_{yz}. 
\end{align}

(6.88)

### 6.6.3 Truncated Momentum Space

In our simulations, we have, as is described in Sect. 6.5, a momentum space that is divided into four bands. We therefore have to calculate

\begin{equation}
J = \sum_n J_n = \sum_n \int V_n \, dk/k^2, 
\end{equation}

(6.89)

where $V_n$ is the volume of the projected subspace in band $n$.

Each band in the truncation has an ellipsoidal projector, symmetric in the $yz$-plane, with maximum value $k_{y,\text{cut}} = k_{z,\text{cut}} = k_{R,\text{cut}}$. In the $x$-direction, each band is centered around $k_x = nQ$ and they all have the same width $\Delta k$.

Because of the cylindrical symmetry of the volume we can simplify the problem by changing to polar coordinates to obtain

\begin{equation}
J_n = \int_{nQ - \Delta k/2}^{nQ + \Delta k/2} \int_0^{\rho_{\text{max}}(\zeta)} \frac{2\pi \rho}{\rho^2 + \zeta^2} d\rho d\zeta.
\end{equation}

(6.90)
6.6. Renormalisation

\[ I = 2\pi \int_0^{nQ + \Delta k/2} (\ln (\rho_{\text{max}}(\zeta) + \zeta^2) - \ln (\zeta^2)) \, d\zeta, \quad (6.91) \]

where \( \rho_{\text{max}} \) is given by

\[ \rho_{\text{max}}^2(\zeta) = k_{R,\text{cut}}^2 \left( 1 - \frac{\zeta^2}{(nQ + \Delta k/2)^2} \right). \quad (6.92) \]

We then get

\[ J_n = 2\pi \int_0^{\Delta k/2} \left( \ln \left( \zeta^2 \left( 1 - \frac{k_{R,\text{cut}}^2}{(\Delta k/2)^2} \right) \right) + 2nQ \zeta + (nQ)^2 + k_{R,\text{cut}}^2 \right) - 2 \ln (\zeta + nQ) \, d\zeta, \quad (6.93) \]

where we have used the fact that the volume \( V_n \) is an ellipsoid and not a sphere, so that \( k_{R,\text{cut}}^2 \neq (\Delta k/2)^2 \).

Since \( \Delta k < Q \), i.e. the bands are not overlapping, this integral has the solution

\[ J_n = 2\pi k_{R,\text{cut}} \sqrt{1 + \tau(nQ) + \tau(k_{R,\text{cut}})} \]

\[ \times \ln \left( \frac{4\tau(k_{R,\text{cut}}) ((nQ)^2 + k_{R,\text{cut}}^2)}{4\tau(k_{R,\text{cut}}) ((nQ)^2 + k_{R,\text{cut}}^2) - \Delta k \tau(k_{R,\text{cut}}) (2nQ - 2k_{R,\text{cut}} \sqrt{1 + \tau(k_{R,\text{cut}}) + \tau(nQ)})} \right) - \frac{4\pi nQ}{\tau(k_{R,\text{cut}})} \ln \left( \frac{nQ + \Delta k/2}{\sqrt{(nQ)^2 + k_{R,\text{cut}}^2}} \right) - 2\pi nQ \ln (nQ (nQ + \Delta k/2)), \quad (6.94) \]

where \( \tau(x) = x^2 / ((\Delta k/2)^2 - 1) \).

For the band centered around \( n = 0 \), this reduces to

\[ J_0 = 2\pi \frac{k_{R,\text{cut}}}{\sqrt{\tau(k_{R,\text{cut}})}} \ln \left( \frac{\Delta k \sqrt{\tau(k_{R,\text{cut}}) + 2k_{R,\text{cut}}}}{\Delta k \sqrt{\tau(k_{R,\text{cut}}) - 2k_{R,\text{cut}}}} \right). \quad (6.95) \]

For the bands centered around \( n \neq 0 \), we can make the approximation

\[ \int \frac{dk}{k^2} \approx \int \frac{dk}{(nQ)^2}; \quad (6.96) \]

Therefore, as long as \( Q \) is fairly large, the only significant contribution to the renormalisation factor will come from the \( n = 0 \) band. To a good order of approximation, we can then write

\[ \Lambda = \frac{J}{4\pi} \approx \frac{J_0}{4\pi} = \frac{k_{R,\text{cut}}}{2\sqrt{\tau(k_{R,\text{cut}})}} \ln \left( \frac{\Delta k \sqrt{\tau(k_{R,\text{cut}}) + 2k_{R,\text{cut}}}}{\Delta k \sqrt{\tau(k_{R,\text{cut}}) - 2k_{R,\text{cut}}}} \right). \quad (6.97) \]
6.6.4 Choice of Renormalisation Parameter

As we have seen in this section, the value of the renormalisation parameter $\Lambda$ is directly dependent on the size of the momentum grid. As is discussed in Sect. 6.5 it is important to include all the relevant physics of the system, but at the same time make sure that the c-field formalism remains valid. A too small value of the momentum cutoffs would mean excluding modes that could have significant population and therefore become important, whereas a larger value of the cutoffs would make the c-field region larger. This would in turn include much more noise in the simulations, which would make any results hard to interpret, and maybe even render the c-field formalism invalid. The momentum grid is therefore chosen as a compromise between these two factors: the momentum modes which are important for the problem, and the inclusion of noise. Thus, the best choice of cutoff is the largest value of that is possible without including too much noise.

6.7 Density-Weighted Density in Terms of C-Fields

The experimental system studied in Chap. 7 does not have a homogeneous density distribution, nor is there an easy way of accurately determining its average density. As mentioned in Sect. 2.4.6 and as will be discussed in greater detail in Sect. 7.1.1, we use the density-weighted density as an estimate of the average density of the system. The calculation of the density-weighted density can be seen as calculating the density by weighting it with the appropriate probability distribution, which in this case is the density itself.

The correct computation of the density-weighted density in the c-field formalism involves some care, since it involves products of four field operators, including both molecule and field operators.

6.7.1 Wigner Ordering

As a preliminary result, consider an operator $A$ with the commutator

$$[A, A^\dagger] = \Delta,$$  \hspace{1cm} (6.98)

and define the operator $N = A^\dagger A$.

For the operator, we know the symmetrically ordered average,

$$\{N^2\}_{\text{sym}} \equiv \{A^\dagger A, A^\dagger A A, A^\dagger A A A, A^\dagger A A A A\}_{\text{sym}}$$

$$= \frac{1}{6}\{A^\dagger A^\dagger A^\dagger A + A A A A^\dagger + A A A A^\dagger A + A A A A^\dagger A + A A A A^\dagger A^\dagger + A A A A^\dagger A^\dagger A^\dagger A^\dagger\},$$  \hspace{1cm} (6.99)
where \( \{ \ldots \}_\text{sym} \) indicates the summation over all possible distinctly different permutations of the operators.

We then find

\[
\{N^2\}_\text{sym} = N^2 + 2\Delta N + \frac{\Delta^2}{2}.
\]  
(6.100)

Since we also have

\[
\{N\}_\text{sym} = N + \frac{\Delta}{2},
\]  
(6.101)

we get

\[
N^2 = \{N^2\}_\text{sym} - 2\Delta \{N\}_\text{sym} + \frac{\Delta^2}{2}.
\]  
(6.102)

We therefore get the averages

\[
\overline{N} = \left\langle \{N\}_\text{sym} - \frac{\Delta}{2} \right\rangle,
\]  
(6.103)

\[
\overline{N^2} = \left\langle \{N^2\}_\text{sym} - 2\Delta \{N\}_\text{sym} + \frac{\Delta^2}{2} \right\rangle,
\]  
(6.104)

where \( \langle \ldots \rangle \) indicates classical averaging over the Wigner function.

### 6.7.2 Atom-Molecule Density-Weighted Density

We now consider the case of a discretised atom field operator \( \hat{\psi}(x, t) \) and a molecule field operator \( \hat{\phi}(x, t) \), with commutators of the same type as (6.98), given by

\[
\left[ \hat{\psi}(x, t), \hat{\psi}^\dagger(x, t) \right] = \Delta_a,
\]  
(6.105)

\[
\left[ \hat{\phi}(x, t), \hat{\phi}^\dagger(x, t) \right] = \Delta_m.
\]  
(6.106)

The average total atom number for this system is given by

\[
\overline{N(t)} = \left\langle \int dx \left[ \hat{\psi}^\dagger(x, t)\hat{\psi}(x, t) + 2\hat{\phi}^\dagger(x, t)\hat{\phi}(x, t) \right] \right\rangle,
\]  
(6.107)

where, as usual, we count a molecule as two atoms. Using the commutation relations, this can be expressed as

\[
\overline{N(t)} = \left\langle \int dx \left( \{\hat{n}_a(x, t)\}_\text{sym} + 2\{\hat{n}_m(x, t)\}_\text{sym} - \frac{\Delta_a}{2} - \Delta_m \right) \right\rangle,
\]  
(6.108)

where \( \{\hat{n}_a(x, t)\}_\text{sym} \) and \( \{\hat{n}_m(x, t)\}_\text{sym} \) are the symmetrically ordered averages

\[
\{\hat{n}_a(x, t)\}_\text{sym} \equiv \left\{ \hat{\psi}^\dagger(x, t)\hat{\psi}(x, t) \right\}_\text{sym},
\]  
(6.109)
\[
\{ \hat{n}_m(x, t) \}_{\text{sym}} \equiv \left\{ \hat{\phi}^*(x, t) \hat{\phi}(x, t) \right\}_{\text{sym}}. 
\] (6.110)

The density-weighted density for the system is given by
\[
\overline{n(t)} = \frac{1}{N(t)} \left\langle \int dx \left( \hat{\psi}^*(x, t) \hat{\psi}(x, t) + 2 \hat{\phi}^*(x, t) \hat{\phi}(x, t) \right)^2 \right\rangle.
\] (6.111)

Using the same approach as in the previous section, we can express this as
\[
\overline{n(t)} = \frac{1}{N(t)} \left\langle \int dx \left( \hat{n}_a^2(x, t) + 4 \hat{n}_m^2(x, t) - 2 \Delta_m \{ \hat{n}_a(x, t) \}_{\text{sym}} - 2 \Delta_a \{ \hat{n}_m(x, t) \}_{\text{sym}} + \Delta_a \Delta_m \right) \right\rangle,
\] (6.112)

where \( \hat{n}_a^2(x, t) \) and \( \hat{n}_m^2(x, t) \) are given by
\[
\overline{n_a^2(x, t)} = \{ \hat{n}_a(x, t) \}_{\text{sym}} - 2 \Delta_a \{ \hat{n}_a(x, t) \}_{\text{sym}} + \frac{\Delta_a^2}{2}, \quad (6.113)
\]
\[
\overline{n_m^2(x, t)} = \{ \hat{n}_m(x, t) \}_{\text{sym}} - 2 \Delta_m \{ \hat{n}_m(x, t) \}_{\text{sym}} + \frac{\Delta_m^2}{2}, \quad (6.114)
\]
and
\[
\{ \hat{n}_a(x, t) \}_{\text{sym}} \equiv \left\{ \hat{\psi}^{12}(x, t) \hat{\psi}^2(x, t) \right\}_{\text{sym}}, \quad (6.115)
\]
\[
\{ \hat{n}_m(x, t) \}_{\text{sym}} \equiv \left\{ \hat{\phi}^{12}(x, t) \hat{\phi}^2(x, t) \right\}_{\text{sym}}. \quad (6.116)
\]

### 6.7.3 Check with Initial State

The initial state corresponds to the two states \( \hat{\psi}(x) \) and \( \hat{\phi}(x) \), given by
\[
\hat{\psi}(x) = \psi_0(x) + \frac{\hat{r}(x)}{\sqrt{2}}, \quad (6.117)
\]
\[
\hat{\phi}(x) = \phi_0(x) + \frac{\hat{s}(x)}{\sqrt{2}}, \quad (6.118)
\]
where
\[
\left\langle |\hat{r}(x)|^2 \right\rangle = \Delta_a, \quad (6.119)
\]
\[
\left\langle |\hat{r}(x)|^4 \right\rangle = 2 \Delta_a^2, \quad (6.120)
\]
\[
\left\langle |\hat{s}(x)|^2 \right\rangle = \Delta_m, \quad (6.121)
\]
\[
\left\langle |\hat{s}(x)|^4 \right\rangle = 2 \Delta_m^2. \quad (6.122)
\]

104
Then we have

\[ \langle \{ \hat{n}_a^2(x) \}_\text{sym} \rangle = \left\langle \left| \psi_0(x) + \frac{\hat{r}(x)}{\sqrt{2}} \right|^4 \right\rangle \]

\[ = |\psi_0(x)|^4 + 2\Delta_a |\psi_0(x)|^2 + \frac{\Delta_a^2}{2}, \quad (6.123) \]

\[ \langle \{ \hat{n}_a(x) \}_\text{sym} \rangle = |\psi_0(x)|^2 + \frac{\Delta_a}{2}, \quad (6.124) \]

\[ \langle \{ \hat{n}_m^2(x) \}_\text{sym} \rangle = \left\langle \left| \phi_0(x) + \frac{\hat{s}(x)}{\sqrt{2}} \right|^4 \right\rangle \]

\[ = |\phi_0(x)|^4 + 2\Delta_m |\phi_0(x)|^2 + \frac{\Delta_m^2}{2}, \quad (6.125) \]

\[ \langle \{ \hat{n}_m(x) \}_\text{sym} \rangle = |\phi_0(x)|^2 + \frac{\Delta_m}{2}, \quad (6.126) \]

\[ \langle [\hat{n}_a(x)]_\text{sym} \{ \hat{n}_m(x) \}_\text{sym} \rangle = \langle [\hat{n}_a(x)]_\text{sym} \rangle \langle [\hat{n}_m(x)]_\text{sym} \rangle \]

\[ = |\psi_0(x)|^2 |\phi_0(x)|^2 + \frac{\Delta_m |\psi_0(x)|^2}{2} \]

\[ + \frac{\Delta_a |\phi_0(x)|^2}{2} + \frac{\Delta_a \Delta_m}{4}. \quad (6.127) \]

Therefore we obtain

\[ \overline{n} = \frac{\int d\mathbf{x} [|\psi_0(x)|^2 + 2|\phi_0(x)|^2]^2}{\int d\mathbf{x} [|\psi_0(x)|^2 + 2|\phi_0(x)|^2]^2}, \quad (6.128) \]

as expected.
Chapter 7

Simulations of Bragg Scattering from $^{85}$Rb

In this chapter, we continue the work presented in previous chapters, and investigate a realistic system, using the numerical methods outlined in Chap. 6. We will apply the coupled atom-molecule c-field formalism outlined in Chap. 4 to the specific case of a recent experiment by Papp et al. [92]. In this experiment, the excitation spectrum of a Bose-Einstein condensate of $^{85}$Rb was measured using Bragg scattering, near the Feshbach resonance at 155 G. This experiment was deliberately designed to explore a region of parameter space in which perturbation theory would not be expected to be valid. Indeed, by tuning the scattering length to large values, they found significant deviations from the Bragg scattering behaviour predicted by the simplest perturbative and mean-field theories.

In Sect. 7.1 we outline the experiment of [92], and present its objective, as well as the main results. We also discuss some of the issues associated with the experiment, which make it particularly difficult to relate to theoretical work. In Sect. 7.2 we describe the set-up we use to simulate the experiment, and list the values of important parameters.

We also compare the results from the atom-molecule simulations with the corresponding simulations for a system of structureless atoms; the method for simulating the structureless atom system is described in Sect. 7.3. In Sect. 7.4 we present the results from our coupled atom-molecule simulations, comparing them to other theoretical predictions, as well as to the experiment. In these simulations, we have omitted the initial noise terms of the truncated Wigner formalism. The corrections that would arise because of this approximation are discussed in Sect. 7.5.
7.1 Introduction

7.1.1 Properties of the Bragg Spectrum

The excitation spectrum of a non-interacting condensate scales quadratically with momentum because of the free-particle behaviour of the quasi-particles. If we instead consider an interacting condensate, the excitation spectrum is shifted from the non-interacting case, due to the atom-atom interactions. The excitation spectrum of a homogeneous condensate for large momentum transfer is given by the sum of the kinetic energy and the chemical potential of the condensate \[118\],

\[
\hbar \omega(k) = \frac{\hbar^2 k^2}{2m} + \frac{4\pi \hbar^2 n a_s}{m},
\] (7.1)

where \(k\) is the photon momentum, \(n\) is the density of the condensate and \(a_s\) is the s-wave scattering length. In the region where (7.1) is valid, it is equivalent to the Bogoliubov excitation spectrum in the limit of large \(k\).

In the case of an inhomogeneous condensate, for example a condensate in a harmonic trapping potential, it was found by Stenger et al. \[118\] that this formula can be used provided \(n\) is interpreted as the density-weighted density of the condensate. The use of the density-weighted density can be theoretically explained by using a local density description of the condensate: A volume element of the condensate at position \(x\) is seen as having a density \(n(x)\). This volume element contributes to a shift from the non-interacting condensate given by

\[
\Delta\omega(x) = \frac{4\pi \hbar^2 n(x) a_s}{m}.
\] (7.2)

The shift of the whole condensate would then be given by the integral

\[
\Delta\omega_{\text{tot}} = \int \Delta\omega(x) n(x) dx,
\] (7.3)

where the contribution of each volume element is weighted with the density (probability) function. This leads to the result

\[
\Delta\omega_{\text{tot}} = \frac{4\pi \hbar^2 a_s}{m} \int (n(x))^2 dx,
\] (7.4)

which is obviously equivalent to using (7.1) with the homogeneous density replaced with the density-weighted density.

Stenger et al. \[118\] found that the prediction (7.1) agreed well with experimental
The prediction (7.1) is expected to be valid as long as:

1. The condensate is dilute \((n a_s^3 \ll 1)\),

2. The excitation is in the free-particle regime \((1/(k \xi) \ll 1)\), where \(\xi = (8 \pi n a_s^{-1/2})\) is the condensate healing length), and

3. The scattering amplitude is momentum independent \((k a_s \ll 1)\) \([92]\).

The aim of the experiment of Papp et al. \([92]\) is to investigate the properties of the Bragg spectrum in a region where the scattering length is large. This means that the condensate interactions cannot be treated as mean-field \((\sqrt{8 \pi n a_s^3} \sim 0.5)\), the excitations are not clearly particle-like \((k \xi \sim 2)\), and the scattering amplitude is not clearly momentum independent \((k a_s \sim 0.8)\).

### 7.1.2 Theoretical Predictions

In the JILA experiment \([92]\), the measured shift of the Bragg spectra from the non-interacting case is compared to available theoretical predictions. In addition to that based on (7.1), several other predictions have been used, some of which are outlined in greater detail in \([107]\).

Since there is no available analytical way of treating a system where the three parameters above — \(n a_s^3\), \(1/(k \xi)\) and \(k a_s\) — are all non-zero, the approach by Papp et al. \([92]\) and Ronen \([107]\) is to find an expression for the Bragg detuning when one or two of the parameters are zero, and the others are non-zero. In Fig. 7.1 these different theoretical predictions are shown for the case of a homogeneous condensate.

The green solid line in Fig. 7.1 corresponds to the simple prediction in (7.1), which is equivalent to letting all three of the above parameters be small. The blue dotted line is obtained by letting \(1/(k \xi)\) be finite, but keeping \(k a_s\) and \(n a_s^3\) small. This is equivalent to the Bogoliubov spectrum given in (2.29).

The magenta dash-dot-dotted line and the red dashed line in Fig. 7.1 are calculated using corrections to the Bogoliubov excitation spectrum based on the work of Beliaev \([6]\). The derivations of these corrections are made using perturbation theory and assuming that \(1/(k \xi)\) is finite and \(na_s^3\) is small. The first correction, plotted as the red dashed line in Fig. 7.1, assumes that \(k a_s\) is finite, but that the diluteness parameter \(n a_s^3\) ¹

¹Note that the value of the diluteness given here is that specified by \([92]\); the diluteness parameter given in that paper has a factor of \(8 \pi\) compared to the usual diluteness parameter.
Figure 7.1: Theoretical predictions for the shift of the peak of the Bragg spectrum for a homogeneous condensate with density $7.6 \times 10^{13}$ cm$^{-3}$. The top axis shows the size of the LHY-correction relative to the condensate chemical potential. The different lines correspond to different approximations, made by keeping one or more parameters small: $k a_s$, $n a_s^3$ and $1/(k \xi)$ all small (green solid line); $k a_s$, $n a_s^3$ small (blue dotted line); $k a_s$ small (magenta dash-dot-dotted line); $n a_s^3$ small (red dashed line); and $1/(k \xi)$ small (black dash-dotted line). The green line corresponds to the result obtained from (7.1). Figure adapted from Fig. 1 in [92].

The calculation of the second Beliaev correction is outlined in detail in [107]. In this case, the diluteness parameter $n a_s^3$ is assumed to take on a finite value, but the scattering amplitude is assumed to be momentum-independent, so that $k a_s = 0$. The result is plotted as the magenta dash-dot-dotted line in Fig. 7.1, showing a clear increase in the excitation energy compared to the Bogoliubov result.

The last prediction in Fig. 7.1 plotted as the black dash-dotted line, corresponds to the excitation spectrum obtained from Hartree–Fock–Bogoliubov theory [51], but modified to include momentum-dependent scattering and beyond mean-field effects. This line therefore corresponds to the regime of $k a_s$ and $n a_s^3$ being finite, but $1/(k \xi)$ being negligible. The predicted line shift in the spectrum can in this case be given analytically as

$$ h \Delta \omega = \frac{4 \pi \hbar^2 n}{m} (2 a_s (k/2) - a_s (1 + \alpha_{\text{LHY}})), \tag{7.5} $$

is zero. The effect of this correction is to decrease the excitation energy of the condensate compared to that obtained from the Bogoliubov calculation.
where $\alpha_{\text{LHY}}$ is the LHY-correction, which is discussed in Sect. 2.1.4 and given by

$$\alpha_{\text{LHY}} \equiv \frac{32}{3\sqrt{\pi}} \sqrt{n a_s^3}. \quad (7.6)$$

In Fig. 7.1 the size of the LHY-correction is indicated on the top of the axis.

It is important to note that, with the sole exception of the Hartree–Fock–Bogoliubov calculation (represented by the black line in Fig. 7.1), all these theoretical approaches predict that the Bragg resonance detuning will increase with increasing interaction strengths. As we shall see in Sect. 7.1.5 this is not the case for the experimental result, where in fact the line shift decreases for large scattering lengths. Regardless, we do not expect these predictions to provide a physical explanation of the experiment, since they are all well outside of their region of validity.

### 7.1.3 Other work

Since the experiment by Papp et al. in 2008, other theoretical models have been developed to explain the results obtained in the experiment, and to predict the Bragg line shift from a strongly interacting Bose–Einstein condensate.

Leskinen et al. [74] explain some of the results of the JILA experiment using a model which describes the coupling between quasiparticles and gapless phonon-like modes. They find that the resonant scattering and absorption effects can explain the broadening of the spectrum of the Bragg pulse, since it allows transitions at higher energies, and that it can also explain the symmetric appearance of the line shape. However, this model does not shed any light on the most important result in the experiment, namely the anomaly in the line shift.

Another theoretical model is presented by Kinnunen et al. [63], who studied Bragg spectroscopy from a uniform and strongly interacting $^{85}\text{Rb}$ condensate using time-dependent Hartree–Fock–Bogoliubov theory. The main result from [63] is presented in Fig. 7.2, showing the line shift as a function of the scattering length. In this approach, they took into account the momentum dependent scattering amplitude, and found that the resonance detuning, or line shift, obtained in this way differs significantly from the prediction based on (7.1), as well as from Bogoliubov theory, as in Sect. 2.4.7. An added change to the excitation spectrum comes from the creation of mobile pairing fields associated with two-particle correlations. However, the difference is nowhere near as dramatic as that seen in the JILA experiment, and does not offer even qualitative agreement with the experimental results.

A recent study by Sarjonen et al., presented in two very similar papers [111, 112], approaches the JILA experiment using an effective atom-atom interaction from two
Figure 7.2: Line shift as a function of the scattering length for various theoretical approaches: Linear response using mean-field shift (7.1) (red solid line); Bogoliubov spectrum (blue dashed line); Hartree–Fock–Bogoliubov (HFB) without the mobile pairing fields $\Delta_{\pm 1}$ (cyan dotted line); and Hartree–Fock–Bogoliubov including the mobile pairing fields (magenta dash-dotted line). Apart from a slightly different density, the red line shown here is the same as the green line in Fig. 7.1. The top axis shows the magnitude of the diluteness parameter, $na_0^3$, which can easily be related to the LHY-correction. Figure adapted from Fig. 5 in [63].

coupled channels, following the method of [67]. They find good agreement with previous experimental values of the binding energy, although the resulting s-wave phase shifts approach the phase shifts from a simple contact potential, which would disagree with the experimentally determined values of the line shift by [92].

Sarjonen et al. go on to neglect the dynamics of the Feshbach resonance bound state, and use a soft sphere model for the local, effective atom-atom interaction potential. Using this method, they obtain excellent agreement with the experimental results of the line shift; however, the parameter values of the potential used are scaled to fit the experimental values of the line shift. Thus, this result does not offer any theoretical prediction about the line shift, but rather a fit to already known experimental values.

Although the results of these other theoretical works are interesting, none of them are able to present a theoretical prediction of the line shift measured in the JILA experiment. Furthermore, none of them treat the full complexity of the experimental situation studied; as we shall discuss in Sect. 7.1.6, the Bragg scattering problem itself, as well as the experimental procedure used by [92], introduce a number of issues when
interpreting the results. None of the theoretical approaches mentioned in this section, or in Sect. 7.1.2 deal with any of these issues. Instead, they study a homogeneous system, and do so without incorporating the full dynamics of the Feshbach resonance.

7.1.4 Outline of Experiment

The JILA experiment uses $^{85}$Rb in the $|F = 2, m_F = -2\rangle$ state. The $^{85}$Rb atoms are sympathetically cooled with $^{87}$Rb in a magnetic trap, followed by evaporative cooling in an optical dipole trap. A single-species Bose–Einstein condensate of approximately 40,000 $^{85}$Rb atoms is then created, with a condensate fraction of 85%.

The optical dipole trap is cigar shaped with an aspect ratio of 46.2 ($\nu_z = 2\pi \times 2.9\text{Hz}$, $\nu_r = 2\pi \times 134\text{Hz}$), and the average density of the condensate created is approximately $2.1 \times 10^{19} \text{m}^{-3}$. The condensate is created at a magnetic field strength of 163 G, where the scattering length is roughly $150a_0$.

Bragg scattering is performed by applying an optical potential to the condensate, in the form of a Bragg pulse. The Bragg pulse consists of two counter-propagating laser beams along the long axis of the condensate. The laser beams have a wavelength of 780 nm, meaning that the momentum imparted to the condensate is

$$\hbar k = 2\hbar \times \frac{2\pi}{780 \times 10^{-9}}.$$  (7.7)

The intensity and duration of the Bragg pulse is chosen such that no more than 10% of the atoms are scattered. With such a small scattered fraction, the scattering process should not cause any dramatic alterations to the properties of condensate, and the linear response can be probed.

In order to enhance the line shift of the Bragg resonance peak, and thus make the beyond-mean-field effects more clearly visible, the density of the condensate is increased before the application of the Bragg pulse. This is done by exciting the radial and axial breathing modes of the condensate by ramping the magnetic field close to the Feshbach resonance. At the inner turning point of the radial breathing mode, the scattering length is ramped to the value of interest, and the Bragg pulse is then applied.

After the Bragg pulse, the scattering length is ramped to a high value ($917a_0$), which ensures that the small fraction of scattered atoms stay in the cloud. Without the strong interactions, these scattered atoms could simply exit the cloud, making them harder to detect. Instead they transfer their momentum to the whole cloud, resulting in a centre of mass motion that can be easily detected. The condensate will then slosh around in the trap, and the total momentum of the condensate can then be inferred by measuring the amplitude of the slosh. This is done using absorption imaging at the axial turning
Figure 7.3: Experimental data of the Bragg spectra for three different scattering lengths from [92]. The figure shows the spectra for $a_s = 100a_0$ (blue triangles), $a_s = 585a_0$ (red circles) and $a_s = 890a_0$ (black squares). Lines are Gaussian fits to the data points. The space- and time-averaged density is approximately $7.6 \times 10^{-13} \text{ cm}^{-3}$, but is not necessarily the same for all three curves. Figure adapted from Fig. 2 in [92].

7.1.5 Experimental Results

By varying the frequency difference of the laser beams and measuring the resulting momentum transfer to the Bose–Einstein condensate, the excitation fraction of the condensate particles is determined. The Bragg spectrum is then obtained by plotting the momentum transfer as a function of the frequency difference. Fig. 7.3 shows the typical spectra for three different scattering lengths, where the experimental data have been fitted to an antisymmetric function assuming a Gaussian shape of each peak.

We see that as the scattering length is increased from $100a_0$ to $585a_0$ (blue and red curve, respectively), the spectral peak is shifted towards higher frequencies. Although, for the even larger scattering length $890a_0$ (black curve), the spectrum is shifted back towards a lower frequency. However, it is not possible to draw any direct conclusions from this result, since the density need not be the same for the three scattering lengths.

As discussed previously, the line shift of the Bragg resonance is the difference in the Bragg peak from the value expected for a non-interacting gas. In this experiment, the ideal gas peak would be at

$$\frac{1}{2\pi} \frac{\hbar k^2}{2m} \approx 15.4 \text{ kHz.}$$  (7.8)
Figure 7.4: Experimental measurements of the Bragg line shift as a function of scattering length. The open circles are the experimental observations, while the solid circles are the experimental data where corrections for the broad thermal atom background have been taken into account. The top axis shows the size of the LHY-correction relative to the condensate chemical potential. The error bars on these points represent fit uncertainties. The lines indicate the theoretical predictions, as in Fig. 7.1, with the density calculated for the trapped gas using a local density approximation. The error bars on the theory lines represent uncertainty in the determination of the density. Some of these error bars have been omitted for clarity. Figure adapted from Fig. 3(a) in [92].

Fig. 7.4 shows the line shift as a function of the scattering length. As in Fig. 7.1, the green solid line corresponds to the prediction from (7.1), and the other lines correspond to the theoretical predictions of [107], which have been calculated here for the space- and time-averaged density for each scattering length. For low scattering lengths, the experimental data agrees well with the theoretical predictions. However, for larger scattering lengths, there is a significant difference between the experimental result and the theoretical predictions. Most importantly, while all but one theoretical calculation predicts that the line shift will increase with stronger interactions, the experimental data shows that there is a decreasing shift for larger scattering lengths.

7.1.6 Interpreting the Experiment

There are several issues that complicate the analysis of the JILA experiment. We will address the most important of these in the following:
1. **Initial state**: The nonlinear effects that were investigated in the experiment are more pronounced the less dilute the condensate is. The density of the initial state in the experiment is therefore enhanced by a series of ramps of the scattering length. Creating an initial state in this way makes the experimental procedure even more complex, and takes the system further away from the simple, homogeneous case studied theoretically by [107] and [63]. Furthermore, the initial state parameters are not explicitly defined, which makes analysis of the line shift result difficult, since this depends on the properties of the condensate at the onset of the Bragg pulse.

2. **Inhomogeneity**: The trapped condensate is spatially inhomogeneous, and also strongly time varying, because of both three-body losses and condensate expansion in the breathing modes, and even as a result of the Bragg scattering process itself (as we shall see in Sect. 7.4.1). Papp *et al.* [92] measure and use space-averaged densities, rather than the density-weighted densities, which (as we noted above) are more appropriate when comparing with results for a homogeneous condensate. In addition to this, they also average densities over the duration of the experiment.

The problem with using the space-averaged density is that, unless the condensate has clearly defined volume, the space-averaged density cannot be accurately determined. In an experiment such as that of [92], the volume is not easily determined and has to be approximated in one way or another.

In [92], the time- and space-averaged density was determined by assuming that the density profile of the condensate is given by a Thomas–Fermi profile with a width given by a variational solution to the Gross–Pitaevskii equation. The variational model, outlined in [93] is, however, not an accurate representation of an exact solution of the Gross–Pitaevskii equation, which even in three dimensions, is not very difficult to find numerically.

Furthermore, it is not clear how accurate a description of the shape of the condensate is given here by a Thomas–Fermi profile. As we shall see in Sect. 7.4.1 in our simulations the shape of the condensate is very different from that given by the Thomas–Fermi approximation, both before and during the application of the Bragg pulse.

3. **Variable pulse length and intensity**: The condensate density varies more rapidly in time as a result of Bragg scattering at larger scattering lengths. By introducing the condition that the density of the condensate cannot change by more than
30% during the Bragg pulse, based on predictions from the variational model, the experiment is forced to use progressively shorter Bragg pulses for larger scattering lengths. To make sure that roughly the same quantity is scattered out each time, the intensity of the pulses is appropriately increased.

In our calculations, we find that the processes involved are sensitive to the duration and intensity of the Bragg pulse, because the condensate expands, because there are three-body losses, and because the spectroscopic resolution improves for longer pulses. It is therefore important to reproduce the experimental parameters as faithfully as possible. Unfortunately, neither the duration nor the intensity of the Bragg pulse are explicitly stated in [92], so we have inferred their values from the spectra and the limits on the number of Bragg-scattered atoms.

4. Time scales: Bragg scattering is a fast process and it is therefore important to consider the other time scales associated with the experiment; if other processes occur on a time scale similar to that of the Bragg scattering, it is likely that those processes are important for the dynamics of the condensate.

There are three time scales that are relevant in this type of experiment, shown in Fig. 7.5 in terms of their corresponding frequencies: The frequency of the applied Bragg pulse, the inverse of the pulse duration and the binding frequency of the bound state in the Feshbach resonance. For large scattering lengths and short Bragg pulses, these frequencies are comparable, and it is therefore very probable that the bound state dynamics become important to the overall dynamics of the experiment.

The unknown parameters make it difficult to model the specific experiment of [92] correctly. However, the inhomogeneity of the system and the fast time scales associated with the Bragg scattering process, introduce an extra complexity to the system which needs to be considered when making any prediction of the line shift. Indeed, as discussed in Sect. 7.1.3, there are no previous theories which have been able to reproduce the experimental results of the line shift in a satisfying way.

7.2 Simulation System Set-Up

We simulate the experiment of Papp et al. [92] using the methods described in Chap. 6. We evolve the atom and molecule fields according to the equations of motion using the RK4IP-P algorithm in three spatial dimensions. In the following section, we describe the set-up for these numerical simulations in detail.
Figure 7.5: Frequency scales in the experiment [92]. The solid line indicates the binding frequencies for different scattering lengths, estimated from the data presented in [27]. The dashed line is the inverse of the duration of the Bragg pulse. The shaded region indicates the range of frequencies \( \omega \) of the optical potential.

Table 7.1: Properties of \(^{85}\text{Rb}\) and the Feshbach resonance used in this simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>In SI-units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass</td>
<td>( m )</td>
<td>84.9 u</td>
<td>1.41 \times 10^{-25} kg</td>
</tr>
<tr>
<td>Background scattering length</td>
<td>( a_{bg} )</td>
<td>-443( a_0 )</td>
<td>-2.34 \times 10^{-8} m</td>
</tr>
<tr>
<td>Resonance position</td>
<td>( B_0 )</td>
<td>155.04 G</td>
<td>0.0155 T</td>
</tr>
<tr>
<td>Resonance width</td>
<td>( \Delta B )</td>
<td>10.7 G</td>
<td>0.107 mT</td>
</tr>
<tr>
<td>Magnetic moment</td>
<td>( \Delta \mu )</td>
<td>-2.33( \mu_B )</td>
<td>-2.16 \times 10^{-23} J/T</td>
</tr>
</tbody>
</table>

7.2.1 Simulation Parameters

In choosing the parameters for our simulation, we follow the experimental set-up as closely as possible, and model a condensate of 40,000 \(^{85}\text{Rb}\) atoms in a trap with cylindrical symmetry and an aspect ratio of 46.2 (\( \nu_z = 2\pi \times 2.9\text{Hz}, \nu_r = 2\pi \times 134\text{Hz} \)). The scattering length ranges from 150\( a_0 \) to 890\( a_0 \), and we use the relationship between the scattering length and the parameters \( g \) and \( \epsilon \) derived in Chap. 6 and given by equations (6.3, 6.4).

The properties of \(^{85}\text{Rb}\) and the Feshbach resonance of interest in these simulations are listed in Tab. 7.1.
7.2.2 Initial State

In the experiment, an initial condensate was created with a scattering length of $150a_0$. The scattering length was then ramped to an unspecified low value, exciting the large-amplitude breathing modes in the condensate. At the inner radial turning point of the breathing mode oscillation, the scattering length was ramped up to the desired value, and the Bragg pulse was applied. Through this process, the condensate becomes much more dense, making the nonlinear effects on the Bragg spectra more clearly visible. However, it is hard to know exactly what the initial state is at the commencement of the Bragg pulse; had the condensate not been compressed in this way, the initial state would have been clearly defined.

Since the initial state of the experiment is not an equilibrium state, it cannot be easily recreated. In our simulations, we create the initial state for the Bragg spectroscopy in such a way as to reconstruct the physics of the experiment. We do this by performing the following steps:

1. We set the scattering length to a small, initially arbitrary, value $a_{\text{init}}$. The exact value of $a_{\text{init}}$ varies depending on the scattering length, but is typically of the order of a few $a_0$, see Tab. 7.2.

2. We numerically solve time-independent equations of motion (6.36, 6.37) for this scattering length, using the Thomas–Fermi equations that we derived in Chap. 5 as the starting position, following the procedure described in Sect. 6.3.

3. We quickly ramp the scattering length up to the value of interest, in the range between $150a_0$ and $890a_0$. The speed of the ramp never exceeds $\dot{a}_s / a_s < 0.25\hbar / ma_s^2$. The density of the condensate after the ramp is listed in Tab. 7.2.

4. We then apply the Bragg pulse while continuing to run the simulation, and calculate the resulting time-average of the density-weighted density for the duration of the Bragg pulse. In our simulations, the density-weighted density $\tilde{n}(t)$ is given by

$$\tilde{n}(t) = \frac{1}{N(t)} \int dx \left( |\psi(x, t)|^2 + 2|\phi(x, t)|^2 \right)^2,$$  \hspace{1cm} (7.9)

$$N(t) = \int dx \left( |\psi(x, t)|^2 + 2|\phi(x, t)|^2 \right).$$  \hspace{1cm} (7.10)

Here $N(t)$ and $\tilde{n}(t)$ involve “effective numbers of atoms”, counting each molecule as two atoms, corresponding to what would in practice be measured in an experiment.
Table 7.2: The initial scattering length and density-weighted densities used for the different scattering lengths in the simulation performed here. Values of the initial scattering length (column 2) for the scattering lengths simulated in this work (column 1). The resulting density after the scattering length has been ramped from the initial value to the desired simulation value are listed in column 3.

<table>
<thead>
<tr>
<th>$a_s [a_0]$</th>
<th>Initial scattering length $[a_0]$</th>
<th>Initial density-weighted density $[10^{19} \text{ m}^{-3}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>0.5</td>
<td>17.4</td>
</tr>
<tr>
<td>300</td>
<td>1.0</td>
<td>13.8</td>
</tr>
<tr>
<td>500</td>
<td>1.5</td>
<td>11.9</td>
</tr>
<tr>
<td>585</td>
<td>1.7</td>
<td>11.4</td>
</tr>
<tr>
<td>695</td>
<td>1.5</td>
<td>11.9</td>
</tr>
<tr>
<td>805</td>
<td>2.0</td>
<td>10.8</td>
</tr>
<tr>
<td>890</td>
<td>2.0</td>
<td>10.8</td>
</tr>
</tbody>
</table>

5. We adjust $a_{\text{init}}$ appropriately, and repeat steps 1-4 until the time-averaged density-weighted density obtained matches that of the experiment.

The experimental space- and time-averaged density is inferred from the predictions of the line shift (Fig. 3(a) in [92]). This varies from $7.6 \times 10^{13} \text{ cm}^{-3}$ for 150$a_0$ to between approximately 4.8 and $8.2 \times 10^{13} \text{ cm}^{-3}$ for 890$a_0$, see Tab. 7.3. We relate the experimental space-averaged density to our density-weighted density by noting that the space-averaged density for a Thomas–Fermi profile is 0.7 times the density-averaged density. The same factor is not necessarily appropriate for other profile shapes, and as we shall see, the condensate in our simulations is quite far from Thomas–Fermi shaped. However, we believe that this nonetheless gives us the best estimate of the density used in [92] that we can reasonably expect to get, since it corresponds to the procedure used in the experiment to estimate the space-averaged density.

### 7.2.3 Time Step

The propagation algorithm used to evolve the equations of motion calculates the fields $\psi$ and $\phi$ at regular time intervals $t_n = t_0 + n\Delta t$. The size of the time step, $\Delta t$, has to be set to be small enough to ensure the differential equations converge. However, too small a value of the time step would make the computation time unreasonable; the parameter $\Delta t$ is therefore chosen as a compromise between these two factors, in general just below the convergence limit. In this work we find a suitable $\Delta t$ for each simulation by monitoring the total atom number (7.10) when evolving the equations of motion without including the three-body loss term, and ensuring that the atom number stays constant to within approximately 0.01% throughout the simulation.
Table 7.3: Experimental average densities (column 3) for different scattering lengths (column 1). The data for the shift (column 2) are taken from Fig. 3(a) in [92]. Column 4 lists the approximate ranges of the average densities, where the values in brackets are our estimates. Column 5 shows the time averages of the density-weighted density that we use in our numerical calculations.

<table>
<thead>
<tr>
<th>(a_s) ([a_0])</th>
<th>(f_{\text{shift}}) [kHz]</th>
<th>Time- and space-average density ([10^{19} \text{ m}^{-3}])</th>
<th>Range ([10^{19} \text{ m}^{-3}])</th>
<th>Time-average density-weighted density ([10^{19} \text{ m}^{-3}])</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>0.9</td>
<td>7.6</td>
<td>7.6</td>
<td>10.857</td>
</tr>
<tr>
<td>300</td>
<td>1.7</td>
<td>7.2</td>
<td>7.2</td>
<td>10.286</td>
</tr>
<tr>
<td>500</td>
<td>2.9</td>
<td>7.3</td>
<td>7.1–7.6</td>
<td>10.429</td>
</tr>
<tr>
<td>585</td>
<td>3.0</td>
<td>6.5</td>
<td>(5.6 – 7.4)</td>
<td>9.286</td>
</tr>
<tr>
<td>695</td>
<td>3.8</td>
<td>6.9</td>
<td>(6.2 – 7.6)</td>
<td>9.857</td>
</tr>
<tr>
<td>805</td>
<td>3.9</td>
<td>6.1</td>
<td>4.9–7.4</td>
<td>8.714</td>
</tr>
<tr>
<td>890</td>
<td>4.6</td>
<td>6.5</td>
<td>(4.8 – 8.2)</td>
<td>9.286</td>
</tr>
</tbody>
</table>

We find that the simulations for smaller scattering lengths — where the molecule field is much smaller than the atom field — require a smaller time step than those for larger scattering lengths, where the molecule field is more significant. We also find that the time step needs to be set to smaller and smaller values the more noise we include in the initial state. These results are hardly surprising; the coupled differential equations we are considering are stiff equations and the accuracy of the numerical solutions are therefore expected to be highly dependent on the step size.

In the simulations where we omit the initial noise, the time step varies from approximately 0.12 \(\mu\)s for a scattering length of 150\(a_0\) to 0.2 \(\mu\)s for a scattering length of 890\(a_0\). For the simulations with noise terms added to the initial modes, typical values of the time step is 0.03 \(\mu\)s for a scattering length of 150\(a_0\) to 0.05 \(\mu\)s for a scattering length of 890\(a_0\).

### 7.2.4 Bragg Pulse

The Bragg pulse, modelled by (6.7), is applied at the start of the simulation with a wave number of \(k = 1.6 \times 10^7 \text{ m}^{-1}\) in the axial direction of the condensate. The pulse durations are not explicitly stated in [92], but can be inferred from the data for the widths of the spectra (Fig. 3(b) in [92]), see Tab. 7.4.

The Fourier transform of the optical potential is given by

\[
\int_0^T V_0 e^{i\omega t} \cos (q \cdot x - \omega_0 t) dt \approx V_0 e^{i q \cdot x} e^{i(\omega - \omega_0) T/2} \sin ((\omega - \omega_0) T/2) \frac{\sin((\omega - \omega_0) T/2)}{\omega - \omega_0}.
\] (7.11)

The pulse duration can then be found by fitting a Gaussian to this result and observ-
Table 7.4: Pulse lengths for different scattering lengths. The data for the width are taken from Fig. 3 in [92].

<table>
<thead>
<tr>
<th>Scattering length $a_s [a_0]$</th>
<th>Width from duration $\Delta f$ [kHz]</th>
<th>Pulse length $t$ [ms]</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>0.8</td>
<td>0.45</td>
</tr>
<tr>
<td>300</td>
<td>1.5</td>
<td>0.24</td>
</tr>
<tr>
<td>500</td>
<td>2.5</td>
<td>0.14</td>
</tr>
<tr>
<td>585</td>
<td>3.0</td>
<td>0.12</td>
</tr>
<tr>
<td>700</td>
<td>3.4</td>
<td>0.11</td>
</tr>
<tr>
<td>800</td>
<td>3.7</td>
<td>0.10</td>
</tr>
<tr>
<td>890</td>
<td>4.0</td>
<td>0.09</td>
</tr>
</tbody>
</table>

Table 7.5: Properties of the Bragg pulse for different scattering lengths.

<table>
<thead>
<tr>
<th>Scattering length $a_s [a_0]$</th>
<th>Duration $t$ [ms]</th>
<th>Amplitude $V_0$ [h kHz]</th>
<th>Scattered fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>0.45</td>
<td>0.13</td>
<td>6.2%</td>
</tr>
<tr>
<td>300</td>
<td>0.24</td>
<td>0.40</td>
<td>6.7%</td>
</tr>
<tr>
<td>500</td>
<td>0.14</td>
<td>0.67</td>
<td>6.5%</td>
</tr>
<tr>
<td>585</td>
<td>0.12</td>
<td>0.80</td>
<td>7.5%</td>
</tr>
<tr>
<td>695</td>
<td>0.11</td>
<td>0.80</td>
<td>6.4%</td>
</tr>
<tr>
<td>805</td>
<td>0.10</td>
<td>0.94</td>
<td>7.1%</td>
</tr>
<tr>
<td>890</td>
<td>0.09</td>
<td>1.07</td>
<td>8.0%</td>
</tr>
</tbody>
</table>

Thus, the pulse duration ranges from 0.09 ms for 890$a_0$ to 0.45 ms for 150$a_0$, see Tab.7.5 In Tab.7.5 we have also listed the Bragg pulse amplitudes, $V_0$, for the different values of the scattering length. The intensities of the Bragg pulse are not stated in [92], but as in the experiment, it is chosen so that there is always between 5% and 10% of the condensate atoms scattered out, see Tab.7.5. Determining the Bragg intensity this way will of course add some uncertainty to our simulations, however, we find that the results are not highly dependent on the exact choice of $V_0$, as long as it is chosen so that the scattered fraction is between 5% and 10%. In comparison to how much the results depend on the density and the pulse duration, the choice of intensity is therefore not of crucial importance.
7.3 Simulations of Structureless Atoms

Table 7.6: Three-body loss parameters for different scattering lengths.

<table>
<thead>
<tr>
<th>Scattering length $a_s [a_0]$</th>
<th>Loss $\gamma$ [cm$^{-7}$/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>$5 \times 10^{-29}$</td>
</tr>
<tr>
<td>300</td>
<td>$1.5 \times 10^{-27}$</td>
</tr>
<tr>
<td>500</td>
<td>$5 \times 10^{-27}$</td>
</tr>
<tr>
<td>585</td>
<td>$1.5 \times 10^{-26}$</td>
</tr>
<tr>
<td>695</td>
<td>$2 \times 10^{-26}$</td>
</tr>
<tr>
<td>805</td>
<td>$2.5 \times 10^{-26}$</td>
</tr>
<tr>
<td>890</td>
<td>$3 \times 10^{-26}$</td>
</tr>
</tbody>
</table>

7.2.5 Three-Body Loss Coefficient

As discussed in Sect. 2.3, the rate of particle loss from the condensate arising from three-body recombination events varies with the scattering length, approximately proportionally to $a_s^4$ [14]. It is also extremely sensitive to the density. There are no exact values of the three-body loss coefficient ($\gamma$ in (6.1)) available; here we have used the theoretical values given by Braaten et al. [15], which qualitatively agreed with previous experimental data from Roberts et al. [106]. However, as is noted in [15], these values have a large uncertainty.

The three-body loss parameter $\gamma$ has been determined by using the corresponding values of the three-body recombination rate $K_3$ given by Braaten et al. [15], see Tab. 7.6.

7.3 Simulations of Structureless Atoms

For comparison with the simulations based on our formalism, we also run simulations based on a simple Gross–Pitaevskii equation. This corresponds to modelling the condensate using a single field $\Psi$, and by letting the interaction strength be determined solely by the scattering length. In the c-field formalism, the equation of motion for the single-component condensate is in this case given by

$$\frac{\partial \Psi(x)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(x) + P_a \{ V_a(x) \Psi(x) \\
+ U_0 |\Psi(x)|^2 \Psi(x) \} - i \gamma |\Psi(x)|^4 \Psi(x), \quad (7.13)$$
where the parameters are the same as in (6.1), except the atom-atom interaction which is now given by

\[
U_0 = \frac{4\pi \hbar^2 a_s}{m \left(1 - 2\Lambda a_s / \pi\right)}.
\] (7.14)

### 7.4 Results of Simulations of the Mean-Field Equations

The underlying equations of motion in the c-field formalism are the same as those of mean-field theory, and the effects quantisation are introduced by the inclusion of fluctuations in the initial state. The inclusion of the fluctuations can cause very dramatic changes in the nature of the solutions, as was found in [89]. In the Bragg scattering problem under study here, we have found that the effects of the quantum fluctuations are in fact rather small. It is therefore logical to study first the solutions of the equations in the absence of the added noise in the initial conditions, which amounts to a mean-field description of the system of atoms and molecules. Indeed, we find that these simulations provide a very satisfactory description of the problem, and that the results agree very well with the experimental results of [92]. The effect of the noise terms is thus a matter of determining relatively small corrections to the mean-field theory, and this will be done in the following section.

#### 7.4.1 General Behaviour

The coordinate space profiles from a typical simulation run are shown in Fig. 7.6. The scattering length is in this case 890\(a_0\). Fig. 7.6(a) shows the radial and axial profiles of the condensate after it has been ramped to the scattering length of interest, at the moment just before the Bragg pulse is applied. Fig. 7.6(b) shows the profiles for the same simulation run, at the end of the Bragg pulse.

As can be clearly seen in Fig. 7.6(a) before the onset of the pulse, the condensate profile in the axial direction is similar in shape to a Thomas–Fermi profile, whereas in the radial direction it is more Gaussian. This is a result of the elongated shape of the condensate, due to the aspect ratio of the trap. As noted in Sect. 7.1.6, this makes any estimate of the average density difficult to justify.

The Bragg pulse is applied in the axial direction; in Fig. 7.6(b) we can clearly see the effect of this as interference fringes in the axial profile of the condensate. In the radial direction we have therefore plotted two distinctly different profiles, corresponding to the crest and trough of the central fringe. We obtain similar profiles with large density variations for each of the different scattering lengths in our simulations.

The particle losses arising from three-body recombination events and the change
7.4. Results of Simulations of the Mean-Field Equations

Figure 7.6: Coordinate space profiles for \( a_s = 890a_0 \) at a time (a) just before the Bragg pulse is applied, and (b) at the end of the Bragg pulse. The left panels show a slice of the condensate in the axial direction, i.e. the direction of the pulse, and the right panels show slices in the radial direction. In the bottom right panel we show two slices, corresponding to the crest (solid line) and trough (dashed line) of the interference fringe centered around \( x = 0 \). The inset in the bottom left panel shows the profile appearance in the region marked by the red box. The parameter \( r_0 \) is the length scale associated with the trap, given by \( r_0 = \sqrt{\hbar/2m\omega_r} \approx 6.665 \times 10^{-7} \text{m} \) (see Sect. 6.2).

In density in our simulations are very different from those predicted by [92], whose prediction is that the density will change by “less than 30%”. In contrast, in our simulations the density changes by up to 70% of the initial density (see Tab. 7.7). Furthermore, in the experiment, the three-body loss is observed to be “typically <30%” [92]; whereas in our simulations the losses never exceed 10% of the total atom number. We believe that the main reason for these differences is the inappropriate model to describe the condensate used in [92]. However, there is also a significant degree of uncertainty in our calculations of the three-body loss, because of the lack of accurate data for the loss rate, and this could also contribute to the discrepancy.

Using our model and the available experimental data of the loss rate, we find that
the three-body loss in this system has a very small effect on the density. Instead, the change in density is mostly due to the expansion of the condensate. Since the small scattering lengths are associated with much longer simulation times than the larger ones, this also explains why we see the biggest change in the density for these, even though the three-body losses are much smaller.

Table 7.7: Condensate three-body loss and density change during the Bragg pulse, for the different scattering lengths.

<table>
<thead>
<tr>
<th>Scattering length $a_s [a_0]$</th>
<th>Three-body loss</th>
<th>Density change</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>1%</td>
<td>70%</td>
</tr>
<tr>
<td>300</td>
<td>2.5%</td>
<td>50%</td>
</tr>
<tr>
<td>500</td>
<td>2.5%</td>
<td>33%</td>
</tr>
<tr>
<td>585</td>
<td>4%</td>
<td>30%</td>
</tr>
<tr>
<td>695</td>
<td>5%</td>
<td>30%</td>
</tr>
<tr>
<td>805</td>
<td>5.5%</td>
<td>26%</td>
</tr>
<tr>
<td>890</td>
<td>6%</td>
<td>24%</td>
</tr>
</tbody>
</table>

7.4.2 Bragg Spectra and Line shift

The Bragg spectrum is obtained by changing the frequency difference, $\omega$, in (6.7), and calculating the momentum transferred to the condensate for each frequency. We calculate the normalised momentum transfer as

$$ P(t) = \frac{1}{N(t)|q|} \int dk \left( |\psi(k, t)|^2 + 2|\phi(k, t)|^2 \right) k. \quad (7.15) $$

Fig. 7.7 shows the normalised momentum transfer calculated in this way as a function of time. Here, the scattering length is $500a_0$ and we are plotting the result for several different values of the Bragg frequency.

Typical Bragg spectra from our simulations are shown in Fig. 7.8. The difference in width between the different spectra is due to the change in duration of the Bragg pulse. The peaks of the spectra in Fig. 7.8 are shifted from the position of the corresponding peaks for the non-interacting gas, located at approximately 15.4 kHz.

In Fig. 7.9, the shifts of the Bragg spectra from result for the non-interacting case are plotted as a function of the scattering length.

For comparison, we have also plotted the experimental results of the Bragg line shift from [92]. Fig. 7.9 also includes the theoretical prediction of the line shift based on (7.1), but using the density-weighted density instead of the space-averaged density used in the experimental paper. For a Thomas–Fermi profile, the density-weighted
7.4. Results of Simulations of the Mean-Field Equations

Figure 7.7: Momentum transfer for $500a_0$ as a function of time for several different values of the Bragg frequency.

As can be seen clearly in the figure, the simulations based on our model show quantitative agreement with the experimental data. We have included error bars on these data points; the error bars indicate the uncertainty in the experimental estimates of the density. Similar error bars should therefore also be included on the other lines in Fig. 7.9, but we have omitted these for clarity.

For small scattering lengths, the molecule field is very small, but nevertheless plays an important role, since its presence gives rise to a positive scattering length, in contrast to the negative background scattering length. The fact that the binding energy is larger at low scattering lengths makes it possible for the molecule field to adiabatically follow the atom field, and thus the condensate behaviour is very similar to that predicted by a Gross–Pitaevskii description. This is clear in Fig. 7.9, where we have included the result from the simulations based on the Gross–Pitaevskii equation (7.13). At larger scattering lengths, however, the bound state evolves more slowly and the atom-molecule simulations become very different from those for structureless atoms.

Finally, in Fig. 7.9 we have included the results from Bogoliubov treatments of the...
ideal case of a uniform condensate, both for the case of a single atom field, as in \[8, 9\],
and in the case of an atom-molecule system, as in Chap. [5]. We find that the atom-molecule Bogoliubov treatment shows surprisingly close agreement with both our simulations and with the experimental data.

### 7.5 Results of Full C-Field Simulations

In the c-field methods, the effect of quantum fluctuations is included by adding stochastic terms to the initial state, corresponding to on average half a particle per mode. In our treatment of Bragg scattering, we will follow the procedure discussed in Sect. 6.3.3 of adding Gaussian random noise, \( r(k) \) and \( s(k) \), with zero mean and unit standard deviation to the initial momentum amplitudes for the atoms (\( \psi_0 \)) and molecules (\( \phi_0 \)), according to

\[
\psi(k) = \psi_0(k) + \frac{r(k)}{\sqrt{2}}, \quad \phi(k) = \phi_0(k) + \frac{s(k)}{\sqrt{2}}. \tag{7.16}
\]

Each simulation run can then be seen as corresponding to a single run of an experiment, and the expectation values of observables are obtained by taking the average of
7.5. Results of Full C-Field Simulations

Scattering length $a$

Line shift [kHz]

Experimental data
Simple shift prediction
Atom Bogoliubov
Atom-molecule Bogoliubov
Atom simulation
Atom-molecule simulation

Figure 7.9: The shift of the peak of the Bragg spectra for different values of the scattering length. The solid lines are results from our simulations, the dashed lines are the experimental results and predictions presented in [92] and the dash-dotted lines are calculations based on the Bogoliubov treatment of Chap. 5. Our atom-molecule simulation (green diamonds) is significantly different from that of the structureless atom (red stars), but agrees well with both the experimental data (black circles) and the atom-molecule Bogoliubov calculation (magenta plusses). The prediction of the line shift based on the excitation spectrum in the large $k$ limit of equation (7.1) (blue squares) shows a very different behaviour for large scattering lengths, as does the structureless Bogoliubov calculation (cyan crosses). The error bars on our atom-molecule calculation indicate the uncertainty in the experimental estimates of the density, as is shown in Tab. 7.3 similar error estimates would apply to the other curves, but have been omitted for clarity.

several different runs. The average of the noise amplitudes is obviously

$$\langle \left| r(k) \right|^2 \rangle = \frac{1}{2}, \quad (7.17)$$

corresponding to half a noise particle per mode.

Fig. 7.10 shows the phase of the spatial atom and molecule fields for a slice in the $xy$-plane for the same system as in Fig. 7.9 at the end of the Bragg pulse. Since the initial stochastic terms are added to the momentum space wavefunctions, and since the molecule projector encompasses a much larger part of momentum space than the atom one, there are many more noise particles in the molecule field than in the atom one. Despite this, and the fact that the molecule field is much smaller than the atom one, there is still a clearly visible phase coherence in the molecule field.
Figure 7.10: Phase plots of a slice of the condensate centered around \( z = 0 \) for a scattering length of \( a_s = 890a_0 \), showing the atom part (top panel) and the molecule part (bottom panel) of the system. The total number of particles is here around 40,000, with approximately 34,000 atoms as atoms, and 6,000 atoms as molecules. The total number of noise particles is 30,000 for the atom field and 500,000 for the molecule field. The parameter \( r_0 \) is the length scale associated with the trap, given by \( r_0 = \sqrt{\hbar/2m\omega_r} \approx 6.665 \times 10^{-7} \text{ m} \) (see Sect. 6.2).

It is remarkable that the noise evident in the phase of the molecule field has very little effect on the results of simulations. The large positive scattering length arises directly from the population of the molecule field, and one might have expected its value to be significantly affected by the quantum fluctuations as they appear in the c-field model. However, we find that the behaviour of the molecule field is strongly dependent of the atom field, and that the molecules cannot be seen as independent particles, but rather as a different form of atoms. The atom field is less dominated by the noise, and since the molecules are strongly coupled to this field, they are not as influenced by the molecule field noise as one would expect.

### 7.5.1 Density-Weighted Density

The way to calculate the density-weighted density in the c-field formalism is described in Sect. 6.7 whose results are in summary:
1. The average total particle number in the simulations using the c-field formalism is given by

\[
\overline{N(t)} = \left\langle \int \, dx \left[ \{ \hat{n}_a(t) \}_\text{sym} + 2 \{ \hat{n}_m(t) \}_\text{sym} - \frac{\Delta_a}{2} - \Delta_m \right] \right\rangle, \tag{7.18}
\]

where \{ \hat{n}_a(x, t) \}_\text{sym} and \{ \hat{n}_m(x, t) \}_\text{sym} are the symmetrically-ordered averages

\[
\{ \hat{n}_a(x, t) \}_\text{sym} \equiv \{ \hat{\psi}^\dagger(x, t) \hat{\psi}(x, t) \}_\text{sym}, \tag{7.19}
\]

\[
\{ \hat{n}_m(x, t) \}_\text{sym} \equiv \{ \hat{\phi}^\dagger(x, t) \hat{\phi}(x, t) \}_\text{sym}. \tag{7.20}
\]

The parameters \( \Delta_a \) and \( \Delta_m \) correspond to the noise on the atom and molecule coordinate space wavefunctions, respectively, given by

\[
\langle |r(k)|^2 \rangle = \Delta_a, \tag{7.21}
\]

\[
\langle |s(k)|^2 \rangle = \Delta_m. \tag{7.22}
\]

As discussed in the previous section, the molecule field has much more initial noise added to it, therefore \( \Delta_m \) will be much larger than \( \Delta_a \).

2. The coordinate space density-weighted density is given by

\[
\overline{n(t)} = \frac{1}{\overline{N(t)}} \left\langle \int \, dx \left[ \overline{n_a^2(x, t)} + 4 \overline{n_m^2(x, t)} - 2\Delta_a \{ \hat{n}_a(t) \}_\text{sym} - 2\Delta_m \{ \hat{n}_m(t) \}_\text{sym} + \Delta_a \Delta_m \right] \right\rangle, \tag{7.23}
\]

where \( \overline{n_a^2(x, t)} \) and \( \overline{n_m^2(x, t)} \) are given by

\[
\overline{n_a^2(x, t)} = \{ \hat{n}_a^2(x, t) \}_\text{sym} - 2\Delta_a \{ \hat{n}_a(x, t) \}_\text{sym} + \frac{\Delta_a^2}{2}, \tag{7.24}
\]

\[
\overline{n_m^2(x, t)} = \{ \hat{n}_m^2(x, t) \}_\text{sym} - 2\Delta_m \{ \hat{n}_m(x, t) \}_\text{sym} + \frac{\Delta_m^2}{2}, \tag{7.25}
\]

and

\[
\{ \hat{n}_a^2(x, t) \}_\text{sym} \equiv \{ \hat{\psi}^4(x, t) \hat{\psi}^2(x, t) \}_\text{sym}, \tag{7.26}
\]

\[
\{ \hat{n}_m^2(x, t) \}_\text{sym} \equiv \{ \hat{\phi}^4(x, t) \hat{\phi}^2(x, t) \}_\text{sym}. \tag{7.27}
\]

We run 30 simulations with noise and compare the density-weighted density obtained from these runs using (7.23) with that obtained in a single simulation run without any stochastic terms added to the initial state. The result for one of these compar-
Figure 7.11: Time evolution of the density-weighted density during the application of the Bragg pulse to a condensate. The scattering length is $a_s = 890a_0$, and the pulse length is 0.09ms. The solid line is calculated using (7.23) for 30 different runs, with error bars indicating the statistical standard error from these runs. The dashed line shows the density-weighted density from a simulation without initial noise. The dotted lines show the time-average of the density-weighted density for the noise free simulation (blue) and for the full simulations (magenta).

As can be seen clearly in the figure, the initial density-weighted density is the same for both the noise-free simulation and the average of the 30 runs with noise. However, as the condensate evolves over time, the density from the c-field simulations is slightly lower than that from the noise-free run. The resulting time-average of the density-weighted density will therefore be slightly higher if we neglect the initial fluctuations, although the size of the change is much less than the experimental uncertainty.

### 7.5.2 Bragg Spectra from C-Field Simulations

For the full c-field simulations, instead of the results in (7.10, 7.15), we calculate the momentum transfer as

$$P(t) = \frac{1}{N(t)|q|} \left\langle \int d\mathbf{k} \left( |\psi(\mathbf{k}, t)|^2 + 2|\phi(\mathbf{k}, t)|^2 - \frac{3}{2} \right) \mathbf{k} \right\rangle,$$  \hspace{1cm} (7.28)
where the factor of $\frac{3}{2}$ is subtracted to account for the initial noise. Similarly, the total number of particles is given by

$$N(t) = \left\langle \int dk \left( |\psi(k, t)|^2 + 2|\phi(k, t)|^2 - \frac{3}{2} \right) \right\rangle,$$

(7.29)

Fig. 7.12 shows the momentum transfer calculated using equation (7.28), where the average has been taken over 30 simulation runs. In comparison, we have also plotted the momentum transfer from a single simulation run without any initial noise terms. The c-field simulations give a spectrum that is slightly narrower than the noise-free simulation and with a slightly lower amplitude. However, the position of the spectral peak is essentially the same for both the simulations with and without initial noise.

In our simulations, we find that averaging over several different c-field simulations in this way gives us results very similar to those obtained by running the same simulation without including the noise. Although the vacuum fluctuations seem to have some small effect on the evolution density, overall, the effect on the condensate dynamics appears to be unimportant to the Bragg scattering experiment. We can therefore be confident that the simulations of the mean-field equations of the atom-molecule system which we did in Sect. 7.4-equivalent to omitting the initial quantum fluctuations—provide a reliable description of the Bragg scattering experiment.
Chapter 8

Conclusion

8.1 Thesis Summary

In this thesis, we have used a truncated Wigner formalism to describe the dynamic behaviour of Bose-gas systems in the vicinity of magnetic Feshbach resonances. The motivation for this work comes from an experiment [92], in which the Bragg excitation spectrum for a gas of $^{85}$Rb with a Feshbach-resonance-enhanced s-wave scattering length was studied. The results of the experiment differed significantly from those predicted by existing theories.

We have modelled the effect of the Feshbach resonance by using a coupled atom-molecule Hamiltonian and have developed a formalism for using this system within the c-field framework. We showed how this Hamiltonian may be used to simulate realistic atom-molecule systems, as long as the binding energy and s-wave scattering length are known. We demonstrated how the mapping of these real parameters to the phenomenological parameters in the Hamiltonian will be dependent on the choice of the cutoff, but that the results obtained in simulations should be essentially independent of the choice of the cutoff parameter.

We then applied the model Hamiltonian to the formulation of the simplest mean-field theory for this model, in particular the Thomas–Fermi approximation to the profile of a trapped condensate. We also used Bogoliubov theory to study the excitation spectrum of Bose–Einstein condensates with Feshbach-resonance-enhanced scattering lengths. Turning our attention to the specific case of Bragg scattering from a Bose–Einstein condensate, we showed how to obtain the Bragg spectrum for a homogeneous atom-molecule system. We found that the Bragg peak shift calculated from our atom-molecule model is significantly different from that obtained by a simple model of structureless atoms.

Finally, we implemented this developed formalism in full numerical calculations.
Chapter 8. Conclusion

of Bragg scattering from an inhomogeneous Bose–Einstein condensate. The results from these simulations were directly comparable to the results from the experiment of Papp et al. [92], and we demonstrated that the experimental data can be reproduced accurately using our formalism.

8.1.1 Discussion

The aim of the experiment of Papp et al. [92] was to probe the behaviour of a Bose–Einstein condensate in the regime where two major simplifications normally made in its theoretical description were not valid:

1. Weak Interactions: This requires that the diluteness parameter, $n a_s^3$, is small. It is important to note that this approximation is necessary not only for the validity of the Gross–Pitaevskii equation, but also for the validity of the local quantum field theory, to which the Gross–Pitaevskii is an approximation.

In the experiment, the condensate was compressed, and the scattering length increased by using a Feshbach resonance, in order to ensure the violation of this condition.

2. Local Interactions: By this, it is meant that the length scale on which processes of interest take place is much larger than that of the interactions. In the experiment, the momentum transfer involved in the Bragg scattering was chosen to be sufficiently large, such that the momentum dependence of the scattering amplitude would be important.

In addition, the parameters of the experiment were chosen so that the relevant quasiparticles, that is, those with momentum corresponding to the Bragg wavenumber, were definitely not in the free particle regime.

In this thesis, we have shown how to take account of all of these factors within a tractable formalism. The most significant aspect of both the experiment and the theory is the clear demonstration that the large scattering lengths generated by Feshbach resonances do not give rise to interactions of the hard-sphere kind, as treated originally by Huang and Yang [56, 57] — indeed, it is remarkable that the classical Huang–Yang theory works so well for systems with Feshbach-resonance-enhanced interactions. For this reason, we investigated stationary states, the Thomas–Fermi approximation and the Bogoliubov excitation spectrum of our model of coupled atoms and molecules, and in fact found that even at large scattering lengths, the corrections were modest, though quite perceptible.

The Bragg scattering experiment is essentially a measurement of the excitation spectrum, and the frequency changes it presents are a measure of the deviation from
the spectrum expected of the corresponding hard sphere model. These corrections are in fact fairly small; only about 10% of the actual Bogoliubov quasi-particle frequencies. The fact that these effects can be measured experimentally is therefore quite remarkable.

The results of our work are very satisfactory. Although the experiment was not designed to test this kind of theory, and thus some significant parameters are hard to estimate, we obtain quantitative agreement with their experimental results, with no fitted parameters.

8.1.2 Relevance of C-field Formalism

One might ask why the implementation of the truncated-Wigner approximation is stressed throughout this thesis, when we discovered that an almost identical result could have been obtained using the much simpler Gross–Pitaevskii style simulation, as seen in Sect. 7.5.

Let us consider the situation as it stood before we started this work. The experiment of Papp et al. [92] was deliberately performed in a region where it was believed most of the standard assumptions used in Bose–Einstein condensation theory were violated. Not surprisingly, in their paper no theory was found which would fit the data.

There were a few papers which attempted to explain the data, without success. We therefore felt we should investigate all possible effects which might be significant, such as the use of Bogoliubov excitations, the inclusion of the inhomogeneity, the effect of fluctuations, and the effect of the molecular basis for the Feshbach resonance. The results we obtained this way disagreed with the experimental data. In the end, we came to the conclusion that the experimenters had incorrectly calculated density, and we therefore adjusted the data to use the density-weighted density. This produced the results of Fig. 7.9, which are in good agreement with our theoretical treatment.

The message of Fig. 7.9 is simple: we present the accumulation of the corrections that we take into account, each of which progressively reduces the line shift at higher scattering lengths. It is true that the c-field calculation and the Bogoliubov calculation could both claim to fit the data, although we find that the c-field fit is better. However, it is also true that the predictions of these two methods are significantly different from each other, and lie on either side of the experimental data.

In Sect. 7.5, we find that the effect of the c-field noise is small; nevertheless the noise itself is very large, and almost swamps the coherent part of the molecular c-field. This is (initially at least) intuitively amazing, and is a result we were very surprised to find. This means we have verified that fluctuations do not play a significant role in Bragg scattering, a fact that was not previously known, and was also very difficult to calculate
by any other method than the c-field method.

The reason for the emphasis on the c-field method is thus twofold:

1. Given that we wish to include the fluctuations, we have to describe how to do this in the c-field formalism, and this requires considerable care, because the procedure is not straightforward.

2. As will be discussed in Sect. 8.2.2, there are other problems waiting for a solution, which have yet to be convincingly described theoretically. The formalism developed in this thesis provides the foundations for future work.

The c-field methods are stressed, therefore, because the objective of the work in this thesis is to formulate a model within a c-field framework of a Bose–Einstein condensate where the scattering length has been altered by a Feshbach resonance, of which Bragg scattering is only one possible application, but one for which interesting experimental data is available.

8.2 Outlook

8.2.1 Relating Theory to Experiment

The JILA experiment set out to test the limits of conventional theory, and convincingly achieved that aim. However, the procedure used was not ideal for comparison with our detailed model.

The most challenging problem is the absence of any measurements of the initial state of the condensate immediately before applying the Bragg pulse. The issue is further complicated by the procedure used to enhance the density of the condensate, before ramping the scattering length to the value used for the Bragg pulse. The result is an initial state for the Bragg scattering which, not being a stationary state, cannot be definitively determined. In order to compare our computations with the experiment we have relied on the time- and space-averaged density measurements implicit in their presentation of the frequency shifts expected from the Huang–Yang theory. We have converted these to the appropriate values of the time-averaged density-weighted density, and using these we achieve our results, which are in very good quantitative agreement with the measured results.

We would consider it of importance in any future experiments to present

1. *Either*: Measurements of the initial state;

2. *Or*: A precise quantitative description of the procedure used to create each initial
state from the initial condensate, which can be reliably modelled as a stationary Bose–Einstein condensate.

The presentation of results as time-averaged quantities should be avoided; these create very significant computational difficulties.

### 8.2.2 Directions for Future Work

In this thesis, the effect of three-body recombination processes on the condensate dynamics is treated in a rather simplistic way; the three-body loss arises from inelastic collisions between atoms and molecules, but in our formalism only the atom field has a term corresponding to the loss of particles. Since the formalism developed here includes both the molecule and atom fields, it provides an opportunity to model the three-body loss process in a more accurate way. We hope to extend our formalism to include the three-body loss mechanism in a more detailed manner in future work.

The methods we have developed in this thesis can clearly be applied to other problems, in which the flexible adjustment of the scattering length afforded by Feshbach resonances has been exploited, for example the Bose-nova problem, and the related problem of bright solitons.

A Bose-nova occurs at the collapse of a Bose–Einstein condensate close to a Feshbach resonance, as the scattering length is tuned to be negative, thus making the interatomic interactions attractive. This phenomenon was studied experimentally by several groups (see for example \[38, 48\]), with later experiments observing the formation and collision of multiple bright soliton waves in the condensate collapse \[29\].

A preliminary theoretical treatment of the Bose-nova problem was made by Haines \[52\], using a similar formalism to the one presented in this thesis. The results indicate the importance of both the molecule field and the quantum fluctuations. However, as is noted in \[52\], more work is needed in order to reproduce the full effects of the Bose-nova seen in experiments, such as the presence of jets and bursts \[38, 105\].

Most other theoretical treatments of the Bose-nova problem use a mean-field Gross–Pitaevskii treatment, which provides some qualitative agreement, but significant quantitative disagreement with the experimental results \[113\]. Alternative methods (see for example \[80, 123\]) showed no dramatic improvement to the Gross–Pitaevskii treatment. A recent experiment \[1\] indicates that the Gross–Pitaevskii treatment may be able to accurately predict the time and scattering length at which the collapse will occur, as well as the rate of particle loss; however, we believe that the treatment of the Feshbach resonance dynamics — as is done in our atom-molecule model — is necessary for a full description of the Bose-nova phenomenon.
Furthermore, it is conceivable that the methodology presented in this thesis could be extended to study the physics of Efimov states in Bose–Einstein condensates. The existence of such three-body bound states was recently confirmed experimentally [70, 65, 99, 127], almost 40 years after the original prediction [42]. The properties of Efimov states in ultra-cold gases have been studied theoretically [18, 17, 15], although the dynamics of such states in the presence of a Bose–Einstein condensate has not previously been explored. By extending our model to include not just two-body bound states, but also three-body bound states, the formalism outlined here might be used to study the dynamics of Efimov states in Bose–Einstein condensates.
Appendix A

Interaction-Picture Integration Algorithm

In this appendix, we review the Projected Fourth-order Runge–Kutta in the Interaction Picture (RK4IP-P) algorithm, which we use to propagate the equations of motion in this thesis. This method is based on the RK4IP algorithm, which was developed by Ballagh [3] for simulating the time-dependent Gross–Pitaevskii equation, and which we discuss in Sect. A.1. We also discuss the projected form of this algorithm that was introduced by Norrie [87]. In Sect. A.2 we go on to present the algorithm in the case of two coupled equations of motion, and give the explicit form of this algorithm that we use in this thesis, developed by Dempsey [34].

A.1 The RK4IP Algorithm

A.1.1 Fourth-Order Runge–Kutta

The differential equations that we are interested in solving are in general of the form

\[
\frac{dg(t)}{dt} = f(g, t), \quad (A.1)
\]

where \(g(t)\) is a vector-valued function and \(f(g, t)\) is the derivative operator of the system. In most cases, these differential equations are impossible to solve analytically, and we will therefore find a solution by propagating the function \(g\) on a discrete time grid, where each point is given by

\[
t_{i+1} = t_i + \Delta t, \quad (A.2)
\]

for some appropriate time step \(\Delta t\).
The fourth-order Runge–Kutta algorithm (RK4) [100] advances the solution from $g(t_i)$ to $g(t_{i+1})$ according to

$$g(t_{i+1}) = g(t_i) + \frac{1}{6} \left[ h_1 + 2(h_2 + h_3) + h_4 \right], \quad (A.3)$$

where in the intermediate steps are given by

$$h_1 = \Delta t f(g(t_i), t_i), \quad (A.4a)$$
$$h_2 = \Delta t f(g(t_i) + h_1/2, t_i + \Delta t/2), \quad (A.4b)$$
$$h_3 = \Delta t f(g(t_i) + h_2/2, t_i + \Delta t/2), \quad (A.4c)$$
$$h_4 = \Delta t f(g(t_i) + h_3, t_i + \Delta t). \quad (A.4d)$$

### A.1.2 Fourth-Order Runge–Kutta in the Interaction Picture

The Fourth-Order Runge–Kutta in the Interaction Picture (RK4IP) algorithm is an efficient algorithm for the temporal integration of differential equations with non-local operators. The algorithm is based on the standard Runge–Kutta approach to evolve operators, and uses the fact that operators which are non-local in position space can be made local by transforming them to momentum space.

The equations of motion used in this thesis are of the general form

$$\frac{i}{\hbar} \frac{d\alpha_j(t)}{dt} = \omega_j \alpha_j(t) + f(\alpha_j, t), \quad (A.5)$$

where the operator $f(\alpha_j, t)$ contains any nonlinear, coupling and perturbation terms. The mode coefficient is transformed to an interaction picture by

$$\alpha_j^I(t) = e^{i\omega_j(t-t_{ref})} \alpha_j(t), \quad (A.6)$$

where $t_{ref}$ is the time of the interaction-picture frame of reference. The differential equation in the interaction picture is then

$$\frac{i}{\hbar} \frac{d\alpha_j^I}{dt} = f^I(\alpha_j^I, t), \quad (A.7)$$

with the interaction-picture operator given by

$$f^I(\alpha_j^I, t) = e^{i\omega(t-t_{ref})} f(\alpha_j^I, t) e^{-i\omega(t-t_{ref})}. \quad (A.8)$$

For each step of the Runge–Kutta algorithm, the system is transformed to the interaction picture, where the slopes $h$ are evaluated, and the system is then transformed
A.1. The RK4IP Algorithm

back. The reference time $t_{\text{ref}}$ can be chosen arbitrarily, but Caradoc–Davies [24] shows how this process can be simplified by choosing the reference time to be $t_{\text{ref}} = t_i + \Delta t/2$. The algorithm for the Fourth-Order Runge–Kutta in the Interaction Picture (RK4IP) is then given by

$$\alpha_j(t_{i+1}) = e^{-i(\Delta t/2)\omega_j} \left( \alpha^1_j(t_i) + \frac{1}{6} \left[ h_{1,j} + 2(h_{2,j} + h_{3,j}) \right] \right) + \frac{1}{6} h_{4,j}, \quad (A.9)$$

where the interaction-picture mode coefficient is

$$\alpha^1_j(t_i) = e^{-i(\Delta t/2)\omega_j} \alpha_j(t_i), \quad (A.10)$$

and the slopes are given by

$$h_{1,j} = -i\Delta t e^{-i(\Delta t/2)\omega_j} f(\alpha_j, t_i), \quad (A.11a)$$
$$h_{2,j} = -i\Delta t f(\alpha^1_j(t_i) + h_{1,j}/2, t_i + \Delta t/2), \quad (A.11b)$$
$$h_{3,j} = -i\Delta t f(\alpha^1_j(t_i) + h_{2,j}/2, t_i + \Delta t/2), \quad (A.11c)$$
$$h_{4,j} = -i\Delta t f(e^{-i(\Delta t/2)\omega_j} \left[ \alpha^1_j(t_i) + h_{3,j} \right], t_i + \Delta t). \quad (A.11d)$$

A.1.3 Projected Fourth-Order Runge–Kutta in the Interaction Picture

It is now straightforward to incorporate the projector into the algorithm. For the specific case of a plane-wave basis, the algorithm for the Projected Fourth-Order Runge–Kutta in the Interaction Picture (RK4IP-P) is given by [87] as

$$\alpha_j(t_{i+1}) = e^{-i(\Delta t/2)k^2_j} \left( \alpha^1_j(t_i) + \frac{1}{6} \left[ h_{1,j} + 2(h_{2,j} + h_{3,j}) \right] \right) + \frac{1}{6} h_{4,j}, \quad (A.12)$$

where the interaction-picture mode coefficient is now

$$\alpha^1_j(t_i) = e^{-i(\Delta t/2)k^2_j} \alpha_j(t_i), \quad (A.13)$$

and the slopes are now given by

$$h_{1,j} = -i\Delta t e^{-i(\Delta t/2)k^2_j} \mathcal{P}_j f(\alpha_j, t_i), \quad (A.14a)$$
$$h_{2,j} = -i\Delta t \mathcal{P}_j f(\alpha^1_j(t_i) + h_{1,j}/2, t_j + \Delta t/2), \quad (A.14b)$$
$$h_{3,j} = -i\Delta t \mathcal{P}_j f(\alpha^1_j(t_i) + h_{2,j}/2, t_j + \Delta t/2), \quad (A.14c)$$
$$h_{4,j} = -i\Delta t \mathcal{P}_j f(e^{-i(\Delta t/2)k^2_j} \left[ \alpha^1_j(t_i) + h_{3,j} \right], t_j + \Delta t). \quad (A.14d)$$
The projector is expressed as
\[ P_j = \begin{cases} 
1 & j \in L \\
0 & j \not\in L 
\end{cases}, \quad (A.15) \]
where \( L \) is the set of indices of the modes that span the low energy subspace below the momentum cutoff.

### A.2 Atom-Molecule RK4IP-P

The algorithm in the previous section can easily be expanded to incorporate a system of two coupled fields. Norrie [87] shows how this is done, and Dempsey [34] uses this method for the specific case of a coupled atom and molecule system. Here we follow these two works.

Using a plane-wave basis is advantageous since there exist high-speed algorithms for Fourier transforms. We express the wavefunctions \( \psi \) and \( \phi \) on a plane-wave basis set
\[
\psi(x, t) = \frac{1}{\sqrt{V}} \sum_l e^{i k_l \cdot x} \alpha_j(t), \quad (A.16) \\
\phi(x, t) = \frac{1}{\sqrt{V}} \sum_l e^{i k_l \cdot x} \beta_j(t). \quad (A.17)
\]
The equations of motion (6.1, 6.2) in their dimensionless form then become
\[
i \frac{d \alpha_j(t)}{dt} = k_j^2 \alpha_j + i P_{a} \frac{1}{\sqrt{V}} \sum_l e^{i k_l \cdot x_l} \left\{ V_a \psi + U_{aa} |\psi|^2 \psi + g \psi \phi^* - i \gamma (|\psi|^2 + 2|\phi|^2) \frac{1}{2} \psi \right\}, \\
i \frac{d \beta_j(t)}{dt} = \frac{k_j^2}{2} \beta_j + i P_{m} \frac{1}{\sqrt{V}} \sum_l e^{i k_l \cdot x_l} \left\{ V_m \psi + g \psi^2 \right\}, \quad (A.18, A.19)
\]
where the spatial and temporal dependencies have been omitted for brevity. The projectors are given by
\[
P_{a} = \begin{cases} 
1 & j \in L_a \\
0 & j \not\in L_a 
\end{cases} \quad \text{and} \quad P_{m} = \begin{cases} 
1 & j \in L_m \\
0 & j \not\in L_m 
\end{cases}, \quad (A.20)
\]
where \( L_a \) and \( L_m \) are the set of indices below the momentum cutoff for the atoms and molecules, respectively.

We write the equations of motion with the simplified notation
\[
i \frac{d \alpha_j(t)}{dt} = k_j^2 \alpha_j(t) + i P_{a} \frac{1}{\sqrt{V}} \sum_l e^{i k_l \cdot x_l} G_a(\psi, \phi, t), \quad (A.21)
\]
\[
\frac{d\beta_j(t)}{dt} = \frac{k_j^2}{2} \beta_j(t) + \sum_j \frac{1}{\sqrt{N}} e^{ik_j x_j} G_m(\psi, \phi, t),
\]

where

\[
G_a(\psi, \phi, t) = V_a \psi + U_{a\alpha} |\psi|^2 \psi + g \psi^* \phi - i \gamma (|\psi|^2 + 2|\phi|^2)^2 \psi,
\]

\[
G_m(\psi, \phi, t) = V_m \psi + g \psi^2.
\]

We can then express the RK4IP-P algorithm as

\[
\alpha_j(t_{i+1}) = e^{-i(\Delta t/2)k_j^2} \left( \alpha_j(t_i) + \frac{1}{6} \left[ h_1^a + 2(h_2^a + h_3^a) \right] + \frac{1}{6} h_4^a \right),
\]

\[
\beta_j(t_{i+1}) = e^{-i(\Delta t/2)k_j^2/2} \left( \beta_j(t_i) + \frac{1}{6} \left[ h_1^m + 2(h_2^m + h_3^m) \right] + \frac{1}{6} h_4^m \right),
\]

where the interaction-picture mode coefficients are

\[
\alpha_j(t_i) = e^{-i(\Delta t/2)k_j^2} \alpha_j(t_i),
\]

\[
\beta_j(t_i) = e^{-i(\Delta t/2)k_j^2/2} \beta_j(t_i),
\]

and the slopes are given by

\[
h_{1,j}^a = -i \Delta t e^{-i(\Delta t/2)k_j^2} \sum_j \frac{1}{\sqrt{N}} e^{ik_j x_j} G_a(\alpha_j(t_i), t_i),
\]

\[
h_{1,j}^m = -i \Delta t e^{-i(\Delta t/2)k_j^2/2} \sum_j \frac{1}{\sqrt{N}} e^{ik_j x_j} G_m(\beta_j(t_i), t_i),
\]

\[
h_{2,j}^a = -i \Delta t \sum_j \frac{1}{\sqrt{N}} e^{ik_j x_j} G_a \left( \alpha_j(t_i) + h_{1,j}^a/2, t_i + \Delta t/2 \right),
\]

\[
h_{2,j}^m = -i \Delta t \sum_j \frac{1}{\sqrt{N}} e^{ik_j x_j} G_m \left( \beta_j(t_i) + h_{1,j}^m/2, t_i + \Delta t/2 \right),
\]

\[
h_{3,j}^a = -i \Delta t \sum_j \frac{1}{\sqrt{N}} e^{ik_j x_j} G_a \left( \alpha_j(t_i) + h_{2,j}^a/2, t_i + \Delta t/2 \right),
\]

\[
h_{3,j}^m = -i \Delta t \sum_j \frac{1}{\sqrt{N}} e^{ik_j x_j} G_m \left( \beta_j(t_i) + h_{2,j}^m/2, t_i + \Delta t/2 \right),
\]

\[
h_{4,j}^a = -i \Delta t \sum_j \frac{1}{\sqrt{N}} e^{ik_j x_j} G_a \left( e^{-i(\Delta t/2)k_j^2} \left[ \alpha_j(t_i) + h_{3,j}^a \right], t_i + \Delta t \right),
\]

\[
h_{4,j}^m = -i \Delta t \sum_j \frac{1}{\sqrt{N}} e^{ik_j x_j} G_m \left( e^{-i(\Delta t/2)k_j^2/2} \left[ \beta_j(t_i) + h_{3,j}^m \right], t_i + \Delta t \right).
\]
A.2.1 Implementation

The memory-efficient implementation of the two-component RK4IP-P algorithm used in this thesis is given in [52]. The explicit form of this algorithm is given in the following:

\[
\begin{align*}
\alpha_j^I & \leftarrow e^{-ik_j^2\Delta t/2}\alpha_j \\
\beta_j^I & \leftarrow e^{-ik_j^2\Delta t/4}\beta_j \\
\alpha_j^H & \leftarrow \text{IFFT}(\alpha_j) \\
\beta_j^H & \leftarrow \text{IFFT}(\beta_j) \\
\zeta_j & \leftarrow \alpha_j^H \\
\alpha_j^H & \leftarrow -i\Delta t \mathcal{P}^a_j e^{-ik_j^2\Delta t/2} \text{FFT}\left(G_a(\alpha_j^H, \beta_j^H, t_i)\right) \\
\beta_j^H & \leftarrow -i\Delta t \mathcal{P}^m_j e^{-ik_j^2\Delta t/4} \text{FFT}\left(G_m(\zeta_j^H, \beta_j^H, t_i)\right) \\
\alpha_j & \leftarrow \alpha_j^I + \frac{1}{6}\alpha_j^H \\
\beta_j & \leftarrow \beta_j^I + \frac{1}{6}\beta_j^H \\
\alpha_j^H & \leftarrow \text{IFFT}(\alpha_j^I + \frac{1}{2}\alpha_j^H) \\
\beta_j^H & \leftarrow \text{IFFT}(\beta_j^I + \frac{1}{2}\beta_j^H) \\
\zeta_j & \leftarrow \alpha_j^H \\
\alpha_j^H & \leftarrow -i\Delta t \mathcal{P}^a_j \text{FFT}\left(G_a(\alpha_j^H, \beta_j^H, t_i + \frac{\Delta t}{2})\right) \\
\beta_j^H & \leftarrow -i\Delta t \mathcal{P}^m_j \text{FFT}\left(G_m(\zeta_j^H, \beta_j^H, t_i + \frac{\Delta t}{2})\right) \\
\alpha_j & \leftarrow \alpha_j + \frac{1}{3}\alpha_j^H \\
\beta_j & \leftarrow \beta_j + \frac{1}{3}\beta_j^H \\
\alpha_j^H & \leftarrow \text{IFFT}(\alpha_j^I + \frac{1}{2}\alpha_j^H) \\
\beta_j^H & \leftarrow \text{IFFT}(\beta_j^I + \frac{1}{2}\beta_j^H) \\
\zeta_j & \leftarrow \alpha_j^H \\
\alpha_j^H & \leftarrow -i\Delta t \mathcal{P}^a_j \text{FFT}\left(G_a(\alpha_j^H, \beta_j^H, t_i + \frac{\Delta t}{2})\right) \\
\beta_j^H & \leftarrow -i\Delta t \mathcal{P}^m_j \text{FFT}\left(G_m(\zeta_j^H, \beta_j^H, t_i + \frac{\Delta t}{2})\right) \\
\alpha_j & \leftarrow \alpha_j + \frac{1}{3}\alpha_j^H \\
\beta_j & \leftarrow \beta_j + \frac{1}{3}\beta_j^H
\end{align*}
\]
\[ \alpha_j^H \leftarrow \text{IFFT}\left(e^{-ik^2_j\Delta t/2} \left(\alpha_j^I + \alpha_j^H\right)\right) \]
\[ \beta_j^H \leftarrow \text{IFFT}\left(e^{-ik^2_j\Delta t/4} \left(\beta_j^I + \beta_j^H\right)\right) \]
\[ \zeta_j \leftarrow \alpha_j^H \]
\[ \alpha_j^H \leftarrow -i\Delta t \mathcal{P}_j^a \text{FFT}\left(G_a(\alpha_j^H, \beta_j^H, t_i + \Delta t)\right) \]
\[ \beta_j^H \leftarrow -i\Delta t \mathcal{P}_j^m \text{FFT}\left(G_m(e^H, \beta_j^H, t_i + \Delta t)\right) \]
\[ \alpha_j \leftarrow e^{-ik^2_j\Delta t/2} \alpha_j + \frac{1}{6}\alpha_j^H \]
\[ \beta_j \leftarrow e^{-ik^2_j\Delta t/4} \beta_j + \frac{1}{6}\beta_j^H \]

Here, FFT denotes a three-dimensional fast Fourier transform and IFFT denotes the inverse transform.

### A.2.2 Practical Experience

Since the RK4IP-P algorithm takes the fields back and forth between position and momentum space, some care must be taken to ensure that the system is well represented in both. This is of particular importance for the system studied in this thesis; we model a condensate which is elongated in one of its spatial dimensions and which has a Bragg pulse applied in the same direction. We must therefore use a grid which is elongated in both position and momentum space. The only way to accomplish this is to use a large number of grid points in the direction of interest. For the work here we are forced to use 2048 grid points in the \(x\)-direction, even though in the \(y\)- and \(z\)-direction it is sufficient to use only 32.

When implementing the coupled atom-molecule RK4IP-P algorithm, we find that the size of the time step \(\Delta t\) is extremely important; if \(\Delta t\) is chosen too large, the solution will quickly diverge. As noted in Sections 7.2.3 and 6.4.5, there is no analytical method for determining the appropriate size of \(\Delta t\), but rather this is accomplished using a method of trial and error. As a condition of convergence, we use the total number of atoms in the system — with a molecule counted as two atoms — and ensure that this does not vary by more than a fraction of a percent when we ignore the effects of three-body loss. The size of the time step will change depending on the system we are looking at; the more even in size the atom and molecule fields are, the smaller the value of \(\Delta t\). If the number of noise particles is decreased we can also reduce the size of the time step significantly.
References


