Coherent Decay of Bose-Einstein Condensates

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ABSTRACT

As the coldest form of matter known to exist, atomic Bose-Einstein condensates are unique forms of matter where the constituent atoms lose their individual identities, becoming absorbed into the cloud as a whole. Effectively, these gases become a single macroscopic object that inherits its properties directly from the quantum world. In this work, I describe the quantum properties of a zero temperature condensate where the atoms have a propensity to pair, thereby leading to a molecular character that coexists with the atoms. Remarkably, the addition of this molecular component is found to induce a quantum instability that manifests itself as a collective decay of the assembly as a whole. As a signature of this phenomenon, there arises a complex chemical potential in which the imaginary part quantifies a coherent decay into collective phonon excitations of a collapsing ground state. The unique decay rate dependencies on both the scattering length and the density can be experimentally tested by tuning near a Feshbach resonance. Being a purely quantum mechanical effect, there exists no mechanical picture corresponding to this coherent many-body process. The results presented can serve as a model for other systems with similar underlying physics.

Thesis Supervisor: Arthur K. Kerman
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To my grandmother,

Immacolata (Margaret) DePetris.

Out of all the places I have lived, her house was the only one that felt like home.

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First, I am especially proud to have worked with my advisor, Arthur Kerman, a man of impeccable scientific achievement. During the course of this thesis, I have availed myself of his knowledge and experience as he was never reluctant to engage in lengthy discussions until the issues at hand were thoroughly understood. Although I had freedom to explore, my ideas still always had to pass a level of scrutiny that has become all to rare in academia these days. In essence, the opportunity of independent thought coupled with rigorous scientific examination have allowed me to grow as a scientist. For that, I will always be grateful.

Also, my fianceé, Ruth D'Oleo, deserves special recognition for generously giving her time by largely relieving me of the everyday chore-like burdens, thus allowing more time to focus on scientific work. As a colleague, she has been instrumental in listening to ideas and providing thoughtful feedback. Sincere thanks are conveyed to my mother, Jeannette DePetris, without whom none of my work would have been possible in the first place. More directly, she has unquestioningly provided both financial and moral support throughout my many undertakings, including this one. Lastly, I am indebted to the taxpayers, as this work was funded through the MIT-Los Alamos Collaborative Research Grant to Develop an Understanding of Bose-Einstein Condensates, Contract No. 19442-001-99-35

George E. Cragg

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Chapter 1

Introduction

1.1 What is Bose-Einstein Condensation?

The phenomenon of Bose-Einstein condensation (BEC) is perhaps best understood through the analogy with coherent light, as found inside a laser cavity. The qualifier "coherent" immediately implies the description of light as a single electromagnetic field, where knowledge of the field at one point in space completely determines it at all other points as well. Hence, coherence describes a kind of connection between all photons of the field.

As learned from de Broglie, material particles, such as atoms, also have a wave-like character to them. When the temperature is lowered, such wave-like behavior begins to emerge as the de Broglie wavelength becomes larger. Given a collection of bosons, it can be the case that the temperature of the system is brought so low that the matter waves of the atoms coincide, essentially coalescing the assembly into a single macroscopic quantum object. Just like the photonic analog, all particles are connected in the resultant coherent state since the constituents can now be viewed as a singular matter field. Like laser light, the matter field can be split then recombined, thus displaying an interference fringe pattern (Fig. 1.1).

However, there are interesting differences between photons and bosonic atoms. Most notably, Maxwell's equations are linear in the electromagnetic field, thus prohibiting any interactions between photons. Indeed, any nonlinearities are introduced by some intervening material. In contrast, the material atomic condensate has nonlinearity built into the system through the interparticle interactions. However, these interactions also render the gas metastable due to recombination events. In dilute atomic vapors, the natural tendency is for the atoms to pair until the lowest energy state is achieved. In alkali metals, this lowest state corresponds to the solid bulk crystalline lattice. The first step from an atomic gas to a solid is a three-body recombinant process, in which two atoms form a deeply bound molecule, which liberates its binding energy through the interaction with the third atom. Based on classical collision arguments, the description of recombinant processes is inconsistent with the defining characteristic of coherence. Once BEC is achieved, all atoms become absorbed into a collective, thus presenting an inconsistency in treating constituent atoms in an independent, kinematic fashion.

The purpose of this thesis is to propose a framework whereby instabilities are understood as a fundamental property intertwined with the coherence of the condensate. To provide a context for these ideas, it is helpful to review the historical development, starting from the original ideas of Bose and Einstein, up through the current efforts in BEC of the alkalis. Followed by this is the modern translation of the ideas originally formulated by Einstein.

Finally, an overview is given of the contribution contained in the present work.

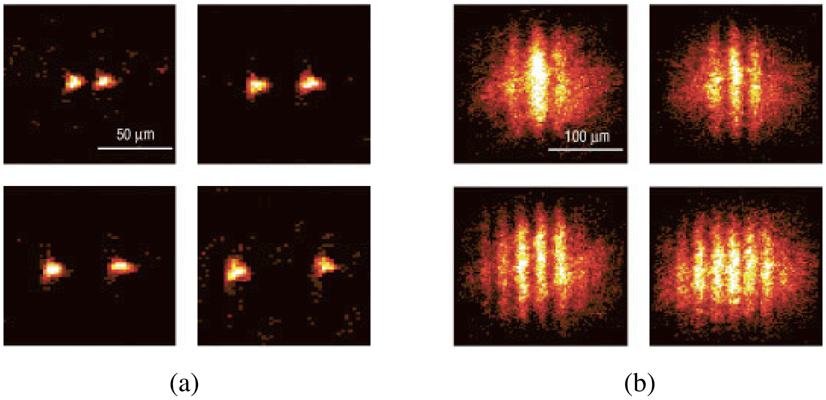

Figure 1.1: A matter-wave interference experiment performed with ^{87}Rb. (a) A BEC is split into two portions, with a variable separation between the two. Hence, each cloud originates from a single condensate thereby establishing a correlation between the two clouds. When released from the substrate based magnetic trap, the expanding clouds impinge on each other, where their coherence displays as the dramatic interference fringes seen in (b). Reprinted by permission from Macmillan Publishers Ltd: *Nature Physics*, T. Schumm, *et al.* Matter-wave interferometry in a double well on an atom chip, **1**:57 © 2005.

1.2 Historical Perspective

In 1924, Satyendra Nath Bose obtained the Planck radiation law by treating photons as individual particles.[1] In this original work, it was found that the number of photons in a particular state depended upon the energy, ε of that state according to

$$N_\varepsilon = \left(e^{\beta\varepsilon} - 1\right)^{-1}, \tag{1.1}$$

where $\beta \equiv 1/(kT)$ as usual. Intrigued by this result, Einstein extended the idea of Bose, treating the case of massive particles with integral spin. Even before the development of quantum mechanics, Einstein proposed using de Broglie's hypothesis to treat particles as waves, just like the case of the photons. Unlike the photonic case, however, the atomic distribution has the form

$$N_\varepsilon = \left(e^{-\beta(\varepsilon-\mu)} - 1\right)^{-1}, \tag{1.2}$$

where the chemical potential, μ must be introduced because of particle number conservation. Using this distribution, Einstein suggested that massive particles could coalesce into a common ground state. However, this idea was initially met with skepticism from the physics

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[1] For a more detailed history from a condensed matter perspective see A. Griffin, "A brief history of our understanding of BEC: From Bose to Beliaev," in M. Inguscio, S. Stringari and C. E. Wieman, eds., *Proceedings of the International School of Physics: Bose-Einstein Condensation in Atomic Gases*, (Amsterdam: IOS Press, 1999), 1-13.

community as it was thought to be an artifact arising in the ideal gas, where interparticle interactions are ignored. In his second paper on the subject, Einstien himself admitted that the differences between distinguishable and indistinguishable state counting "express indirectly a certain hypothesis on a mutual influence of the molecules which for the time being is of a quite mysterious nature"[1].

The idea of BEC remained dormant for more than a decade until, in 1938, Pyotr L. Kapitza, John F. Allen and Don Misener published some experiments concerning the superfluid nature of ^{4}He, emerging below the transition temperature of 2.17 K. In the period 1935-37, Fritz London introduced the idea of a macroscopic wave function, pertaining to a quantum state on a macroscopically large scale. Consequently, when he heard of the ^{4}He experiments, London postulated that some sort of condensate was responsible for the observed superfluid transition. Interacting with London, Lazlo Tiza came up with the "two-fluid" concept, describing the condensate as a new degree of freedom which could move coherently without friction, thereby giving rise to the superfluid behavior.

On the theoretical side, the 1940's and 50's saw much work on interacting Bose systems. However, most of these results were perturbative and thus restricted to weak interactions. Working independently, Eugene P. Gross and Lev P. Pitaevskii put forth a macroscopic energy functional approach to treat interacting Bose gases. This resulted in the famed Gross-Pitaevsii equation[2], describing the time evolution of the condensate field. Forty years later, this equation remains one of the preferred approaches for dealing with interacting Bose systems. In another long lasting development, Elliott H. Lieb and Werner Liniger found and exact solution for the one dimensional case of bosons with a contact interaction[3]. Even today, this is the only interaction model where an exact solution has been found.

Up to this point, superfluid ^{4}He was one of the few systems that could be used to verify the theories underpinning BEC. Not long after its development, laser light was proposed as a mechanism to slow and cool atoms. In the early 80's, many experiments were being performed using lasers in deflecting and slowing atomic beams. These efforts culminated in the invention of optical molasses, a technique capable of producing microkelvin temperatures in the alkalis. Soon thereafter, the technique of evaporative cooling was developed, allowing the first direct observation of atomic BEC in ^{23}Na, ^{87}Rb and ^{7}Li[4]. This development prompted a host of new studies into BEC, both experimental and theoretical.

1.3 Bosonic vs. Fermionic Composites

In nature, all particles can be classified as either integral spin bosons or half integral spin fermions. Unlike bosons, fermions must obey the Pauli Exclusion Principle which states that no two of them may simultaneously occupy the same quantum state. This fact is reflected in their distribution function, the Fermi-Dirac distribution:

$$N_\varepsilon = \left(e^{\beta\varepsilon} + 1\right)^{-1}, \tag{1.3}$$

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[1] Albert Einstein, as quoted in E. A. Cornell (1999), p. 16.

[2] For more details on the Gross-Pitaevsii equation, see one of the original works E. P. Gross (1963). An overview is also given in Section 4.4

[3] E. H. Lieb (1963).

[4] The 2001 Nobel Prize was awarded for the works of K. B. Davis (1995) and M. H. Anderson (1995). At the same time, Randy Hulet's group at Rice provided evidence for atomic condensation of the attractive isotope ^{7}Li: C. C. Bradley (1995).

which differs from the Bose-Einstein distribution by the sign in the denominator.

Atoms are comprised of a nucleus of protons and neutrons surrounded by an electron cloud. All three particles, protons, neutrons and electrons, are fermionic in nature. However, the composite atoms have a character dependent upon the overall spin of the isotope as a whole. For electrically neutral atoms, the proton number equals the electron number, indicating that an even or odd neutron number determines whether an isotope is bosonic or fermionic, respectively. In addition, two fermionic atoms may pair to form a bosonic molecule, which would then be amenable to molecular condensation.

1.4 Spatially Uniform, Ideal Bose Gas

In ordinary room temperature gases, the atoms move at speeds of about 300m/s. As such, they display behavior consistent with the classical picture of a collection of billiard balls bouncing into each other. However, as the gas is cooled, quantum effects begin to dominate. The emergence of this otherwise hidden nature can be quantified by a ratio of the mean thermal wavelength, $\lambda_{th} \equiv h/\sqrt{2\pi mkT}$, to the interparticle spacing. In fact, the degeneracy parameter,

$$\rho\lambda_{th}^3 = \frac{\rho h}{(2\pi mkT)^{3/2}}\,, \tag{1.4}$$

crops up in the various expressions for the physical properties of the system. In the limit $\rho\lambda^3 \to 0$, such properties will be classical in nature, whereas the opposite extreme, $\rho\lambda^3 \sim 1$, indicates quantum mechanical behavior. In the latter regime, we show the emergence of a Bose-Einstein condensate for a non-interacting (ideal) collection of Bose particles, distributed according to the function in (1.2). Using Einstein's distribution, the grand partition function is[1]

$$\mathscr{Q} = \prod_{\varepsilon}\left(1 - ze^{-\beta\varepsilon}\right)^{-1}, \tag{1.5}$$

where the product is over all the energy eigenvalues, ε, and as usual, the fugacity is defined as $z \equiv e^{\mu/kT}$. By the relationship $PV/(kT) = \ln\mathscr{Q}$, the system's thermodynamics follows from the grand partition function. Using (1.5) we have

$$\frac{PV}{kT} = -\sum_{\varepsilon}\ln\left(1 - ze^{-\beta\varepsilon}\right). \tag{1.6}$$

Also, the total number of particles is given by

$$N = \sum_{\varepsilon}\langle n_\varepsilon\rangle = \sum_{\varepsilon}\frac{1}{z^{-1}e^{\beta\varepsilon} - 1}\,. \tag{1.7}$$

For large volumes, the spectrum of the single particle states is nearly continuous, thereby permitting a replacement of the sums with integrals, weighted by the density of states in the vicinity of energy ε:

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[1] Further details are available in most texts on statistical mechanics. See, for example, R. K. Pathria (1996), p. 158.

$$n(\varepsilon) = \frac{2\pi V}{h^3}\,(2m)^{3/2}\varepsilon^{1/2}\,. \tag{1.8}$$

Substitution of the density of states into the continuum versions of (1.6) and (1.7) results in

$$\frac{P}{kT} = -\frac{2\pi}{h^3}\,(2m)^{3/2}\int\limits_0^\infty \varepsilon^{1/2}\ln\bigl(1 - ze^{-\beta\varepsilon}\bigr)d\varepsilon - \frac{1}{V}\ln(1-z) \tag{1.9a}$$

$$\frac{N}{V} = \frac{2\pi}{h^3}\,(2m)^{3/2}\int\limits_0^\infty \frac{\varepsilon^{1/2}d\varepsilon}{z^{-1}e^{\beta\varepsilon}-1} + \frac{1}{V}\,\frac{z}{1-z}\,. \tag{1.9b}$$

Because the density of states is proportional to $\varepsilon^{1/2}$, a zero weight is assigned to the ground state. Equation (1.9b) accounts for this since the zero energy contribution is separated out by the term $z/(1-z)$. However, (1.9a), is only a valid description of the excited states, for which $\varepsilon \neq 0$. Both of these results may be expressed in terms of the Bose-Einstein functions, $g_\nu(z)$[1]

$$\frac{P}{kT} = \frac{1}{\lambda^3}\,g_{5/2}(z) \tag{1.10a}$$

$$\frac{N-N_0}{V} = \frac{1}{\lambda^3}\,g_{3/2}(z)\,, \tag{1.10b}$$

where N_0 is the population of the ground state. Recognizing the emergence of a Bose-Einstein condensate comes from an analysis of the particle number expression (1.10b). Since the fugacity, z, can only range between zero and one, the maximum value of $g_{3/2}(z)$ is $g_{3/2}(1) = \zeta(3/2) \simeq 2.612$, where ζ is the famed Riemann Zeta function. Thus, the number of excited state particles is

$$N_e = N - N_0 \leq \frac{(2\pi mkT)^{3/2}}{h^3}\zeta\left(\frac{3}{2}\right). \tag{1.11}$$

If the actual number of particles is larger than N_e, then the excited states will receive up to N_e of them while the remainder, $N_0 = N - N_e$, will be pushed into the ground state. The fugacity is found from the ground state contribution of (1.9b),

$$N_0 = \frac{z}{1-z} \Rightarrow z = \frac{N_0}{N_0+1}\,. \tag{1.12}$$

which gives $z \approx 1$ for large N_0. This accumulation of particles into the state $\varepsilon = 0$ is what is known as Bose-Einstein condensation. From this analysis, the atomic condensation transition can be expressed by an inequality in the total particle number,

$$N > VT^{3/2}\frac{1}{h^3}(2\pi mk)^{3/2}\zeta\left(\frac{3}{2}\right). \tag{1.13}$$

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[1] See Pathria, p. 159.

This expression may be rearranged to give the critical temperature, T_c, at which atomic condensation occurs,

$$T < T_c = \frac{h^2}{2\pi mh}\left[\frac{\rho}{\zeta\big(3/2\big)}\right]^{2/3}. \tag{1.14}$$

For $T < T_c$, the system can be regarded as a mixture of an uncondensed phase, composed of the N_e particles distributed over the excited states, plus a condensed phase consisting of N_0 particles in the ground state. Shown in Fig. (1.2) is the temperature dependence of the particle fraction in each of these phases.

It is interesting to note that a uniform one or two dimensional Bose gas will not undergo BEC at any nonzero temperature. This is evident in the corresponding density of states, which for two dimensions has the form $\rho(\varepsilon) = 2\pi mA/h^2$, where A is the area. In this case, the number of particles is

$$N = \frac{z}{1-z} - \frac{2\pi mkT}{h^2}\ln(1-z)\,. \tag{1.15}$$

Since both terms diverge as $z \to 1$, there is no macroscopic occupancy of the ground state for any $T > 0$. A similar result can be obtained in the one-dimensional case. However, the above results only apply to uniform systems, since in the presence of boundaries or confining fields, atomic condensation is possible in one, two or three dimensions in general.[1]

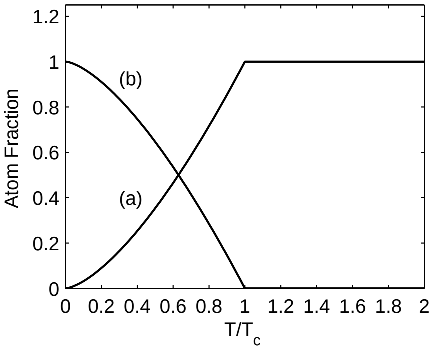

Figure 1.2: This figure is a plot of the condensate (b) and noncondensate (a) fractions as a function of the normalized temperature, T/T_c. At zero temperature, the normal fraction vanishes leaving a pure BEC.

1.5 Overview

This thesis puts forth a new description of atomic condensate losses as a coherent phenomenon intrinsic to the macroscopic wave function. However, almost any new idea or development cannot exist inside a vacuum, for no contact with familiar results would render it inapproachable. Moreover, it is always good practice to explain results starting from well-established fundamentals, as it is often the case that what is already known can be recast in a form that accentuates the introduction of the new hypothesis. Therefore, this

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[1] See J. Oitmaa, p.48.

exposition is a combination of new results inside a scaffolding of preexisting knowledge, much of which I learned along the way. While this approach is of course dominated by my own experiences and way of thinking, I hope to have been successful in keeping the presentation general enough to be useful to others in similar fields.

Because non-ideal many-body systems are essentially built up from the pairwise interactions among the particles, a logical place to begin is from a description of two-body scattering, the subject of Chapter 2. Additionally, the two-body problem can be regarded as the zero density limit of the multiple particle assembly. Therefore, through this mapping, it can be expected that a known two-body result has a correspondence with a many-body equation of state. Lastly, simplified interaction potentials are evaluated in terms of their consistency with the low-energy scattering physics. From this comparison, it is seen that a separable potential has advantage over the conventional zero-range delta function model.

After the two-body results, the language and general many-body formalisms are reviewed in Chapter 3. Ending with a description of the coherent states provides a natural transition into the variational Gaussian formalism discussed in Chapter 4. In this chapter, the many-body trial wave functional is presented where the variational parameters are the Gaussian width and mean fields. This formalism is used in all subsequent calculations of the work. Explicitly specifying a form of the wave functional provides a straightforward way of calculating the uniform excitation spectrum as a small oscillation expansion about the stationary uniform state.

Chapter 5 uses the previous machinery in the analysis of a zero-range model of the ^{85}Rb system, which is inherently unstable due to its innately negative scattering length. By tuning a Feshbach resonance, as described in Chapter 2, the scattering length can be made effectively positive, resulting in what is believed to be a stable condensate. In spite of the positive scattering length, it is found that the lowest energy solution still tends toward collapse. However, the usual low-density result can be obtained by allowing the chemical potential to range into the complex plane. Physically, this result is interpreted as a coherent decay, with the imaginary part quantifying the decay rate, or decoherence rate, into collective phonon excitations of the collapsing ground state.

Considering a non-zero range potential, Chapter 6 discusses the applicability of this theory to observed condensate losses in general. Chapter 7 then details the collective phenomenon of macroscopic quantum tunneling, known to occur in condensate species having negative scattering lengths. Subsequently, these results are applied to the collapsing molecular condensate found in the ^{85}Rb system. Finally, Chapter 8 concludes with the Bose-Hubbard model as well as fermionic superfluids. This final chapter puts forth some calculations that were thought about during the process of refining the current work. As such, they are not intended as direct applications of this thesis topic, but should be considered as spin off directions, potentially supporting distinct but related efforts. At the end, appendices are included which contain the details behind several expansions employed in this work.

Chapter 2

Two-Body Scattering

Microscopic models of many-atom assemblies are first conceived through the two-body analyses of the interparticle interactions. Through this connection, a many-body Hamiltonian may be postulated where subsequent analysis determines the properties of the collection. Finally, the model is validated through a careful comparison between prediction and experiments, so far as can be done with preexisting empirical knowledge. However, the first step in this process begins with the development of model potentials that adequately describe the scattering physics.

To accomplish this description, Section 2.1 provides a concise review of single particle quantum mechanics, which is used as a basis for both the two and many-body cases. Next, Section 2.2 serves to connect all the elements of scattering theory[1] required to understand the relationship between the scattering length and the associated interaction potential. Following this is a discussion of the low-energy scattering which provides geometric interpretations for the s-wave scattering length and effective range. Using these identifications, it then becomes possible to formulate simplified models of the two-body interaction, which can be used in simplifying the many-body model. In Section 2.5, bound states and resonances are identified as poles of the $\mathcal{T}$-matrix, where the distinction between the two is provided by their location on the complex plane.

Up to this point, all that has been considered pertains to the case of a single channel outcome in which two particles enter in a particular state or channel, scatter, then reemerge in the same channel. However, in any scattering reaction, there may be a number of different channels or outcomes which characterize the event. Hence, an analysis is undertaken in which the energetically favored channel of the scattering state is coupled to the energetically unfavorable state of a bound molecule. This coupled channels analysis forms the basis for the description of the Feshbach resonance, from which can arise coupled many-body superfluids having a mixed atom-molecule character. Lastly, numerical examples are presented, providing the parameters of some of the relevant isotopes used in current experiments.

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[1] Introductory treatments of quantum scattering may be found in J. J. Sakurai (1994), Chap. 7, and Cohen-Tannoudji (1977), Chap. VIII. The former presents the Lippmann-Schwinger operator approach, whereas the latter leans heavily toward the partial wave expansions.

2.1 Quantum Mechanics of Single Particles

To begin, it is helpful to review some single-particle quantum mechanics, as the fundamental concepts of this theory will be relied upon in subsequent many-particle generalizations. In quantum mechanics, the state of a particle, or any other object for that matter, is represented by an abstract state vector belonging to a linear vector space known as a Hilbert space, $\mathscr{H}$. One common feature to all quantum systems lies in the fact that the set of all single particle state vectors forms a Hilbert space.

To solidify the notion of the Hilbert space, it is necessary to state its defining characteristics. One important property of $\mathscr{H}$ is that it can be spanned by a countable orthonormal basis, $\{|n\rangle : n \text{ an integer}\}$. Mathematically, this means

$$\langle n|n'\rangle = \delta_{nn'} \quad \text{orthonormality}\,, \tag{2.1a}$$

$$\sum_n |n\rangle\langle n| = \mathbb{1} \quad \text{closure}\,. \tag{2.1b}$$

In the second equation, $\mathbb{1}$ refers to the identity operator acting on $\mathscr{H}$. As a consequence of the closure property, every vector, $|\psi\rangle \in \mathscr{H}$, can be expanded in terms of the basis $\{|n\rangle\}$:

$$|\psi\rangle = \sum_n \psi_n |n\rangle\,. \tag{2.2}$$

Known as the coordinates of $|\psi\rangle$ in the $\{|n\rangle\}$ representation, the expansion coefficients ψ_n, are given by the inner product $\psi_n = \langle n|\psi\rangle$, which are in general complex.

Connecting quantum theory to the physical world requires the association of observables or measurable quantities with Hermitian operators, $\hat{\mathcal{O}}$, that act on $\mathscr{H}$. If the system is in some state $|\psi\rangle$, then a measurement of $\mathcal{O}$ obtains the inner product value $\mathcal{O} = \langle\psi|\hat{\mathcal{O}}|\psi\rangle$ on average. In other words, $\hat{\mathcal{O}}$ is the operator associated with the observable $\mathcal{O}$, quantified by the expectation value $\langle\psi|\hat{\mathcal{O}}|\psi\rangle$. Some observables have eigenvectors that form an orthonormal basis spanning $\mathscr{H}$, although most do not have this property. For instance, the position and momentum of a particle are physically measurable quantities with corresponding operator representations, denoted as $\hat{\mathbf{x}}$ and $\hat{\mathbf{k}}$, respectively[1]. These operators have no normalizable or "proper" eigenvectors at all. Fortunately, through the work of Dirac, it is possible to work with the "improper" vectors, or vectors of infinite length, in forming a basis of $\mathscr{H}$. We introduce the improper eigenvectors of $\hat{\mathbf{x}}$ as $|\mathbf{x}\rangle$, which are defined to satisfy the normalization and completeness conditions

$$\langle\mathbf{x}|\mathbf{x}'\rangle = \delta(\mathbf{x}-\mathbf{x}')\,, \tag{2.3a}$$

$$\int_{\mathbf{x}} |\mathbf{x}\rangle\langle\mathbf{x}| = \mathbb{1}\,, \tag{2.3b}$$

in analogy with (2.1). Hence, the coordinate space expansion of a proper Schrödinger vector is given by

---

[1] We will call the vector $\hat{\mathbf{k}}$ the momentum although the actual momentum is $\hat{\mathbf{p}} = \hbar\hat{\mathbf{k}}$.

$$|\psi, t\rangle = \int_{\mathbf{x}} \psi(\mathbf{x}, t)|\mathbf{x}\rangle\,, \tag{2.4}$$

where we use the notation $\int_{\mathbf{x}} = \int d^3x$. The coefficient, $\psi(\mathbf{x}, t) = \langle \mathbf{x}|\psi, t\rangle$ is the spatial wave function, or the probability amplitude, where $|\psi(\mathbf{x}, t)|^2 d^3x$ is the probability of finding the particle within the volume d^3x at the location $\mathbf{x}$ and at the time t. Given this identification, normalization demands that we require $\int d^3x |\psi(\mathbf{x}, t)|^2 = 1$.

In a similar fashion it is possible to introduce momentum eigenvectors $|\mathbf{k}\rangle$ which are normalized as $\langle \mathbf{k}|\mathbf{k}'\rangle = \delta(\mathbf{k} - \mathbf{k}')$. This normalization combined with the completeness of the $\{|\mathbf{x}\rangle\}$ basis gives

$$\begin{aligned}\int_{\mathbf{x}} \langle \mathbf{k}|\mathbf{x}\rangle\langle \mathbf{x}|\mathbf{k}'\rangle &= \delta(\mathbf{k} - \mathbf{k}') \\ &= \int_{\mathbf{x}} e^{-i\mathbf{x}\cdot(\mathbf{k}-\mathbf{k}')}\,.\end{aligned} \tag{2.5}$$

The last line is just the Fourier integral representation[1] of the Dirac delta function, from which we identify

$$\langle \mathbf{x}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{x}}\,. \tag{2.6}$$

In the coordinate basis, the action of the momentum operator is determined by operating $\hat{\mathbf{k}}$ on some arbitrary ket $|\psi\rangle$, then projecting the result onto $\langle \mathbf{x}|$:

$$\begin{aligned}\langle \mathbf{x}|\hat{\mathbf{k}}|\psi\rangle &= \int'_{\mathbf{k}} \langle \mathbf{x}|\mathbf{k}\rangle\langle \mathbf{k}|\hat{\mathbf{k}}|\psi\rangle \\ &= \int'_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}\mathbf{k}\,\psi(\mathbf{k})\,.\end{aligned} \tag{2.7}$$

Recognizing the Fourier transform[2] of $\psi(\mathbf{x})$ in (2.7), this can be written as

$$\langle \mathbf{x}|\hat{\mathbf{k}}|\psi\rangle = -i\nabla_{\mathbf{x}}\psi(\mathbf{x})\,. \tag{2.8}$$

Thus, in the coordinate basis we have[3]

$$\hat{\mathbf{x}} \to \mathbf{x} \tag{2.9a}$$

$$\hat{\mathbf{k}} \to -i\nabla_{\mathbf{x}}\,. \tag{2.9b}$$

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[1] Throughout, we use the Fourier transform normalization convention such that $\delta(\mathbf{k} - \mathbf{k}') \equiv \int_{\mathbf{x}} exp\{-i\mathbf{x} \cdot (\mathbf{k} - \mathbf{k}')\}$, where the $(2\pi)^{-3}$ factor is accounted for in the inverse, $\delta(\mathbf{x} - \mathbf{x}') \equiv (2\pi)^{-3} \int_{\mathbf{k}} exp\{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')\}$.

[2] A primed integration sign is used to denote the $(2\pi)^{-3}$ factor.

[3] These identifications will be useful in the functional Schrödinger picture. Compare with Eqs. (4.7).

Determining the time evolution of a quantum system requires the solution of an operator equation on the state $|\psi, t\rangle$. In nonrelativistic quantum mechanics, particles obey the Schrödinger equation

$$-i\hbar\frac{\partial}{\partial t}|\psi, t\rangle = \hat{H}|\psi, t\rangle\,, \tag{2.10}$$

where $\hat{H}$ is the Hamiltonian, given by the sum of the kinetic energy operator $\hat{T} = (\hbar^2/2m)\,\hat{\mathbf{k}}^2$ and the external potential energy $\hat{V}$:

$$\begin{aligned}\hat{H} &= \hat{T} + \hat{V}\\ &= -\frac{\hbar^2}{2m}\,\hat{\mathbf{k}}^2 + \hat{V}\end{aligned} \tag{2.11}$$

For conservative systems, where the Hamiltonian is independent of time, the Schrödinger equation (2.10) admits the general solution

$$\begin{aligned}|\psi, t\rangle &= \sum_{n=0}^{\infty}\frac{1}{n!}\Big(\frac{-i\hat{H}t}{\hbar}\Big)^n|\psi\rangle\\ &= e^{-i\hat{H}t/\hbar}|\psi\rangle\\ &\equiv \hat{U}(t)|\psi\rangle\,.\end{aligned} \tag{2.12}$$

The operator $e^{-i\hat{H}t/\hbar} \equiv \hat{U}(t)$ is identified as the time evolution operator, whereas $|\psi\rangle$ is just the state of the system at $t = 0$. Since $\hat{H}$ is self-adjoint ($\hat{H}^\dagger = \hat{H}$) it follows that the evolution operator is unitary, or norm preserving. If $|\psi, t\rangle$ is stationary with respect to the energy (i.e. if $\langle\psi, t|\hat{H}|\psi, t\rangle$ is a constant), then it follows that $|\psi, t\rangle$ is an eigenstate of $\hat{H}$. Denoting the energy eigenvalue by E permits a recasting of (2.12) as

$$\begin{aligned}|\psi, t\rangle &= \sum_{n=0}^{\infty}\frac{1}{n!}\Big(-i\frac{Et}{\hbar}\Big)^n|\psi\rangle\\ &= e^{-iEt/\hbar}|\psi\rangle\,,\end{aligned} \tag{2.13}$$

which, when substituted into (2.10) gives the time-independent Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle\,. \tag{2.14}$$

Using Eqs. (2.9) and (2.11), the coordinate space representation of this eigenvalue equation is given as a second order differential equation for the wave function $\psi(\mathbf{x})$:

$$\Big[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\Big]\,\psi(\mathbf{x}) = E\,\psi(\mathbf{x})\,. \tag{2.15}$$

Knowing the potential, $V(\mathbf{x})$, plus the boundary conditions allows a complete solution to be determined. However, in many cases it turns out that V is quite complicated or not completely known in advance. Faced with this dilemma, it may seem that the Schrödinger equation is impossible to solve, especially in situations involving multiple particles that mutually interact. Fortunately, it is possible to introduce simplified interparticle pseudopotentials that permit an extraction of the salient physics without resorting to a full calculation that would be complicated by details of the potential. Furthermore, schemes have been developed to find the relevant physical information without actually solving the Schrödinger equation. One of these methods relies on the well-known theorem that states that taking the expectation value of the Hamiltonian with some arbitrary state, $|\psi\rangle$, results in a value that is greater than or equal to the ground state energy, $E_0 \geq \langle\psi|\hat{H}|\psi\rangle$. By making a good guess at a wave function that "closely" approximates the ground state, it is possible to obtain a close estimate of the true ground state energy. Typically, the trial wave function is chosen to have a convenient form dependent upon some initially undetermined parameters. Stationarizing $\langle\hat{H}\rangle$ with respect to these parameters reveals the optimal values for these unknowns. In Chapter 4, we use a generalization of this approach to deal with many-particle assemblies.

2.2 General Scattering Formalisms

2.2.1 Relative and Center of Mass Motion

Having reviewed some single particle preliminaries, we now consider the two-body system of masses m_1 and m_2, interacting through a mutual potential $V(\mathbf{x_1}-\mathbf{x_2})$. The Hamiltonian for this system is given by the sum two single particle Hamiltonians [compare with (2.15)] as

$$\hat{H} = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\mathbf{x_1}-\mathbf{x_2})\,. \tag{2.16}$$

Clearly, the corresponding two-particle wave function is an element of the Hilbert space $\mathscr{H}_2$, which is formed by the tensor product of the single particle spaces:

$$\mathscr{H}_2 = \mathscr{H} \otimes \mathscr{H}\,. \tag{2.17}$$

Because the potential is dependent upon the relative coordinate, $\mathbf{r} = \mathbf{x_1} - \mathbf{x_2}$, the wave function cannot be represented as a product of the single particle amplitudes, $\psi(\mathbf{x_1}, \mathbf{x_2}) \neq \phi(\mathbf{x_1})\phi(\mathbf{x_2})$. Alternatively, the Hamiltonian in (2.16) may be expressed in terms of the relative coordinate, $\mathbf{r}$, and the center of mass coordinate, $\mathbf{R} = m_1\mathbf{x_1} + m_2\mathbf{x_2}$, thus giving

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla_{\mathbf{R}}^2 - \frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2 + V(\mathbf{r})\,. \tag{2.18}$$

By this change of coordinate, the system has been decoupled, thus allowing the total wave function to be expressed as separable product of a relative amplitude and a center of mass amplitude, corresponding to a free particle of mass M and a relative particle of mass μ, where

$$M = m_1 + m_2\,, \tag{2.19a}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}\,. \tag{2.19b}$$

This rearrangement suggests an alternative decomposition of the two-body Hilbert space as

$$\mathscr{H}_2 = \mathscr{H}_{cm} \otimes \mathscr{H}_{rel} \tag{2.20}$$

where $\mathscr{H}_{cm}$ is a Hilbert space of plane wave states and $\mathscr{H}_{rel}$ is the space spanned by the eigenfunctions of the Hamiltonian with potential $V(\mathbf{r})$. Since the free particle is just the plane wave associated with the movement of the center of mass, it is not physically interesting and will therefore be ignored in subsequent discussions. Instead we confine our attention to the center of mass where the relative motion is equivalent to an effective one-body problem of a mass μ scattering off of a central potential, $V(\mathbf{r})$, located at the origin.

2.2.2 Asymptotic Scattering States

As we will be concerned with systems composed of identical particles, it is at first desirable to understand the scattering of two masses interacting through a potential V. As shown in the previous section, this is equivalent to being in the center of mass where the scattering is simply that of a mass $m/2$ scattering off a fixed force center. To understand the quantum description of this process, it is helpful to use the classical analog as a guide.

Assume that particles scatter from some target at time $t = 0$. At times long before or long after the event, the target has no influence, rendering the motion essentially free. As depicted in Fig. (2.1), the rectilinear motions long before, $t \to -\infty$, or long after the interaction, $t \to +\infty$, are referred to as the *in* or *out* asymptotes, respectively.

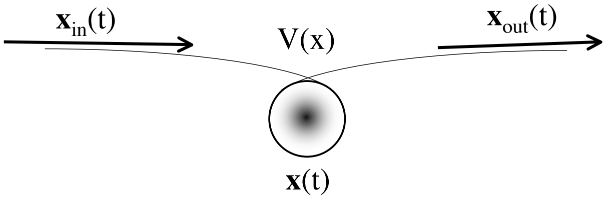

Figure 2.1: The in $\mathbf{x}_{in}(t)$ and the out $\mathbf{x}_{out}(t)$ asymptotes associated with the trajectory $\mathbf{x}(t)$. At times long before or after the interaction, the classical orbit approaches the respective in or out linear trajectories.

In atomic systems, the actual "orbit" is physically uninteresting due to the small length ($\sim 10^{-8}$ m) and time ($\sim 10^{-10}$ s) scales over which the potential has an appreciable influence. Therefore, it would be more useful to characterize a scattering event by its asymptotes rather than try to solve for the complete trajectory. To this end, a mapping is sought relating every in or out asymptote with an actual orbit. However, this mapping will not be onto because the inverse does not always exist, as is readily seen from the fact that bound orbits do not have asymptotes.

This description carries over into the quantum case with the orbit replaced by an amplitude. Denoting the full and free Hamiltonians as $\hat{H} = \hat{H}_0 + \hat{V}$ and $\hat{H}_0 = (\hbar^2/2m)\hat{\mathbf{k}}^2$, the respective time evolution operators [Eq. (2.12)] are given by $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ and $\hat{U}_0(t) = e^{-i\hat{H}_0 t/\hbar}$, from which the in and out asymptotes are seen to be

$$\hat{U}(t)|\psi\rangle \xrightarrow[t\to-\infty]{} \hat{U}_0(t)|\psi_{in}\rangle \tag{2.21a}$$

$$\hat{U}(t)|\psi\rangle \xrightarrow[t\to+\infty]{} \hat{U}_0(t)|\psi_{out}\rangle\,. \tag{2.21b}$$

By the above equations, it follows that the actual orbit, $\hat{U}(t)|\psi\rangle$ (with $|\psi\rangle$ the $t=0$ state), has the time dependent in and out asymptotes, $\hat{U}_0(t)|\psi_{in}\rangle$ and $\hat{U}_0(t)|\psi_{out}\rangle$, respectively. By using (2.21) it is possible to define the required mapping of the asymptotes onto the actual state at $t=0$:

$$|\psi\rangle = \lim_{t\to-\infty} U(t)^{\dagger} U_0(t)|\psi_{in}\rangle = \Omega_+|\psi_{in}\rangle \tag{2.22a}$$

$$|\psi\rangle = \lim_{t\to+\infty} U(t)^{\dagger} U_0(t)|\psi_{out}\rangle = \Omega_-|\psi_{out}\rangle\,, \tag{2.22b}$$

where we have dropped the hats on U and U_0. Known as the Møller operators, $\Omega_\pm = \lim_{t\to\mp\infty} U(t)^{\dagger} U_0(t)$, map any vector in the Hilbert space, $\mathscr{H}_{cm} \equiv \mathscr{H}$, to the actual $t=0$ state that would evolve from or to that vector.

Some comments are in order regarding the Hilbert space on which the Møller operators act. As noted above, the set of states with asymptotes, called the scattering states, together with the bound states span $\mathscr{H}$, the set of all states. To provide a distinction between these various spaces, we denote the subspace of bound states as $\mathscr{B}$, the subspace of states with in asymptotes as $\mathscr{R}_+$, and the subspace of states with out asymptotes as $\mathscr{R}_-$. Not surprisingly, the vectors in $\mathscr{R}_+ \bigcup \mathscr{R}_-$ are orthogonal to those in $\mathscr{B}$, or in set notation

$$\mathscr{R}_+ \perp \mathscr{B}\,; \qquad \mathscr{R}_- \perp \mathscr{B}\,. \tag{2.23}$$

In all that follows, the scattering theory will be assumed to be *asymptotically complete*, a condition in which $\mathscr{R}_+ = \mathscr{R}_- = \mathscr{R}$. Hence, for each $|\psi_{in}\rangle$ or $|\psi_{out}\rangle$ in $\mathscr{H}$, there corresponds a unique scattering state, $|\psi\rangle$. Conversely, for each $|\psi\rangle \in \mathscr{R}$, there are in and out asymptotes, $|\psi_{in}\rangle$ and $|\psi_{out}\rangle$. Note that even bound states, $\{|n\rangle\}$ in $\mathscr{H}$ can represent an asymptote after an application of the Møller operator: $|\psi_{in/out}\rangle = \Omega_\pm|n\rangle$.

2.2.3 The Scattering Operator

The $t=0$ amplitude can be expressed by either of its two asymptotes through the action of the appropriate Møller operator. Naturally, this leads to the construction of the scattering operator which relates the in asymptote to the out one. Because the Møller operators are unitary, Eqs. (2.22) give $|\psi_{out}\rangle = \Omega_-^{\dagger}|\psi\rangle = \Omega_-^{\dagger}\Omega_+|\psi_{in}\rangle = \mathcal{S}|\psi_{in}\rangle$, thus defining the scattering operator as

$$\mathcal{S} = \Omega_-^{\dagger}\Omega_+\,, \tag{2.24}$$

which can be shown to be unitary directly from the properties of $\Omega_\pm$. To understand the physical interpretation of $\mathcal{S}$, consider the in and out asymptotes given by $|\phi\rangle$ and $|\chi\rangle$, respectively. As such, the corresponding actual scattering states are $\Omega_+|\phi\rangle$ and $\Omega_-|\chi\rangle$. Hence, the probability amplitude for the process $|\phi\rangle \to |\chi\rangle$ is given by the overlap between the actual scattering states:

$$\begin{aligned} P(\phi \to \chi) &= \langle\chi|\Omega_-^\dagger \Omega_+|\phi\rangle \\ &= \langle\chi|\mathcal{S}|\phi\rangle\,, \end{aligned} \tag{2.25}$$

which is simply the $\mathcal{S}$ matrix element.

Furthermore, the action of the $\mathcal{S}$ operator conserves the energy in the system, as can be demonstrated by using the relation

$$H\Omega_\pm = \Omega_\pm H_0\,. \tag{2.26}$$

Known as the intertwining relation, this result can be proven in the following steps

$$\begin{aligned} e^{i\frac{Ht'}{\hbar}}\,\Omega_\pm &= e^{i\frac{Ht'}{\hbar}}\left[\lim_{t\to\mp\infty} e^{i\frac{Ht}{\hbar}}\,e^{-i\frac{H_0 t}{\hbar}}\right] \\ &= \lim_{t\to\mp\infty}\left[e^{i\frac{H(t'+t)}{\hbar}}\,e^{-i\frac{H_0 t}{\hbar}}\right] \\ &= \lim_{t\to\mp\infty} e^{i\frac{H(t'+t)}{\hbar}}\,e^{-i\frac{H_0(t'+t)}{\hbar}}\,e^{i\frac{H_0 t'}{\hbar}} \\ &= \Omega_\pm\,e^{i\frac{H_0 t'}{\hbar}} \end{aligned} \tag{2.27}$$

Taking derivatives with respect to t' establishes the desired result (2.26). If the in and out asymptotes are $|\psi_{in}\rangle$ and $|\psi_{out}\rangle$, then the mean out energy is $\langle\psi_{out}|H_0|\psi_{out}\rangle = \langle\psi_{in}|\mathcal{S}^\dagger H_0 \mathcal{S}|\psi_{in}\rangle$. Using the relation (2.26), we have $\mathcal{S}H_0 = \Omega_-^\dagger\Omega_+ H_0 = \Omega_-^\dagger H\Omega_+ = H_0\Omega_-^\dagger\Omega_+ = H_0\mathcal{S}$. Since $\mathcal{S}^\dagger\mathcal{S} = \mathbb{1}$ it follows that $\langle\psi_{out}|H_0|\psi_{out}\rangle = \langle\psi_{in}|H_0|\psi_{in}\rangle$, which verifies that the mean in energy is equal to the mean out energy for states mapped by the action of $\mathcal{S}$. Having established these properties of the $\mathcal{S}$ operator, it is appropriate to analyze the form of its matrix element $\langle\mathbf{k}|\mathcal{S}|\mathbf{k}'\rangle$. To explore this representation, it is most convenient to use the Green's operator, G, and the $\mathcal{T}$ operator, which are reviewed in the next few sections. In doing so, various relationships arise between the commonly used scattering quantities.

2.2.4 Green's Operator

Associated with the free Hamiltonian, $H_0 = \hat{\mathbf{p}}^2/(2m)$, and the full Hamiltonian, $H = \hat{\mathbf{p}}^2/(2m) + \hat{V}$, are the respective Green's operators:

$$G_0(\xi) = (\xi - H_0)^{-1}\,, \tag{2.28a}$$

$$G(\xi) = (\xi - H)^{-1}\,, \tag{2.28b}$$

defined for all ξ where the inverses exist. Since the Hamiltonian is always a Hermitian operator, these definitions are valid for any $\mathrm{Im}\{\xi\} \neq 0$. Multiplication of (2.28b) by $\xi - H$ gives $(\xi - H)G(\xi) = \mathbb{1}$, which has a coordinate space representation as

$$\left[\nabla^2_{\mathbf{x}} - V(\mathbf{x}) + \xi\right]\langle \mathbf{x}|G(\xi)|\mathbf{x}'\rangle = \delta(\mathbf{x}-\mathbf{x}') \tag{2.29}$$

thus showing that the coordinate representation of the Green's operator is just the Green's function of the corresponding differential operator.

If $\langle\phi|G(\xi)|\chi\rangle$ is an analytic function of ξ for all states $\langle\phi|$ and $|\chi\rangle$, then it is said that $G(\xi)$ is an analytic operator. By its construction, the Green's operator is therefore analytic everywhere except for the eigenvalue spectrum of its associated Hamiltonian. Hence, knowledge of G is equivalent to solving the eigenvalue problem. To understand how these eigenvalues manifest in the Green's operator, consider an explicit representation of $G(\xi)$ in the angular momentum eigenbasis $\{|E,\ell,m\rangle\}$:

$$\begin{aligned} G(\xi) &= (\xi - H)^{-1}\mathbb{1} \\ &= \int_0^\infty dE \sum_{\ell,m} \frac{|E,\ell,m\rangle\langle E,\ell,m|}{\xi - E} \end{aligned} \tag{2.30}$$

As seen from this form, the corresponding Green's function will have a branch cut along the positive real axis ($\mathrm{Re}\{\xi\} \geq 0$), representing the continuum of H. Bound states occur for some discrete set of values $E_n < 0$, which indicate the Green's function poles [Fig. 2.2)]. In fact, the poles of $G(\xi)$ will be used to calculate the binding energy of the coupled atom-molecule problem of Sec. 2.6.2.

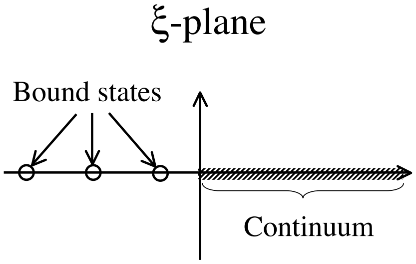

Figure 2.2: The complex ξ plane. In general, the Green's operator $G(\xi)$ of Eq. (2.28b) is analytic except at points along the real ξ axis that correspond to bound state poles for $\xi < 0$, and a continuum branch cut for $\xi \geq 0$.

Because knowledge of $G(\xi)$ solves the eigenvalue problem, it would be most useful to relate $G(\xi)$ from known operators. To accomplish this, first observe that the free Green's operator is explicitly known, as it is diagonal in momentum space,

$$G_0(\xi)|\mathbf{k}\rangle = (\xi - H_0)^{-1}|\mathbf{k}\rangle \tag{2.31}$$

$$= \frac{1}{\xi - E_k}|\mathbf{k}\rangle\,. \tag{2.32}$$

Since $G^{-1} = \xi - H = G_0^{-1} - V$, it becomes a simple matter to express G in terms of G_0 and V. Multiplying this identity on the left by G_0 and on the right by G obtains

$$G = G_0 + G_0 V G\,. \tag{2.33a}$$

Similarly, multiplying on the left by G and on the right by G_0 leads to

$$G = G_0 + G V G_0\,. \tag{2.33b}$$

Both (2.33a) and (2.33b) are referred to as the Lippmann-Schwinger equation for G. It must be remembered, however, that solving either for G is as difficult as obtaining an answer directly from the original eigenvalue problem.

2.2.5 Solutions from the Green's Operator

The full Hamiltonian has a solution that may be expressed in terms of the Green's operator. From the in asymptote, $|\phi\rangle$, the actual $t = 0$ state is

$$\begin{aligned} |\phi -\rangle &= \Omega_- |\phi\rangle \\ &= \lim_{t\to+\infty} U(t)^\dagger U_0(t)|\phi\rangle \\ &= |\phi\rangle + \frac{i}{\hbar}\int_0^\infty dt' U(t')^\dagger V U_0(t')|\phi\rangle\,. \end{aligned} \tag{2.34}$$

This last equality is obtained by integrating the time derivative of Ω_-, since $\partial_t\{\lim_{t\to\infty} U(t)^\dagger U_0(t)\} = \lim_{t\to\infty} U(t)^\dagger (iH/\hbar - iH_0/\hbar)U_0(t) = (i/\hbar)\lim_{t\to\infty} U(t)^\dagger V U_0(t)$. For some sufficiently small number, ε, the scattering state will be unchanged by the replacement of V by $Ve^{-\varepsilon|t|/\hbar}$, permitting a recasting of (2.34) as[1]

$$|\phi -\rangle = |\phi\rangle + \frac{i}{\hbar}\lim_{\varepsilon\downarrow 0} \int_{\mathbf{k}}\!\!{}' \int_0^\infty dt' \Big[e^{-\varepsilon t'/\hbar} U(t')^\dagger V U_0(t')\Big] |\mathbf{k}\rangle\langle\mathbf{k}|\phi\rangle\,. \tag{2.35}$$

Because $|\mathbf{k}\rangle$ is an (improper) eigenstate of the free Hamiltonian, H_0, the operator in square braces can be written as $e^{-i(E_k - i\varepsilon - H)t'/\hbar}V$, thus allowing the time integral to be performed explicitly

$$\begin{aligned} \int_0^\infty dt' e^{-i(E_k - i\varepsilon - H)t'/\hbar} V &= -i\hbar(E_k - i\varepsilon - H)^{-1} V \\ &= -i\hbar G(E_k - i\varepsilon) V\,, \end{aligned} \tag{2.36}$$

where use has been made of the Green's function (2.28b). Substitution of (2.36) into (2.35) yields the Green's operator expression for the scattering state in terms of its in asymptote, $|\phi\rangle$:

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[1] The downward arrow indicates that ε tends to zero along the positive real axis.

$$|\phi-\rangle = \Omega_-|\phi\rangle = |\phi\rangle + \lim_{\varepsilon\downarrow 0} \int_{\mathbf{k}}' G(E_k - i\varepsilon)\, V|\mathbf{k}\rangle\langle\mathbf{k}|\phi\rangle\,. \tag{2.37a}$$

Alternatively, it would have been possible to start with $|\phi\rangle$ as the out asymptote, in which case the scattering state is given as

$$|\phi+\rangle = \Omega_+|\phi\rangle = |\phi\rangle + \lim_{\varepsilon\downarrow 0} \int_{\mathbf{k}}' G(E_k + i\varepsilon)\, V|\mathbf{k}\rangle\langle\mathbf{k}|\phi\rangle\,. \tag{2.37b}$$

Equations (2.37) naturally suggest the definition of another useful object called the $\mathcal{T}$ operator.

2.2.6 The $\mathcal{T}$ Operator

Introduction of the $\mathcal{T}$ operator facilitates a compact expression for the $\mathcal{S}$ matrix elements. Moreover, the $\mathcal{T}$ matrix is itself a very convenient device which will be used in discussing the scattering length, pseudopotentials and bound states later on. With a plane wave state as the in asymptote, the action of $\mathcal{T}$ is *defined* as that of the potential operator on the full scattering state, $|\psi\rangle$:

$$T|\mathbf{k}\rangle = V|\psi\rangle\,. \tag{2.38}$$

To illustrate the utility in this definition, note that in matrix form, (2.37) can be written as $|\psi\rangle = |\mathbf{k}\rangle + G(\xi)V|\mathbf{k}\rangle$. Multiplying both sides by V, then using (2.38) along with the fact that $|\mathbf{k}\rangle$ is arbitrary, obtains $\mathcal{T}$ in terms of G and V:

$$\mathcal{T}(\xi) = V + V\,G(\xi)\,V\,. \tag{2.39}$$

From this result it is clear that $\mathcal{T}$ shares the same analytic behavior as $G(\xi)$, since it too is analytic for all ξ not in the spectrum of H. This property will be used when calculating the binding energy from the poles of $\mathcal{T}$.

Some important identities are obtained from (2.39). Multiplication on the left by the free Green's operator gives

$$\begin{aligned} G_0\,\mathcal{T} &= (G_0 + G_0\,V\,G)\,V \\ &= GV\,. \end{aligned} \tag{2.40a}$$

Similarly, multiplication on the right side by G_0 gives

$$\begin{aligned} \mathcal{T}G_0 &= V\,(G_0 + G\,V\,G_0) \\ &= VG\,. \end{aligned} \tag{2.40b}$$

where the last equalities in (2.40a) and (2.40b) follow from (2.33a) and (2.33b), respectively. Substitution of (2.40a) into (2.39) leads to the Lippmann-Schwinger equation for $\mathcal{T}$:

$$\mathcal{T} = V + VG_0\mathcal{T}\,. \tag{2.41}$$

If the potential is sufficiently weak, a solution may be obtained by iteration, where the first step is the Born approximation, $\mathcal{T} \simeq V$. Inserting this back into the Lippmann-Schwinger equation gives the second iteration, $\mathcal{T} \simeq V + VG_0V$. Continuing this process, known as Picard's method, results in the Born series

$$\mathcal{T} = V + VG_0V + VG_0VG_0V + \ldots . \tag{2.42}$$

Finally, there is sufficient background in place to discuss the S matrix element.

2.2.7 The S Matrix

The G and $\mathcal{T}$ operators are convenient constructions allowing for efficient calculation of the $\mathcal{S}$ matrix element in momentum space. By definition,

$$\begin{aligned}\langle \mathbf{k}|\mathcal{S}|\mathbf{k}'\rangle &= \langle \mathbf{k}|\Omega_-^\dagger \Omega_+|\mathbf{k}'\rangle \\ &= \lim_{\substack{t\to\infty \\ t'\to-\infty}} \langle \mathbf{k}|\big(e^{iH_0t/\hbar}e^{-iHt/\hbar}\big)\big(e^{iHt'/\hbar}e^{-iH_0t'/\hbar}\big)|\mathbf{k}'\rangle \, .\end{aligned} \tag{2.43}$$

Ordering in the limits is immaterial, so it is permissible to set $t' = -t$ then let $t \to \infty$:

$$\langle \mathbf{k}|\mathcal{S}|\mathbf{k}'\rangle = \lim_{t\to\infty} \langle \mathbf{k}|e^{iH_0t/\hbar}e^{-2iHt/\hbar}e^{-iH_0t/\hbar}|\mathbf{k}'\rangle \tag{2.44}$$

As was done in Eq. (2.35), the operator is expressed as the integral of its derivative, where the derivative is $\partial_t e^{iH_0t/\hbar}\, e^{-2iHt/\hbar}\, e^{iH_0t/\hbar} = -(i/\hbar)(e^{iH_0t/\hbar}\, V\, e^{-2iHt/\hbar}\, e^{iH_0t/\hbar} + e^{iH_0t/\hbar}\, e^{-2iHt/\hbar}\, V\, e^{iH_0t/\hbar})$. Also, V gets replaced by $Ve^{-\varepsilon t/\hbar}$, thus giving

$$\begin{aligned}\langle \mathbf{k}|\mathcal{S}|\mathbf{k}'\rangle &= \delta(\mathbf{k}-\mathbf{k}') - \frac{i}{\hbar}\lim_{\varepsilon\downarrow 0}\int_0^\infty dt e^{-\varepsilon t}\langle \mathbf{k}|(\ldots)|\mathbf{k}'\rangle \\ &= \delta(\mathbf{k}-\mathbf{k}') - \frac{i}{\hbar}\lim_{\varepsilon\downarrow 0}\int_0^\infty dt \langle \mathbf{k}|V\, e^{i(E_{k'}+E_k+i\varepsilon-2H)t/\hbar} + e^{i(E_{k'}+E_k+i\varepsilon-2H)t/\hbar}\, V|\mathbf{k}'\rangle \\ &= \delta(\mathbf{k}-\mathbf{k}') + \frac{1}{2}\lim_{\varepsilon\downarrow 0}\langle \mathbf{k}|V\, G\Big(\frac{E_{k'}+E_k}{2}+i\varepsilon\Big) + G\Big(\frac{E_{k'}+E_k}{2}+i\varepsilon\Big)\, V|\mathbf{k}'\rangle \, .\end{aligned} \tag{2.45}$$

Using the relations (2.40) along with the identity $\lim_{\varepsilon\downarrow 0}\{(E_{k'}-E_k+i\varepsilon)^{-1} + (E_k - E_{k'} + i\varepsilon)^{-1}\} = -2\pi i\delta(E_{k'}-E_k)$, obtains the matrix element as

$$\langle \mathbf{k}|\mathcal{S}|\mathbf{k}'\rangle = \delta(\mathbf{k}-\mathbf{k}') - 2\pi i\delta(E_{k'}-E_k)\lim_{\varepsilon\downarrow 0}\langle \mathbf{k}|\mathcal{T}(E_k+i\varepsilon)|\mathbf{k}'\rangle \, . \tag{2.46}$$

The first term in $\mathcal{S}(\mathbf{k},\mathbf{k}')$ is a delta function, or the amplitude for the particle to pass through without scattering, whereas the second term is proportional to the scattering amplitude. As expected, the two delta functions assure energy conservation. More precisely, the second term is associated with the on-shell $\mathcal{T}$ matrix, defined only for those momenta on the energy shell $|\mathbf{k}|^2 = |\mathbf{k}'|^2$. One may wonder why it is necessary to bother with the full $\mathcal{T}$ matrix, as only the on-shell components seem to contribute to the scattering. The answer is twofold. First, although $\mathcal{S}$ does describe the scattering process, the delta functions make it a highly singular equation, whereas the Lippmann-Schwinger equation for the full $\mathcal{T}$ matrix (2.41) is not. Therefore, it is convenient to generalize $\mathcal{T}$ in obtaining nonsingular expressions. Second, the off-shell components of $\mathcal{T}$ are relevant in more complicated multi-channel scattering processes. Thus far, we have only been concerned with single channel scattering in which two particles go in then come out. However, there do exist situations where reactions occur involving the emergence of new particles in the out asymptote.

2.2.8 Stationary Scattering States and the Scattering Amplitude

We denote $|\mathbf{k}\pm\rangle = \Omega_\pm|\mathbf{k}\rangle$ as the scattering state associated with the in or out asymptote, depending on whether the respective + or - sign is taken. Operating with the full Hamiltonian gives

$$\begin{aligned} H|\mathbf{k}\pm\rangle &= H\Omega_\pm|\mathbf{k}\rangle \\ &= \Omega_\pm H_0|\mathbf{k}\rangle \\ &= E_k|\mathbf{k}\pm\rangle\,, \end{aligned} \tag{2.47}$$

where the second line follows from the intertwining relation (2.26). This shows that $|\mathbf{k}\pm\rangle$ are indeed eigenvectors of H, with the same eigenvalues as the free Hamiltonian. By the results (2.37), these stationary states are expressed in terms of Green's operators as $|\mathbf{k}\pm\rangle = |\mathbf{k}\rangle + G(E_k \pm i\varepsilon)\,V|\mathbf{k}\rangle$. Since it is also true that $G(E_k \pm i\varepsilon)\,V|\mathbf{k}\rangle = G_0(E_k \pm i\varepsilon)\,\mathcal{T}|\mathbf{k}\rangle = G_0(E_k \pm i\varepsilon)\,V|\mathbf{k}\pm\rangle$, the stationary state is

$$|\mathbf{k}\pm\rangle = |\mathbf{k}\rangle + G_0(E_k \pm i\varepsilon)\,V|\mathbf{k}\pm\rangle\,, \tag{2.48}$$

with the corresponding wave function

$$\psi_{\mathbf{k}}(\mathbf{x}) = \langle\mathbf{x}|\mathbf{k}\pm\rangle = \langle\mathbf{x}|\mathbf{k}\rangle + \int_{\mathbf{x}'} \langle\mathbf{x}|G_0(E_k \pm i\varepsilon)|\mathbf{x}'\rangle V(\mathbf{x}')\langle\mathbf{x}'|\mathbf{k}\pm\rangle\,. \tag{2.49}$$

To proceed further requires the matrix element of the free particle Green's operator in coordinate space:

$$\begin{aligned} \langle\mathbf{x}|G_0(\xi)|\mathbf{x}'\rangle &= \int'_{\mathbf{k}} \langle\mathbf{x}|G_0(\xi)|\mathbf{k}\rangle\langle\mathbf{k}|\mathbf{x}'\rangle \\ &= \int'_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{\xi - E_k}\,. \end{aligned} \tag{2.50}$$

Taking $\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}') = k|\mathbf{x}-\mathbf{x}'|\cos\theta$, then integrating over the full solid angle yields

$$\langle \mathbf{x}|G_0(\xi)|\mathbf{x}'\rangle = \frac{i}{4\pi^2|\mathbf{x}-\mathbf{x}'|}\int\limits_{-\infty}^{\infty} dkk\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{k^2-\xi}$$

$$= -\frac{1}{4\pi}\frac{e^{i\sqrt{\xi}\,|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}\,, \tag{2.51}$$

where the last line was accomplished by complex contour integration[1]. With $\xi = k^2 \pm i\varepsilon$, this is inserted back into (2.49):

$$\langle \mathbf{x}|\mathbf{k}\pm\rangle = \langle \mathbf{x}|\mathbf{k}\rangle - \frac{1}{4\pi}\int\limits_{\mathbf{x}'}' \frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}V(\mathbf{x}')\langle \mathbf{x}'|\mathbf{k}\pm\rangle\,. \tag{2.52}$$

The asymptotic behavior for large $|\mathbf{x}|$, is obtained from the usual expansion

$$|\mathbf{x}-\mathbf{x}'| = (x^2 - 2\mathbf{x}\cdot\mathbf{x}' + x'^2)^{1/2} = x\Big[1 - \frac{\mathbf{x}\cdot\mathbf{x}'}{x^2} + \ldots\Big]\,. \tag{2.53}$$

Substituting this into (2.52), then keeping the leading term in the denominator while retaining the first two terms of the exponent, gives

$$\langle \mathbf{x}|\mathbf{k}\pm\rangle \xrightarrow[x\to\infty]{} \langle \mathbf{x}|\mathbf{k}\rangle - \frac{1}{4\pi}\frac{e^{\pm ikx}}{x}\int\limits_{\mathbf{x}'} e^{\mp ik\hat{\mathbf{x}}\cdot\mathbf{x}'}V(\mathbf{x}')\langle \mathbf{x}'|\mathbf{k}\pm\rangle$$

$$= e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{4\pi}\langle \pm k\hat{\mathbf{x}}|V|\mathbf{k}\pm\rangle\frac{e^{\pm ikx}}{x}\,. \tag{2.54}$$

Since, for the case of $|\mathbf{k}+\rangle$, $V|\mathbf{k}+\rangle = \mathcal{T}(E_k + i\varepsilon)|\mathbf{k}\rangle$, (2.54) becomes

$$\langle \mathbf{x}|\mathbf{k}\pm\rangle \xrightarrow[x\to\infty]{} e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{4\pi}\langle k\hat{\mathbf{x}}|\mathcal{T}(E_k + i\varepsilon)|\mathbf{k}\rangle\frac{e^{ikx}}{x}$$

$$= e^{i\mathbf{k}\cdot\mathbf{x}} + f(\theta,\varphi)\,\frac{e^{ikx}}{x}\,, \tag{2.55}$$

where the scattering amplitude is defined by

$$f(\theta,\varphi) \equiv -\frac{1}{4\pi}\langle k\hat{\mathbf{x}}|\mathcal{T}(E_k + i\varepsilon)|\mathbf{k}\rangle \tag{2.56}$$

As the polar angles (θ,φ) are those between $\hat{\mathbf{x}}$ and $\mathbf{k}$, the scattering amplitude quantifies the angular dependence of the scattered wave. This quantity is intimately related to the cross section, the only measurable quantity in a scattering experiment.

---

[1] Either the upper or the lower semi-circular contour can be chosen at this point, as we have not yet specified on which side of the real axis ξ lies on.

2.2.9 Cross Section and the Scattering Amplitude

In any scattering experiment, all that is known is that particles with some reasonably well-defined momentum impinge upon a target from which it is possible to measure the resultant flux of the scattered particles. Put another way, all that can be measured is the probability that particles in some incoming state $\psi_{in}(\mathbf{x})$ are deflected into some element of solid angle, $d\Omega$, about the scattering center. Due to the fact that there is no precise knowledge of the incoming state, an average is taken over all reasonable incoming states, thus leading to the notion of the differential cross section.

Assuming the incoming asymptote is a plane wave along the $z-$axis, the asymptotic functions can be written

$$\psi_{in}(\mathbf{x}) = e^{ikz} \tag{2.57a}$$

$$\begin{aligned}\psi_{out}(\mathbf{x}) &= \psi_{in}(\mathbf{x}) + \psi_{sc}(\mathbf{x}) \\ &= e^{ikz} + f(\theta,\varphi)\frac{e^{ikx}}{x}\,.\end{aligned} \tag{2.57b}$$

The situation can be visualized in Figure (2.3).

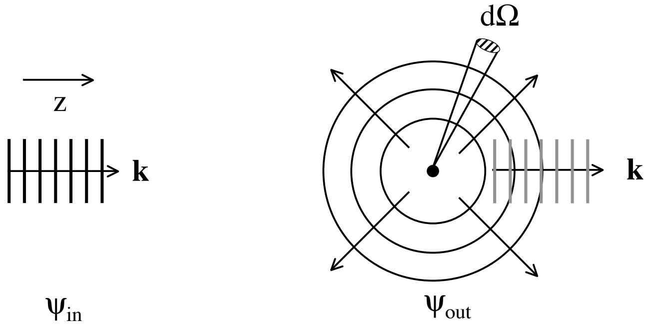

Figure 2.3: The in and out asymptotes of the stationary scattering states. The in asymptote is a plane wave, whereas the scattering asymptote is a sum of an outward traveling spherical wave and an attenuated in asymptote. From the spherical component, a particle flux equal to $|f(\theta,\varphi)|^2 d\Omega$ is scattered into the solid angle $d\Omega$ at (θ,φ).

Using the forms of ψ_{in} and ψ_{sc}, it is possible to calculate the particle flux associated with the incoming and scattering states

$$\begin{aligned}\mathbf{j}_{in} &= -\frac{i\hbar}{m}\big[\psi_{in}^*\nabla\psi_{in} - (\nabla\psi_{in}^*)\psi_{in}\big] \\ &= \frac{2\hbar k}{m}\hat{\mathbf{z}}\end{aligned} \tag{2.58a}$$

$$\begin{aligned}\mathbf{j}_{sc}\cdot d\mathbf{S} &= -\frac{i\hbar}{m}\left[\psi_{sc}^*\frac{\partial}{\partial x}\psi_{sc} - \Big(\frac{\partial}{\partial x}\psi_{sc}^*\Big)\psi_{sc}\right]x^2 d\Omega \\ &\xrightarrow[x\to\infty]{} |\mathbf{j}_{in}||f(\theta,\varphi)|d\Omega\,.\end{aligned} \tag{2.58b}$$

By definition, the differential cross section, $\sigma(\theta,\varphi)$, is the fraction of the incident flux scattered into the solid angle $d\Omega$ at (θ,φ). From (2.58b) it is seen that $\sigma(\theta,\varphi)$ is simply the absolute square of the scattering amplitude

$$\sigma(\theta,\varphi) = |f(\theta,\varphi)|^2\,, \tag{2.59a}$$

with the total cross section given by an integral over the solid angle

$$\sigma_T = \int |f(\theta,\varphi)|^2 d\Omega\,. \tag{2.59b}$$

Thus, solving the scattering problem is equivalent to finding the scattering amplitude $f(\theta,\varphi)$ for a given potential, $V(\mathbf{x})$. If $V(\mathbf{x})$ can be replaced by a simple enough form, then finding the amplitude can be effectively accomplished directly from the Lippmann-Schwinger equation (2.41). Such simplified pseudopotentials will be discussed in Sec. 2.4.

2.2.10 The Partial Wave Series

Another important representation of scattering theory involves the expression of the incoming and outgoing states as a sum over spherical waves. The effect of the potential is then naturally incorporated through the phase shifts of the outgoing waves relative to the incoming waves. To connect this approach to the $\mathcal{T}$ and $\mathcal{S}$ operators, first consider a spherical wave basis is generated by the orthonormal eigenvectors $\{|E,\ell,m\rangle\}$ of the complete set of commuting observables H_0, L^2 and L_z, where the respective eigenvalues are given by E, $\ell(\ell+1)$ and m. Because the scattering operator $\mathcal{S}$ commutes with H_0 and $\mathbf{L}$, it must be diagonal in the spherical wave basis:

$$\langle E,\ell,m|\mathcal{S}|E',\ell',m'\rangle = \delta(E-E')\delta_{\ell\ell'}\delta_{mm'}\,s_\ell(E)\,, \tag{2.60}$$

where the unitarity of $\mathcal{S}$ allows the eigenvalue to be written in terms of the partial wave shift, $\delta_\ell(E)$, of the ℓth partial wave:

$$s_\ell(E) = e^{2i\delta_\ell(E)}\,. \tag{2.61}$$

Projecting the free particle Schrödinger equation onto spherical coordinates obtains the normalized spatial wave functions as

$$\langle\mathbf{x}|E,\ell,m\rangle = i^\ell\Big(\frac{k}{\pi}\Big)^{1/2}\frac{1}{kx}\,\hat{j}_\ell(kx)\,Y_\ell^m(\hat{\mathbf{x}})\,, \tag{2.62}$$

where i^ℓ is conventional and $\hat{j}_\ell(kx) = kxj_\ell(kx)$ is the Riccati-Bessel function with $j_\ell(kx)$ the spherical Bessel function. Also, $Y_\ell^m(\hat{\mathbf{x}})$ is the spherical harmonic with the argument denoting the polar angles (θ, φ) of the unit vector $\hat{\mathbf{x}}$. From the normalization, $\langle E, \ell, m|E', \ell', m'\rangle = \delta(E - E')\delta_{\ell\ell'}\delta_{mm'}$[1], it is possible to derive the momentum space representation

$$\langle \mathbf{k}|E, \ell, m\rangle = (2\pi)^{3/2}\Big(\frac{k}{2}\Big)^{-1/2}\delta(E_k - E)Y_\ell^m(\hat{\mathbf{k}})\,, \tag{2.63}$$

where the factor of $(2\pi)^{3/2}$ is in keeping with the Fourier transform convention of (2.5). According to Eqs. (2.46) and (2.55), the amplitude, $f(\theta, \varphi)$, is expressible as

$$\langle \mathbf{k}|(\mathcal{S} - 1)|\mathbf{k}'\rangle = -2\pi i\delta(E_k - E_{k'})\lim_{\varepsilon\downarrow 0}\langle \mathbf{k}|\mathcal{T}(E_k + i\varepsilon)|\mathbf{k}\rangle \tag{2.64}$$

$$= 8\pi^2 i\delta(E_k - E_{k'})f(\theta, \varphi)\,. \tag{2.65}$$

On the other hand, $\mathcal{S} - 1$ can be expressed using (2.60) and (2.63):

$$\begin{aligned}\langle \mathbf{k}|\mathcal{S} - 1|\mathbf{k}'\rangle &= \int dE\sum_{\ell,m}\langle \mathbf{k}|(\mathcal{S} - 1)|E, \ell, m\rangle\langle E, \ell, m|\mathbf{k}'\rangle\\ &= \int dE\sum_{\ell,m}\langle \mathbf{k}|(s_\ell(E_{k'}) - 1)|E, \ell, m\rangle\langle E, \ell, m|\mathbf{k}'\rangle\\ &= \frac{16\pi^3}{k}\delta(E_k - E_{k'})\sum_{\ell,m}Y_\ell^m(\hat{\mathbf{k}'})\big[s_\ell(E_{k'}) - 1\big]Y_\ell^m(\mathbf{k})^*\\ &= \frac{4\pi^2}{k}\delta(E_k - E_{k'})\sum_{\ell=0}^{\infty}(2\ell + 1)\big[s_\ell(E_{k'}) - 1\big]P_\ell(\cos\theta)\,.\end{aligned} \tag{2.66}$$

In writing the final line of (2.66), use has been made of the addition theorem for spherical harmonics[2]. Equating (2.64) with (2.66) gives the partial wave expansion of the scattering amplitude

$$f(\theta, \varphi) = \sum_{\ell=0}^{\infty}(2\ell + 1)f_\ell(E_k)P_\ell(\cos\theta)\,, \tag{2.67}$$

from which a partial wave amplitude can be identified as

$$\begin{aligned}f_\ell(E) &= \frac{s_\ell(E) - 1}{2ik}\\ &= \frac{e^{2i\delta_\ell(E)} - 1}{2ik}\\ &= \frac{1}{k}e^{i\delta_\ell(E)}\sin\delta_\ell(E)\,.\end{aligned} \tag{2.68}$$

---

[1] Using the orthonormality relations $\int d\Omega Y_\ell^m(\theta, \varphi)^* Y_\ell^m(\theta, \varphi) = 1$ and $\int x^2 dx j_\ell(kx)j_\ell(k'x) = (\pi/2k^2)\delta(k - k') = (\pi/k)\delta(E - E')$, this can be explicitly verified from (2.62).

[2] With $P_\ell(\cos\theta)$ the Legendre polynomial and θ the angle between $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$, the addition theorem is $\sum_m Y_\ell^m(\hat{\mathbf{k}})Y_\ell^m(\hat{\mathbf{k}}')^* = \frac{2\ell+1}{4\pi}P_\ell(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')$.

The expansion (2.67) can be regarded as a statement that the full amplitude is a sum of the contributions, $f_\ell(E)$, from each partial wave, where knowledge of the corresponding phase shifts, $\delta_\ell(E)$, determines the full amplitude. From this perspective, all scattering quantities have a dependence on the phase shifts.

Finally, the differential cross section can be related to the phase shifts by

$$\begin{aligned}\sigma(\theta,\varphi) &= |f(\theta,\varphi)|^2 \\ &= \frac{1}{k^2}\left|\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell(E)}\sin\delta_\ell(E)P_\ell(\cos\theta)\right|^2 .\end{aligned} \tag{2.69}$$

Evaluation of the total cross section is straightforward,

$$\begin{aligned}\sigma_T &= \int d\Omega |f(\theta,\varphi)|^2 \\ &= \frac{2\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell(E) .\end{aligned} \tag{2.70}$$

Physically, the phase shifts' meaning emerges when the partial wave expansion of the free radial wave function is compared with the analogous expansion of the asymptotic scattered wave function.

2.2.11 Free Radial Wave Function

Although the normalized solution to the free $[V(\mathbf{x}) = 0]$ case has been written down in (2.62), it is nonetheless instructive to examine the general solutions of the free radial equation. For spherically symmetric potentials, the wave function $\langle \mathbf{x}|E,\ell,m\rangle$ can be written as a product of a spherical harmonic and a radial function:

$$\langle \mathbf{x}|E,\ell,m\rangle = \frac{u^f_{\ell,k}(x)}{x}Y^m_\ell(\hat{\mathbf{x}}) , \tag{2.71}$$

which, when substituted into the time independent Schrödinger equation reduces to the radial equation

$$\left[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + k^2\right]u^f_{\ell,k}(x) = 0 . \tag{2.72}$$

Due to the $1/x$ form of the wave function, we must impose the boundary condition

$$u^f_{\ell,k}(0) = 0 . \tag{2.73}$$

The solution that solves (2.72) and (2.73) is given by the Riccati-Bessel function,

$$\begin{aligned}\hat{j}_\ell(kx) &\equiv kx\, j_\ell(kx) \\ &= (kx)^{\ell+1}\sum_{n=0}^{\infty}\frac{\left[-(kx)^2/2\right]^n}{n!(2\ell+2n+1)!!} ,\end{aligned} \tag{2.74}$$

which is seen to vanish as $x^{\ell+1}$ at the origin. The other solution behaves like $x^{-\ell}$ as $x \to 0$, and is given by the Riccati-Neumann function:

$$\begin{aligned}\hat{n}_\ell(kx) &\equiv kx\, n_\ell(kx)\\ &= (kx)^{-\ell}\sum_{n=0}^{\infty}\frac{1}{n!}\Big[\frac{-(kx)^2}{2}\Big]^n(2\ell-2n-1)!!\,.\end{aligned} \tag{2.75}$$

At large distances from the scattering center ($x \to \infty$), we expect the radial solution to approach plane waves, a limiting behavior that is captured by the Riccati-Hankel functions:

$$\begin{aligned}\hat{h}_\ell^{\pm} &= \hat{n}_\ell(kx) \pm i\hat{j}_\ell(kx)\\ &\xrightarrow[x\to\infty]{} e^{\pm i(kx-\ell\pi/2)}\,.\end{aligned} \tag{2.76}$$

As suggested by (2.76), the asymptotic forms of $\hat{n}_\ell(kx)$ and $\hat{j}_\ell(kx)$ are given by

$$\hat{n}_\ell(kx) \xrightarrow[x\to\infty]{} \cos(kx-\ell\pi/2) \tag{2.77a}$$

$$\hat{j}_\ell(kx) \xrightarrow[x\to\infty]{} \sin(kx-\ell\pi/2)\,. \tag{2.77b}$$

Having outlined some general solutions of (2.72), we now proceed to expand the plane waves, $|\mathbf{k}\rangle$ in terms of spherical partial waves:

$$\begin{aligned}|\mathbf{k}\rangle &= \int dE\sum_{\ell m}|E,\ell,m\rangle\langle E,\ell,m|\mathbf{k}\rangle\\ &= 4\pi^{3/2}\frac{1}{\sqrt{k}}\sum_{\ell m}|E_k,\ell,m\rangle Y_\ell^m(\hat{\mathbf{k}})^*\,,\end{aligned} \tag{2.78}$$

which follows from (2.63). Projection onto the coordinate space gives the partial wave expansion of the plane wave function,

$$\begin{aligned}\langle\mathbf{x}|\mathbf{k}\rangle &= 4\pi^{3/2}\frac{1}{\sqrt{k}}\sum_{\ell,m}\langle\mathbf{x}|E,\ell,m\rangle Y_\ell^m(\hat{\mathbf{k}})^*\\ &= 4\pi\sum_{\ell,m}i^\ell\frac{1}{kx}\hat{j}_\ell(kx)Y_\ell^m(\hat{\mathbf{x}})Y_\ell^m(\hat{\mathbf{k}})^*\\ &= \frac{1}{kx}\sum_\ell(2\ell+1)i^\ell\hat{j}_\ell(kx)P_\ell(\hat{\mathbf{x}}\cdot\hat{\mathbf{k}})\,,\end{aligned} \tag{2.79}$$

where use has been made of (2.62) as well as the addition theorem for spherical harmonics. Next, we outline the partial wave scattering states, thus illustrating the phase shift when compared with the free form.

2.2.12 Partial Wave Scattering States

Just as $|E, \ell, m\rangle$ are the eigenstates of angular momentum (L^2, L_z) and the free Hamiltonian, H_0, we use the Møller operator to define

$$|E, \ell, m+\rangle = \Omega_+ |E, \ell, m\rangle \tag{2.80}$$

as the eigenvectors of L^2, L_z and the full Hamiltonian H. In analogy with the free case (2.62), the normalized scattering wave function is written as a separable product

$$\langle \mathbf{x}|E, \ell, m+\rangle = i^\ell \Big(\frac{k}{\pi}\Big)^{1/2} \frac{1}{kx} u_{\ell,k}(kx) Y_\ell^m(\hat{\mathbf{x}}) \,, \tag{2.81}$$

with the full radial function $u_{\ell,k}(kx)$ that satisfies

$$\Big[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} - V(x) + k^2\Big] u_{\ell,k}(x) = 0 \,, \tag{2.82}$$

where $u_{\ell,k}(x) \to u^f_{\ell,k}(x)$ as $V(x) \to 0$. Just as in Eq. (2.79), the corresponding full wave function is

$$\langle \mathbf{x}|\mathbf{k}+\rangle = \frac{1}{kx} \sum_\ell (2\ell+1) i^\ell u_{\ell,k}(kx) P_\ell(\hat{\mathbf{x}} \cdot \hat{\mathbf{k}}) \,, \tag{2.83a}$$

with (2.55) giving the asymptotic form as

$$\xrightarrow[x\to\infty]{} e^{i\mathbf{k}\cdot\mathbf{x}} + f(\theta, \varphi)\, \frac{e^{ikx}}{x} \,. \tag{2.83b}$$

Inserting the partial wave expansions of the plane wave (2.79) and the scattering amplitude (2.67) yields

$$\langle \mathbf{x}|\mathbf{k}+\rangle \xrightarrow[x\to\infty]{} \frac{1}{kx} \sum_\ell (2\ell+1) \big[i^\ell \hat{j}_\ell(kx) + k f_\ell(E_k) e^{ikx}\big] P_\ell(\hat{\mathbf{x}} \cdot \hat{\mathbf{k}}) \tag{2.84}$$

A comparison of this expression with (2.83a), reveals the asymptotic radial wave function to be

$$u_{\ell,k}(kx) \xrightarrow[x\to\infty]{} \hat{j}_\ell(kx) + k f_\ell(E_k) e^{i(kx - \ell\pi/2)} \tag{2.85}$$

Replacing $\hat{j}_\ell(kx)$ by its asymptotic form (2.77b) and using the definition $k f_\ell(E_k) = (exp\{2i\delta_\ell(k)\} - 1)/(2ik)$, obtains

$$u_{\ell,k}(kx) \xrightarrow[x\to\infty]{} e^{i\delta_\ell(k)} \sin\Big[kx - \frac{\ell\pi}{2} + \delta_\ell(k)\Big] \,. \tag{2.86}$$

In a comparison with the free radial asymptote,

$$\hat{j}_\ell(kx) \xrightarrow[x\to\infty]{} \sin\Big[kx - \frac{\ell\pi}{2}\Big] \,, \tag{2.87}$$

it is seen that the potential has the effect of shifting the phase of the ℓth partial wave function by $\delta_\ell(k)$. For attractive potentials, the particles are more likely to be closer to the scattering center. Hence, the wave function should be "pulled into" the potential, resulting in a positive phase shift, $\delta_\ell(k) > 0$. Conversely, repulsive interactions "push outward" on the particles, leading to a negative phase shift. The relation between the potential and the wave-function geometry can be further developed through the s-wave scattering length parameter.

2.3 Scattering Length and Effective Range

In this section, we define the scattering length and the effective range, parameters used in the specification of pseudopotentials. Through this description, it will be seen how these quantities are related to the s-wave phase shift and the $\mathcal{T}$ matrix.

2.3.1 Scattering Length

The scattering length is best illustrated by considering the asymptotic form of the scattered state. Beginning with the full radial equation

$$\left[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} - V(x) + k^2\right] u_{\ell,k}(x) = 0\,, \tag{2.88}$$

it is seen that far from the scattering center, $x \to \infty$, the potential and the centrifugal term are negligible. Equivalently, this situation describes the s-wave ($\ell = 0$) scattering of particles outside the region of influence of the potential. In either case, the low-energy ($k \to 0$) solution approaches a linear form, denoted by $v_0(x)$:

$$\frac{d^2 v_0}{dx^2} = 0 \Rightarrow v_0(x) \propto x - a\,, \tag{2.89}$$

Here, the parameter a is called the s-wave scattering length which has the geometrical interpretation as the point at which the asymptotically linear radial wave function intercepts its coordinate axis[1]. Figure. (2.4) demonstrates the relationship between the scattering length and the potential. For attractive potentials, a can be either positive or negative, but for repulsive interactions, a must be non-negative[2].

The low-energy (small k) expansion of the radial function $x\,\langle \mathbf{x}|\mathbf{k}+\rangle$ determines a in terms of the phase shift. Including only the s-wave contribution in the sum (2.83a), we have

$$\begin{aligned} x\,\langle \mathbf{x}|\mathbf{k}+\rangle \xrightarrow[x\to\infty]{} & \frac{1}{k}\sin\bigl[kx + \delta_0(k)\bigr] \\ \propto & \frac{1}{k}\sin\delta_0(k) + x\cos\delta_0(k) \quad (k \to 0)\,. \end{aligned} \tag{2.90}$$

Matching the normalization of this asymptotic expression to the linear form in (2.89) requires a division by $\cos\delta_0(k)$, from which we have

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[1] This defines the "zero-energy" scattering length, which we identify simply as the scattering length. Alternatively, a can be defined as the first zero of the radial wave function, thus making it an energy dependent quantity.

[2] We define an attractive or repulsive potential as $V(x) < 0;\ \forall x$ or $V(x) > 0;\ \forall x$, respectively. Actual potentials may have both attractive and repulsive parts, depending on x, but we restrict our attention to the simplified case of either pure attraction or pure repulsion, which is justified in sufficiently dilute systems where particles only feel the effect of the long-range tail.

$$v_k(x) = x + \frac{1}{k}\tan\delta_0(k)\,. \tag{2.91}$$

Alternatively, we can use the form in (2.83b),

$$v_k(x) = x + f(\theta,\varphi)\,. \tag{2.92}$$

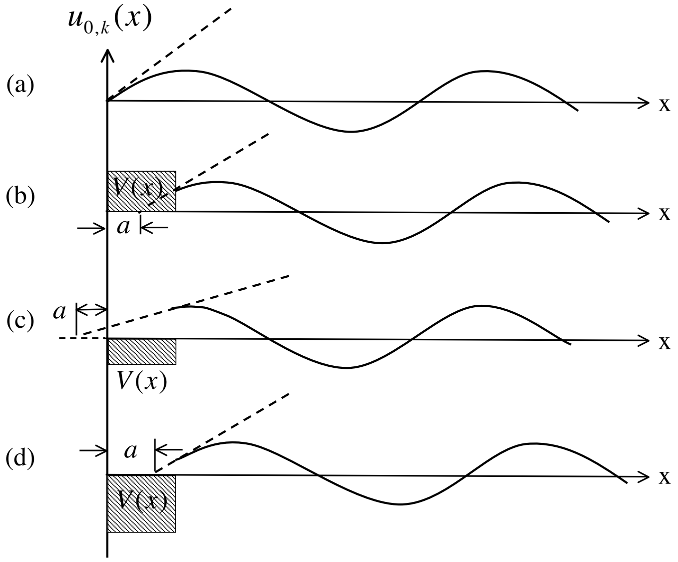

Figure 2.4: At points outside the influence of the potential, $V(x)$, this schematic depicts the s-wave ($\ell = 0$) radial wave function (solid line) and the corresponding "zero energy" linear asymptote (dashed line) . Part (a) shows the free forms of both. For a repulsive potential, (b) indicates a negative phase shift (compared with (a)), as the wave function is "repelled" by the potential. The point where the zero energy line intersects the radial axis is the scattering length, a, which must be non-negative for repulsion. Note that as the range of $V(x)$ shrinks to zero, so does the scattering length. For an attractive potential, (c) shows that the intercept can land on the other side of the axis, indicating a negative scattering length. As the well depth increases, (d) shows that the wave function can get "pulled in" far enough to give a positive value for a. Thus, for attractive potentials, the scattering length may have either sign.

At this point it is worth remembering that we have calculated all quantities in the center of mass frame, which, by the results of Sec. 2.2.1, is equivalent to particles of reduced mass $m/2$ [Eq. (2.19b)] impinging on a potential fixed at the origin. Consequently, the equations developed thus far have all been on the energy scale of $\hbar^2/m$. However, in the many-body treatment, we will be on the scale of the full particle mass, a discrepancy that translates into an extra factor of 1/2 multiplying the $\mathcal{T}$ matrix in (2.56)[1]. Taking this factor into account we henceforth use the relation

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[1] This extra factor of 1/2 comes from the denominator of the free-particle Green's operator (2.50) where E_k is $2k^2$ in the full mass scaling.

$$f(\theta, \varphi) \equiv -\frac{1}{8\pi} \langle k\hat{\mathbf{x}} | \mathcal{T}(E_k + i\varepsilon) | \mathbf{k} \rangle \,. \tag{2.93}$$

A comparison of (2.91), (2.92) and (2.93) with (2.89) leads to the following expression for the scattering length

$$a = \frac{1}{8\pi} \lim_{\mathbf{k}=\mathbf{k}' \to 0} \langle \mathbf{k} | \mathcal{T} | \mathbf{k}' \rangle \tag{2.94a}$$

$$= -\lim_{\mathbf{k} \to 0} \frac{1}{k} \tan \delta_0(k) \,. \tag{2.94b}$$

Calculated from the center of mass $\mathcal{T}$ matrix, the total s-wave cross section is simply

$$\sigma_0 = 4\pi a^2 \,, \tag{2.95}$$

which is that of a hard sphere of radius a.

2.3.2 Effective Range

Realizing an effective distance or range over which the potential acts requires a comparison between the asymptotic and the full s-wave radial functions. To generate the required expressions, recall the full $\ell = 0$ radial wave equation,

$$-\frac{d^2 u_k}{dx^2} + \left[V(x) - k^2 \right] u_k = 0 \,, \tag{2.96a}$$

where its "zero energy" counterpart is

$$-\frac{d^2 u_0}{dx^2} + V(x) u_0 = 0 \,. \tag{2.96b}$$

Multiplying (2.96a) by u_0 and (2.96b) by u_k, then taking the difference results in

$$\frac{d}{dx} \left(u_k u_0' - u_0 u_k' \right) = k^2 u_k u_0 \,. \tag{2.97}$$

Analogous equations for v_k are obtained by taking $V(x) \equiv 0$ in (2.96a) and (2.96b), resulting in the asymptotic counterpart to Eq. (2.97):

$$\frac{d}{dx} \left(v_k v_0' - v_0 v_k' \right) = k^2 v_k v_0 \,. \tag{2.98}$$

Subtracting (2.98) from (2.97), then integrating over x from 0 to ∞ gives

$$\left(u_k u_0' - u_0 u_k' - v_k v_0' + v_0 v_k' \right) \Big|_0^\infty = k^2 \int_0^\infty \left(u_k u_0 - v_k v_0 \right) dx \,. \tag{2.99}$$

Just as in the free case (2.73), the boundary conditions on u are $u_k(0) = u_k'(0) = 0$, whereas Eqs. (2.89) and (2.91) give $v_0(0) = -a$, $v_0'(0) = 1$, $v_k(0) = (1/k) \tan \delta_0(k)$, and $v_k'(0) = 1$. After inserting these boundary conditions, Eq. (2.99) is multiplied by $(k/a) \cot \delta_0(k)$. A slight rearrangement of terms yields

$$k\cot\delta_0(k) = -a^{-1} + k^2\left[-\frac{k}{a}\cot\delta_0(k)\int\limits_0^\infty \big(v_k v_0 - u_k u_0\big)dx\right]. \tag{2.100}$$

The integral can be viewed as measure of the difference between the linear asymptotes and the radial functions that include the full influence of the potential. As the term in square brackets has dimensions of length, it can therefore be thought of as the distance over which the potential extends its influence. More generally, this argument can simply be seen as an expansion of the quantity $k\cot\delta_0(k)$,

$$k\cot\delta_0(k) = -a^{-1} + \frac{1}{2}r_0k^2 + \dots\,, \tag{2.101}$$

where the coefficient r_0 is identified as the effective range.

2.4 Pseudopotentials

Thus far, we have reviewed the relationships between various quantities used to describe scattering processes. All such quantities are determined by the interparticle potential, which must be specified in order for quantitative statements to be made. Therefore, in this section a couple of model potentials are developed where the goal is to arrive at the simplest possible form without sacrificing any of the underlying physics present in the full expression of $V(x)$. The first model is the commonly used delta-function pseudopotential, whereas the second is the more realistic separable potential.

2.4.1 Delta-Function Model

The zero-range delta function approach derives from considering some fundamental length scales of the problem under consideration. Typical atomic condensates are fairly dilute systems with peak number densities on the order of $\rho \sim 10^{14}$ cm^{-3}, thus corresponding typical interparticle spacings of $\rho^{-1/3} \sim 0.2\mu$m. Because this spacing is much larger than the van der Waals tail of $\sim$ 1nm, it is physically sensible to consider a zero-range model. Additionally, condensates are formed at temperatures low enough such that only the "zero energy" states are dominant in the scattering.

We already know that in regions away from the influence of the potential the low-energy wave function behaves as $1 - a/x$. If the potential has zero range, then at any infinitesimal distance outside the scattering center the wave function assumes this form. To construct an effective potential, this boundary condition is imposed on the wave function, ψ:

$$\psi(x) \xrightarrow[x\to 0]{} 1 - \frac{a}{x}\,. \tag{2.102}$$

At very small separations, x, this boundary condition implies

$$x^2\,\frac{\partial\psi}{\partial x} \to a\frac{\partial(x\psi)}{\partial x}\,. \tag{2.103}$$

Integrating both sides over the solid angle gives

$$\int x^2\,\frac{\partial\psi}{\partial x}d\Omega = \int \nabla^2_{\mathbf{x}}\,\psi\,d\mathcal{V}\,, \tag{2.104a}$$

for the left side, and

$$\int a\,\frac{\partial(x\psi)}{\partial x}d\Omega = 4\pi a\int \delta(\mathbf{x})\,d\mathcal{V}\,, \tag{2.104b}$$

for the right side. Arriving at (2.104b) requires the use of the boundary condition (2.102). Equating (2.104a) with (2.104b) gives an effective zero-range Schrödinger equation,

$$\nabla^2_{\mathbf{x}}\psi - 4\pi a\,\delta(\mathbf{x})\psi = 0\,, \tag{2.105}$$

from which the delta function pseudopotential is identified as

$$V(\mathbf{x}) = 4\pi a\,\delta(\mathbf{x})\,. \tag{2.106}$$

Initially used in neutron-proton scattering[1], this pseudopotential has found wide application in the description of atomic condensation. Indeed it has been described as "the single most important result in the whole of the physics of the dilute ultracold alkali gases[2]." In spite of its proposed successes, this form does have significant drawbacks. First, zero range is implicit in its definition, precluding a limit from being taken. From a mathematical point of view, it is preferable to have a range parameter that can be explicitly taken to zero, thus allowing a study of analytic properties when such a limit is performed. More importantly, the delta function model does not capture the low-energy scattering physics as outlined by Fig. (2.4). First, a zero-range repulsive potential corresponds to zero scattering length, a condition obviously violated by (2.106). Additionally, according to the delta function model only the sign of the scattering length determines whether an interaction is attractive or repulsive. However, attractive interactions can admit a scattering length of either sign. A more realistic model can be obtained by using a separable form.

2.4.2 Separable Potential

As its name suggests, the separable potential has a matrix element given by

$$\langle\mathbf{k}|V|\mathbf{k}'\rangle = \lambda v(\mathbf{k})v(\mathbf{k}')\,, \tag{2.107}$$

where $v(\mathbf{k})$ is called the form factor[3]. Both the range of the potential, b, and its strength, λ, are related to the s-wave scattering length, a_{bg},[4] by way of the $\mathcal{T}$ matrix (2.94a),

$$8\pi a_{bg} = \langle\mathbf{k}|\mathcal{T}(E+i\varepsilon)|\mathbf{k}'\rangle|_{\mathbf{k}=\mathbf{k}'=0}\,. \tag{2.108}$$

In turn, the $\mathcal{T}$ matrix is obtained in solving the Lippmann-Schwinger equation, $\mathcal{T} = V + VG_0\mathcal{T}$, where the momentum space free particle Green's function is given by $\delta(\mathbf{k}'' - \mathbf{k}''')/(E_k + i\varepsilon - 2\,k''^2)$. Using a separable form for $\mathcal{T}$ results in

---

[1] Blatt and Weisskopf (1952), p. 75.

[2] Leggett (2000), p. 319.

[3] The normalization of $v(\mathbf{k})$ is $v(0) = 1$, but any nonzero value can be taken without changing any of the results.

[4] We use a_{bg} instead of a in order to distinguish the background scattering length from the full scattering length obtained when molecular coupling is introduced.

$$\mathcal{T}(\mathbf{k},\mathbf{k}') = \frac{v(\mathbf{k})\,\lambda\,v(\mathbf{k}')}{1+\lambda \displaystyle\int_{\mathbf{k}''}' \frac{v(\mathbf{k}'')^2}{2k''^2 - E_k - i\varepsilon}}\,. \tag{2.109}$$

Substitution of (2.109) into (2.108) gives the relationship between the background parameters:

$$\frac{1}{8\pi a_{bg}} = \frac{1}{\lambda} + \frac{1}{b}\,, \tag{2.110}$$

where the range, b, is defined by $1/b \equiv \int v(\mathbf{k})^2/(2k^2)$[1]. From Eq. (2.110) it is evident that the separable potential is consistent with the low-energy scattering conditions illustrated in Fig. (2.4). In the zero range limit, we must have $a_{bg} \to 0$ for repulsive ($\lambda > 0$) interactions. Also, since b is always positive, it follows that attractive interactions ($\lambda < 0$) can admit scattering lengths of either sign. In the limit $b \to 0$, the strength must be allowed to approach zero from the negative side, $\lambda \to 0^-$, resulting in either a positive or a negative scattering length.

By examining the effective range expansion, we can justify the association of the parameter b with a range. To simplify the calculations, a spherical step function is chosen for the form factor, having a momentum cutoff K:

$$v(\mathbf{k}) = \begin{cases} 1 & k \le K \\ 0 & k > K\,. \end{cases} \tag{2.111}$$

With this form of v, the range is inversely related to the momentum cutoff as

$$\frac{1}{b} = \int_{\mathbf{k}}' \frac{1}{2k^2} = \frac{K}{4\pi^2}\,. \tag{2.112}$$

Recall that the scattering amplitude is given by a sum over all partial waves, $f(\theta,\varphi) = k^{-1}\sum_\ell (2\ell+1)e^{i\delta_\ell(k)}\sin\delta_\ell(k)P_\ell(\cos\theta)$. If only the s-waves contribute, this reduces to $f = -(8\pi)^{-1}\mathcal{T}(k,k) = k^{-1}e^{i\delta_0(k)}\sin\delta_0(k)$, thus suggesting [see (2.100)] that the effective range can be found by an expansion of the ratio of real to imaginary parts of $\mathcal{T}$:

$$\cot\delta_0(k) = \frac{\mathrm{Re}\{\mathcal{T}(k,k)\}}{\mathrm{Im}\{\mathcal{T}(k,k)\}} \tag{2.113}$$

Taking the step function form factor of (2.111) and identifying $E = 2k^2$, the diagonal $\mathcal{T}$ matrix is found to be[2]

$$\mathcal{T}(k,k) = \left[\frac{1}{8\pi a_{bg}} + \frac{k^2}{4\pi^2}\int_0^K \frac{dk'}{k'^2 - k^2}\right]^{-1}\,. \tag{2.114}$$

---

[1] For an equivalent relationship between the scattering length, the strength and the range, see Kokkelmans, Milstein, *et al.* (2002).

[2] The limit $\varepsilon \downarrow 0$ has already been taken.

Using a partial fraction decomposition, the integral is $\int dk'/(k'^{\,2} - k^2) = (2\,k)^{-1}(\ln|k - K| - \ln|k + K| + i\pi)$. Expanding the logarithms for small k, then taking the ratio of real to imaginary $\mathcal{T}$ obtains

$$k \cot \delta_0(k) = -\frac{1}{a_{bg}} + \frac{2}{\pi}\frac{1}{K}k^2 + \dots\,, \tag{2.115}$$

giving the effective range

$$r_0 = \frac{4}{\pi K} = \pi^{-3} b\,, \tag{2.116}$$

which justifies its association with b.

2.5 Bound States and Resonances

By rewriting the radial wave function as an incoming plus outgoing wave, much headway is gained in the identification and analysis of bound states and resonances. Such a viewpoint is facilitated by the introduction of the Jost function.

2.5.1 Jost Function

From the decomposition $\hat{\jmath}_\ell = (1/2i)(\hat{h}^+ - \hat{h}^-)$, the radial wave function of (2.84) can be written in the illuminating form[1]

$$u_{\ell,k}(kx) \xrightarrow[x\to\infty]{} \frac{i}{2}\left[\hat{h}_\ell^-(kx) - s_\ell(k)\hat{h}_\ell^+(kx)\right]. \tag{2.117}$$

Asymptotically, the Riccati-Hankel functions behave as

$$\hat{h}_\ell^\pm \xrightarrow[x\to\infty]{} e^{\pm i(kx - \ell\pi/2)}\,, \tag{2.118}$$

which suggest that $\hat{h}_\ell^\pm$ are just generalizations of the exponentials. In analogy with the decomposition $\sin x = (i/2)(e^{-ikx} - e^{ikx})$, the regular wave function is constructed as

$$\varphi_{\ell,k}(kx) \xrightarrow[x\to\infty]{} \frac{i}{2}\left[\mathscr{F}_\ell(k)\,\hat{h}_\ell^-(kx) - \mathscr{F}_\ell(k)^*\hat{h}_\ell^+(kx)\right], \tag{2.119}$$

where the coefficients, $\mathscr{F}_\ell(k)$, called Jost functions, have been introduced to keep $\varphi_{\ell,k}$ real. In addition, the Jost function is simply the proportionality, $\varphi_{\ell,k}(kx) = \mathscr{F}_\ell(k)u_{\ell,k}(kx)$, from which the $\mathcal{S}$ matrix can be written as the ratio

$$s_\ell(k) = \frac{\mathscr{F}_\ell(k)^*}{\mathscr{F}_\ell(k)}\,. \tag{2.120}$$

Using $s_\ell(k) = e^{2i\delta_\ell(k)}$, the phase of $\mathscr{F}_\ell(k)$ is seen to be equal to the negative phase shift since

$$\mathscr{F}_\ell(k) = |\mathscr{F}_\ell(k)|e^{-i\delta_\ell(k)}\,. \tag{2.121}$$

---

[1] Compare with (2.85). Both forms are equivalent in the limit $x \to \infty$.

When no scattering state solution exists, the $\mathcal{S}$ matrix is undefined, possibly indicating the presence of a bound state. Identifying the $\mathcal{S}$ matrix as the ratio in (2.120) provides a convenient way to study the singular points through the zeros of the Jost function. Even though the momentum, k, is regarded as a real quantity, it is nonetheless useful to consider the analytic continuation of $\mathscr{F}$ into the complex k plane since zeros occurring for $\mathrm{Im}\{k\} < 0$ sometimes have physical interpretations as well. Similar issues arise in the many-body problem, as it will be seen that certain solutions do admit a complex valued chemical potential, the counterpart of complex k^2. It is therefore hoped that insight gained from the analogous two-body case will help clarify some of these many-body results. For this reason, time is spent describing the zeros of $\mathscr{F}_\ell(k)$ for complex k.

2.5.2 Bound States

By the structure of the Green's operator, it has already been indicated that poles in the $\mathcal{S}$ matrix correspond to bound states (Fig. 2.2). This relationship also emerges from the regular form of the radial wave function, $\varphi_{\ell,k}(kx)$, which reduces to an outward traveling spherical wave at points where $\mathscr{F}_\ell(k) = 0$[1]. By the asymptotic form of the Riccati-Hankel function, the regular wave function becomes $\varphi_{\ell,k}(kx) \to -(i/2)\mathscr{F}_\ell(k)^* e^{i(kx-\ell\pi/2)}$. To avoid divergence, it must be the case that $\mathrm{Im}\{k\} > 0$, as this corresponds to an exponentially decaying solution that is normalizable. As a solution to the Schrödinger equation, this implies that the Hamiltonian has an eigenstate of energy k^2. Because this eigenvalue must be real, it follows that k is purely imaginary, $k = i\sqrt{E}$, and the energy of the bound state is $-E$.

2.5.3 Resonances

In contrast to a bound state, a resonance is associated with a state where the energy of the projectile is larger than the depth of the potential well. At an appropriate energy, the particle may be trapped for a time in the vicinity of the potential before it escapes. The formation of this metastable state causes a large variation in the cross section, which can be mathematically understood as arising from a complex-valued zero of the Jost function for $\mathrm{Im}\{k\} < 0$. To understand the correspondence between the abrupt peak and the complex pole, recall the definition of the partial wave cross section

$$\sigma_\ell(k) = 4\pi(2\ell+1)\frac{1}{k^2}\sin^2\delta_\ell(k)\,, \tag{2.122}$$

which becomes peaked when $\delta_\ell(k) = \pi/2$. Suppose that the Jost function has a pole at some point $k_0 = k_r - ik_i$, in the lower half plane, close to the real axis. Expanding around this point gives

$$\mathscr{F}_\ell(k) \approx \left(\frac{d\mathscr{F}_\ell}{dk}\right)_{k_0}(k-k_0) \tag{2.123}$$

By (2.121), the phase shift is

---

[1] It can be shown that this zero is always simple for a bound state, see Newton (2002), p. 346.

$$\begin{aligned}\delta_\ell(k) &= -\arg[\mathscr{F}_\ell(k)] \\ &= -\arg\left[\frac{d\mathscr{F}_\ell(k)}{dk}\right]_{k_0} - \arg(k-k_0) \\ &= \delta_{bg} + \delta_{res}(k)\,, \end{aligned} \tag{2.124}$$

where the phase shift decomposes into a background part $\delta_{bg} = -\arg(d\mathscr{F}_\ell/dk)|_{k_0}$ and a resonant part, $\delta_{res}(k) = -\arg(k-k_0)$. For simplicity, the Breit-Wigner form will be assumed where $\delta_{bg} = 0$, thus making $\delta_\ell(k) = \delta_{res}(k)$. When the projectile momentum, k, is equal to k_r, the cross section achieves its maximum. How abruptly this happens depends on the width of the resonance as determined by the magnitude of k_i, the imaginary part of k_0. As implied by Fig. (2.5), the resonance width will grow or increase in proportion to k_i.

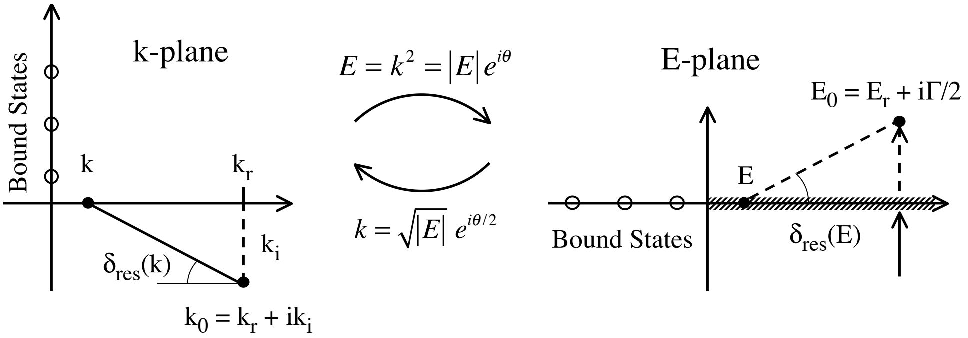

Figure 2.5: Bound states and resonances in the complex planes of momentum, k, and energy, E. In the k plane, bound states are poles on the imaginary axis, whereas resonances occur for $\mathrm{Re}\{k\} > 0$ and $\mathrm{Im}\{k\} < 0$. Due to the two-to-one mapping, the corresponding E plane comprises two sheets with a boundary given by a branch cut from 0 to ∞. The bound states lie on the first for $\mathrm{Re}\{E\} < 0$, while resonances correspond to poles immediately across the cut. As the incoming momentum, k, or energy, E, moves across the real axis, the phase shift becomes $\pi/2$ at the point where $k = k_r$. How abruptly this happens depends upon how close k_i (Γ) is to the axis. Thus, the resonance width is given by the imaginary part of k_0 or E_0.

Alternatively, these arguments can be recast in terms of the energy, E. Since the mapping from k to E is two-to-one, any function of k maps into a function of E on a two-sided Riemann sheet [see Fig. (2.5)]. With θ as the phase of E, there exists the relationship

$$E = |E|e^{i\theta} = k^2 \Rightarrow k = \sqrt{|E|}e^{i\theta/2}\,, \tag{2.125}$$

whence it follows that $\mathrm{Im}\{k\} > 0$ maps onto the first Riemann sheet, $0 < \theta < 2\pi$. Likewise, $\mathrm{Im}\{k\} < 0$ corresponds to the second sheet, $2\pi < \theta < 4\pi$, where the branch cut from 0 to ∞ marks the boundary between the two sheets. In this language, bound states occur on the negative real axis ($\theta = \pi$) of the first sheet, whereas a resonance is associated with a point on the second sheet, just across the cut. At a resonance, the off-shell energy is given as

$$E_0 \equiv -\gamma_0^2 = E_r + i\frac{\Gamma}{2}\,, \tag{2.126}$$

where Γ is the imaginary part that quantifies the resonance width as well as the lifetime of the resonant state.

2.5.4 Decay of the Resonant State

The expansion of the Jost function (2.123) could have just as well been done in terms of the energy

$$\delta_{res}(E) = -\arg(E - E_0)\,, \tag{2.127}$$

for $\delta_{bg} = 0$. Recalling that the $\mathcal{S}$ matrix eigenvalue is $e^{2i\delta_{res}}$, we have $\sqrt{s_\ell(E)} = \cos\delta_{res} + i\sin\delta_{res}$. Reading off the sine and cosine from Fig. (2.5), $s_\ell(E)$ is found to be

$$s_\ell(E) = \frac{E - E_r - i\Gamma/2}{E - E_r + i\Gamma/2}\,, \tag{2.128}$$

where the corresponding partial wave amplitude is

$$\begin{aligned} f_\ell(E) &= \frac{s_\ell - 1}{2ik} \\ &= -\frac{1}{2k}\frac{\Gamma}{E - E_r + i\Gamma/2}\,. \end{aligned} \tag{2.129}$$

The decay of the resonant state is illustrated by considering the time dependent asymptotic form of the wave function

$$\begin{aligned} \psi(\mathbf{x}, t) &= \langle \mathbf{x}|U(t)|\psi\rangle \\ &= \int_{\mathbf{k}}' \phi(\mathbf{k}) e^{-iE_k t/\hbar}\langle \mathbf{x}|\mathbf{k}+\rangle \\ &\xrightarrow[x\to\infty]{} \int_{\mathbf{k}}' \phi(\mathbf{k}) e^{-iE_k t/\hbar}\Big[e^{i\mathbf{k}\cdot\mathbf{x}} + f(E,\theta)\,\frac{e^{ikx}}{x}\Big] \\ &= \psi_{in}(\mathbf{x}, t) + \psi_{sc}(\mathbf{x}, t) \end{aligned} \tag{2.130}$$

Assuming that all other phase shifts are negligible, the total amplitude can be approximated by just one partial wave

$$f(E, \theta) \approx (2\ell + 1) f_\ell(E) P_\ell(\cos\theta)\,. \tag{2.131}$$

The scattered wave function in (2.130) is given by

$$\psi_{sc}(\mathbf{x},t) = \text{const.}\frac{\Gamma}{x}\int_{\mathbf{k}}' \phi(\mathbf{k})\frac{P_\ell(\hat{\mathbf{x}}\cdot\hat{\mathbf{k}})}{k(E-E_r+i\Gamma/2)}\, e^{i(kx-Et)}\,. \tag{2.132}$$

Since $\phi(\mathbf{k}) = \langle \mathbf{k}+|\psi\rangle$ can be expanded in terms of spherical harmonics, the angular integrals separate out and we are left with an integral over E involving a pole at $E_r - i\Gamma/2$. Performing contour integration, it can be seen that the pole leads to a scattered wave probability $|\psi_{sc}(\mathbf{x},t)|^2$ that has a decay constant of Γ. Thus, we see that the imaginary part of the energy quantifies the decay rate of the resonance. When describing the problem of interacting bosons, it will be seen that the many-body analog of this state corresponds to a system with a complex valued chemical potential.

2.6 Coupled-Channels Analysis

2.6.1 General Description

In this section, we consider a two-channel reaction in which the bound state and the scattering state Hilbert spaces are coupled. The situation can be depicted schematically as in Fig. (2.6).

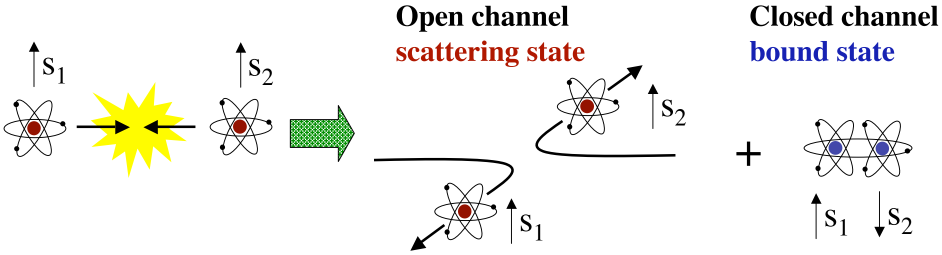

Figure 2.6: A schematic showing the possible outcomes or channels of a two-body collision. In the open channel, two particles go in and two emerge. There is, however, the possibility that a bound state may be formed, with a different electronic spin configuration than the incoming atoms. When the Zeeman energy of the bound state is tuned close to that of the incoming state, the presence of the former becomes appreciable. In general, what we call "the bound state" may be either a molecule or a resonance. Note that angular momentum is conserved by considering the rotational degree of freedom of the molecular state.

Due to the difference in spin configurations, a unique potential exists both for the scattered atoms and the molecular state [see Fig. (2.7)]. A complete elaboration of this scenario requires the description of a couple of new parameters. In particular, the molecular binding energy, E, is the energy difference between the bound state and two free atoms relative to the molecular potential whereas the detuning, ϵ, is defined as the same, but relative to the scattering potential. In systems with a magnetic Feshbach resonance, the detuning, and hence the binding energy, can be adjusted using the Zeeman interaction in the presence of an externally applied magnetic field. Consequently, the detuning varies linearly with the field through the species dependent proportionality, η/a_{bg}^2

$$\epsilon = \frac{\eta}{{a_{bg}}^2}(B - B1), \tag{2.133}$$

where $B1$ is some offset field denoting the zero in the energy difference.

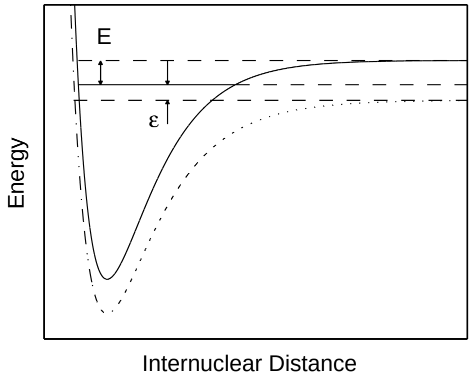

Figure 2.7: Schematic showing the potential of the closed channel (solid curve) with that of the open channel (dash-dot curve). The binding energy E and the detuning ϵ are shown relative to the free level of each case.

Due to the coupling, the complete two-body wave function is represented by the sum of functions from each space,

$$|\psi\rangle = \left|\psi^P\right\rangle + \left|\psi^Q\right\rangle, \tag{2.134}$$

where $\left|\psi^P\right\rangle$ is the scattering space projection while $\left|\psi^Q\right\rangle$ is the that of the bound space. Accordingly, it is most convenient to introduce projection operators P and Q onto the respective Hilbert spaces, such that $\left|\psi^P\right\rangle \equiv P\,|\psi\rangle$ and $\left|\psi^Q\right\rangle \equiv Q\,|\psi\rangle$. Using the standard relationships, $P = P^\dagger$, $Q = Q^\dagger$ and $Q^\dagger Q + P^\dagger P = 1$, the projection of the Schrödinger equation, $H\,|\psi\rangle = E\,|\psi\rangle$ onto the scattering space gives

$$H_{PP}\left|\psi^P\right\rangle + H_{PQ}\left|\psi^Q\right\rangle = E\left|\psi^P\right\rangle, \tag{2.135}$$

where we have defined $H_{PP} \equiv PHP$ and $H_{PQ} \equiv PHQ$. Similarly, the bound space counterpart is

$$H_{QQ}\left|\psi^Q\right\rangle + H_{QP}\left|\psi^P\right\rangle = E\left|\psi^Q\right\rangle. \tag{2.136}$$

The scattering space projection of the Hamiltonian contains both kinetic, T and potential V pieces, which in momentum space become

$$\begin{aligned}\left\langle \mathbf{k}\left|H_{PP}\right|\psi^{P}\right\rangle &= \int_{\mathbf{k}'}' \left\langle \mathbf{k}\left|T+V\right|\mathbf{k}'\right\rangle \left\langle \mathbf{k}'\,\middle|\,\psi^{P}\right\rangle \\ &= 2\,k^{2}\psi(\mathbf{k}) + \int_{\mathbf{k}'}' \left\langle \mathbf{k}\left|V\right|\mathbf{k}'\right\rangle \psi(\mathbf{k}')\,. \end{aligned} \tag{2.137}$$

Assuming the total bound state projection to be a linear combination of the basis functions, $\{|\phi_n\rangle\}$, we have

$$\left|\psi^{Q}\right\rangle = \sum_{n} c_n \left|\phi_n\right\rangle . \tag{2.138}$$

With the separable potential of Eq. (2.107), the momentum space representation of Eq. (2.135) is

$$\left(2\mathbf{k}^{2}-E\right)\psi(\mathbf{k}) + \lambda v(\mathbf{k}) \int_{\mathbf{k}'}' v(\mathbf{k}')\psi(\mathbf{k}') + \sum_{n} c_n \left\langle \mathbf{k}\left|H_{PQ}\right|\phi_n\right\rangle . \tag{2.139}$$

Elimination of the coupling term requires an examination of the bound state projection of the Schrödinger equation given by Eq. (2.136). Since the $\{|\phi_n\rangle\}$ are eigenstates of H_{QQ}, their eigenvalues quantify the energy difference between their binding energy and the lowest-lying scattering state. Recognizing these quantities as detunings, given in Eq. (2.133), we project the molecular equation (2.136) onto one of the basis states, $|\phi_n\rangle$, thus solving for the coefficients, c_n,

$$c_n = -\frac{\lambda\alpha_n}{\epsilon_n - E} \int_{\mathbf{k}'}' v(\mathbf{k}')\psi(\mathbf{k}'), \tag{2.140}$$

which implicitly defines the coupling constants through

$$H_{QP}\left|\mathbf{k}'\right\rangle = \sum_{j} \lambda\alpha_j v(\mathbf{k}')\left|\phi_j\right\rangle . \tag{2.141}$$

In elucidating the vanishing of the coupling with the interparticle interactions, the coupling strength is chosen as a product between the parameter α and the atom-atom interaction strength, λ. Substitution of the coefficients into Eq. (2.139) gives

$$\left(2\mathbf{k}^{2}-E\right)\psi(\mathbf{k}) + \left(\lambda - \lambda^{2}\sum_{n}\frac{\alpha_n^{2}}{\epsilon_n - E}\right) v(\mathbf{k}) \int_{\mathbf{k}'}' v(\mathbf{k}')\psi(\mathbf{k}') = 0, \tag{2.142}$$

thus illustrating the effect of coupling to many-body bound states. In subsequent analyses, it will be assumed that the effect of the highest lying molecular state is dominant over the ones below. Alternatively, taking a single resonance may be thought of as the net effect on the system of all real bound states. In either case, a coupled two-channel analysis suffices. Comparing Eq. (2.142) with the usual single channel result ($\alpha = 0$), it can be seen that the binding to molecules is included in the analysis by the replacement,

$$\lambda \to \lambda - \frac{\lambda^2\alpha^2}{\epsilon - E}. \tag{2.143}$$

Hence, this prescription is used to include the possibility of binding to a molecular state.

2.6.2 Molecular Binding Energy

The full T-matrix is found by the substitution of (2.143) into Eq. (2.109), thus giving

$$\langle 0\,|\mathcal{T}|\,0\rangle = \frac{v(0)\left(\lambda - \dfrac{\lambda^2\alpha^2}{\epsilon - E}\right)v(0)}{1 + \left(\lambda - \dfrac{\lambda^2\alpha^2}{\epsilon - E}\right)\displaystyle\int_{\mathbf{k}}' \frac{v(\mathbf{k})^2}{2\mathbf{k}^2 - E - i\varepsilon}}. \tag{2.144}$$

Since the poles of the T-matrix locate the bound states, the binding energies are given by the values of E where the denominator vanishes. Repeated application of Eq. (2.110) in conjunction with some algebraic manipulations unveils the following equation for the zeros,

$$\frac{1}{8\pi a_{bg}} - \frac{\gamma_0^2}{2}\int_{\mathbf{k}}' \frac{1}{k^2}\frac{v(\mathbf{k})^2}{k^2 + \gamma_0^2} + \frac{\alpha^2}{\epsilon + 2\gamma_0^2 - \lambda\alpha^2} = 0, \tag{2.145}$$

where the binding energy has been defined as $-E = 2\gamma_0^2$. For negative background scattering lengths, the limit of zero range, $b \to 0$, may be taken where, according to (2.110) and (2.111), $\lambda \to 0^-$ and $v(\mathbf{k}) \to 1$. In this limit, Eq. (2.145) reduces to a cubic equation in the square root of the binding energy[1],

$$\left(\epsilon + 2\gamma_0^2\right)\left(\frac{1}{a_{bg}} - \gamma_0\right) = 8\pi\alpha^2. \tag{2.146}$$

2.6.3 Full Scattering Length

Using the $E = 0$ form of Eq. (2.143) in Eq. (2.110) results in an expression for the effective scattering length due to the presence of the molecular state,

$$\frac{1}{a(\epsilon)} = \frac{1}{a_{bg}} + \frac{8\pi\alpha^2}{\epsilon - \lambda\alpha^2}. \tag{2.147}$$

Defining the resonance width, ΔB, and the resonant field, B_0, in terms of the detuning proportionality, η, offset field, $B1$, and the coupling parameter, α, such that

$$\begin{aligned} \Delta B &= 8\pi a_{bg}^3\alpha^2/\eta \\ B_0 &= B1 - \Delta B + \frac{\lambda\alpha^2 a_{bg}^2}{\eta}, \end{aligned} \tag{2.148}$$

allows the scattering length to be put into the standard form, explicitly dependent on the magnetic field,

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[1] In evaluating this integral, we have taken $k = \gamma_0 \tan u$, so that only roots with $\gamma_0 > 0$ are permissible.

$$a(B) = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right). \tag{2.149}$$

2.6.4 Two-Body Interactions Modeled by a Resonance

Upon closer inspection, Eq. (2.142) indicates a way of modeling the background interactions directly from a single resonance. If there were no potential present, but only a resonance with coupling parameter g and detuning ε, Eq. (2.142) would become

$$\left(2\mathbf{k}^2 - E\right)\psi(\mathbf{k}) + \frac{g^2}{\epsilon_n - E} v(\mathbf{k}) \int_{\mathbf{k}'}' v(\mathbf{k}')\psi(\mathbf{k}') = 0. \tag{2.150}$$

Choosing a detuning far enough away from the binding energy, $|\varepsilon| \gg |E|$, the effective interaction strength is $\approx -g^2/\varepsilon$ which can be chosen equal to the original separable potential strength, λ.

Although it may appear that the two-body interactions can be replaced with a single resonance, it must be pointed out that this is an alternative way of modeling the physics that gives rise to the background scattering length, not a substitute for a potential. In reality, both potential and resonances would be responsible for the background value. However, in the zero-range limit, it will be seen that this substitution is identical to having a potential. As a consequence, a substantial simplification of the many-body Hamiltonian results.

2.7 Numerical Examples

Due to the fact that the interaction range is a free parameter in the preceding analysis, our initial attention will be confined to species with negative background scattering lengths, where the limit of zero-range can be taken. Therefore, both binding energy and scattering length plots will be given for the bosonic species of ^{85}Rb and the fermionic species ^{6}Li.

Table 2.1 gives the parameter values of some common BEC isotopes[1]. Note that, unlike the case of ^{85}Rb, ^{6}Li has a sign discrepancy in the full scattering length as it is described by the form $a(B) = a_{bg}[1 + |\Delta B|/(B - B_0)]$. In order to accommodate both cases in Eq. (2.147), it is necessary to denote the resonance width as a negative quantity in the ^{6}Li case.

Isotope	a_{bg} (a_0)	η (G^{-1})	B_0 (G)	ΔB (G)
^{85}Rb	-450	-30	154.6	11
^{87}Rb	109.6	2.3	1007.34	0.17
^{23}Na	64.3	0.245	907	1
^{6}Li	-1405	18.2	834	-300

Table 2.1: Table showing numerical parameter values for some common isotopes used in atomic BEC, where a_0 is defined as the Bohr radius.

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[1] The parameter values of ^{85}Rb were obtained from S. J. J. M. F. Kokkelmans (2002) and E. A. Donley (2002), whereas those of ^{87}Rb and ^{23}Na were found in V. A. Yurovsky (2003) and V. A. Yurovsky (1997), respectively. Finally, the ^{6}Li parameters came from M. Bartenstein (2004) and from Fig. 2.8.

The origin of the scattering length expressions' sign difference arises from the Zeeman proportionality, η. As shown in Fig. (2.8), the nearly zero molecular state energy crosses the Zeeman energy of two free atoms from below threshold. As such, the energy difference between the "bare" molecules and the free atoms is negative below threshold ($B < B1$), hence, by Eq. (2.133), there must be positive value of η determined from the magnitude of the slope of the free atom Zeeman energy. On the other hand, the molecular ^{85}Rb state crosses its continuum state from above threshold, thereby giving a negative η.

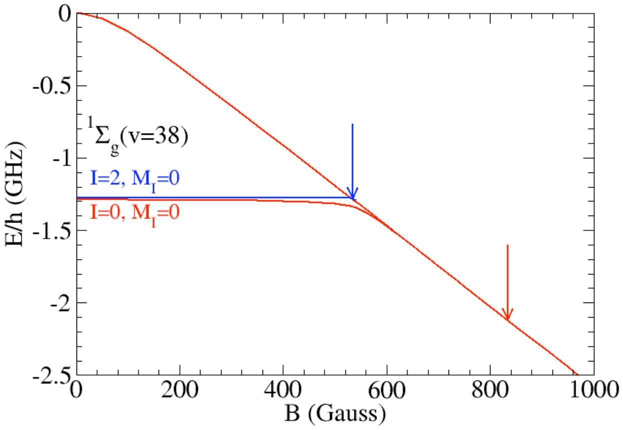
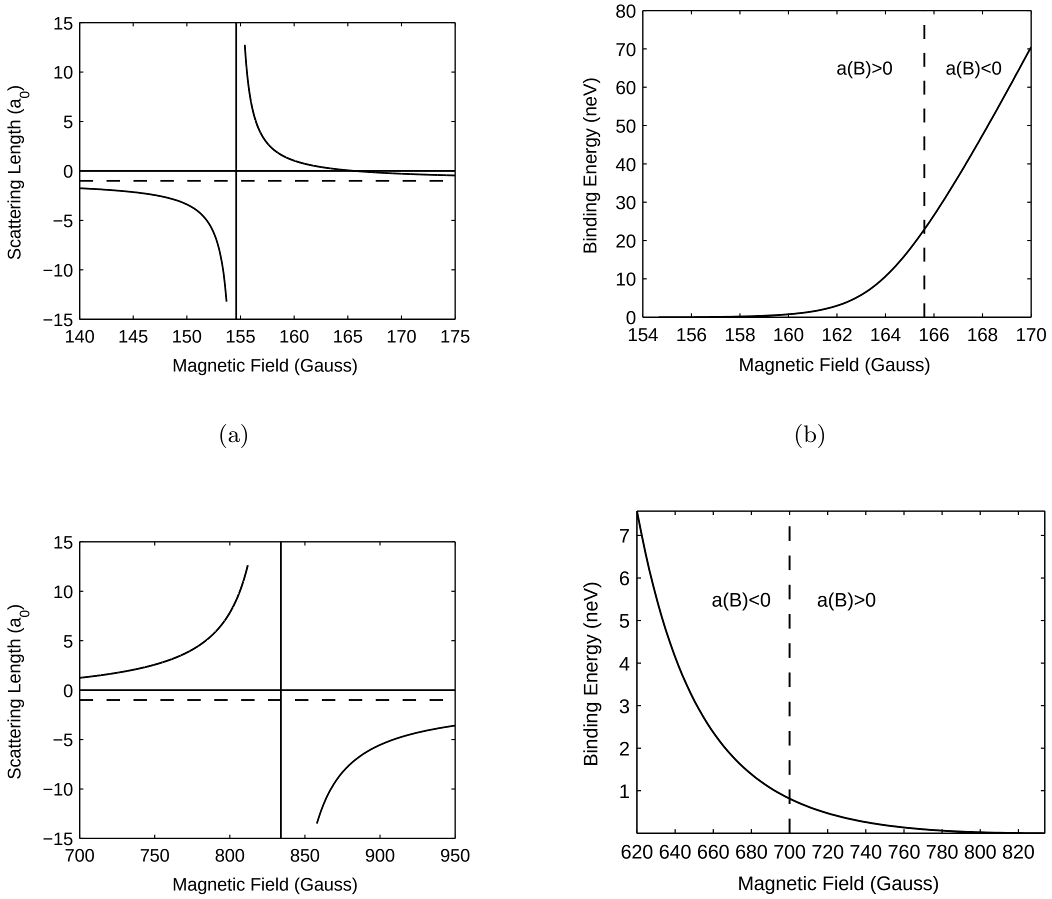


Figure 2.8: Figure showing ^{6}Li$_2$ molecular levels near threshold. The line starting at $E = B = 0$ shows the Zeeman energy of two separated atoms, while the narrow resonance at 534 G and the broad resonance at 834 G start as two different, but nearly degenerate spin components of the $\nu = 38$ vibrational level of the singlet Σ_g molecular state. The magnetic moment of the "bare" molecular state, that is the state without interactions with the continuum, is zero. Thus the detuning or energy difference between the bound and free states is due primarily to the Zeeman interaction of the two free atoms. The $I = 2$ spin component interacts very weakly with the continuum, becoming the narrow resonance $\Delta B \approx .01$ G as threshold is crossed near $534G$, shown by the upper arrow. In contrast, the $I = 0$ spin component interacts more strongly with the continnuum, yielding the broad 300 G resonance given in Table 2.1. In the latter case, the threshold crossing is depicted by the lower arrow at 834 G. Note that in the above figure, threshold occurs at $B = B_0$ whereas, we have a shifted value ($B = B1$), given by the detuning definition of Eq. (2.133). This figure was provided through private correspondence with P.S. Julienne.

Using the numerical values from Table 2.1, Eqs. (2.146) and (2.147) are employed in generating plots for the binding energies and full scattering lengths, respectively.



(a) (b)

(c) (d)

Figure 2.9: For the case of ^{85}Rb, (a) shows the full scattering length of Eq. (2.147), with the horizontal dashed line as the normalized asymptotic background value and the solid vertical indicating the location of the resonance at 154.6 G. (b) With a vertical, dashed boundary line separating the region of positive from that of negative scattering length, a plot is shown of the ^{85}Rb binding energy for the zero-range case of Eq. (2.146). Approaching the resonance, both the scattering length and molecular size become unbounded, indicating an increasingly weakly bound molecular state. Confirming this intuition, the binding energy is seen to increase from zero on resonance. For the case of ^{6}Li, parts (c) and (d) show the respective analogs of (a) and (b).

Chapter 3

Many-Body Formalisms

The purpose of this chapter is to provide a context for the many-body variational formalism used in the analysis of atomic systems at zero temperature. In Sec. 3.1, the many-body state vectors are constructed as direct products of the single particle states. Section 3.2 then discusses the second quantized form of the operators that act on these states. Since the ladder operators create and destroy particles, the entire Hilbert space can be generated by their action on the vacuum state. Hence, it is most convenient to work in the Fock space, which has an indefinite particle number. By counting particles in the appropriate way, the creation and annihilation operators can be used as a basis for the many-body operators. Finally, Section 3.4 describes coherent states for both the bosonic and fermionic cases, where the former will be used in constructing a variational Gaussian ansatz in the analysis of model Hamiltonians.

3.1 State Vectors

Having reviewed the essential features of one-body quantum mechanics, the extension to many particles becomes a straightforward generalization[1]. To construct a basis for the many-body state, we define the N particle Hilbert space as a tensor product on the N single particle spaces

$$\mathscr{H}_N = \underbrace{\mathscr{H} \otimes \mathscr{H} \otimes \ldots \otimes \mathscr{H}}_{N} \,. \tag{3.1}$$

Basis vectors constructed in this way are then simply tensor products of the orthonormal bases of each single particle space:

$$|\beta_1 \ldots \beta_N) = |\beta_1\rangle \otimes \ldots \otimes |\beta_N\rangle \,, \tag{3.2}$$

where completeness is inherited from the individual bases,

$$\sum_{\beta_1 \ldots \beta_N} |\beta_1 \ldots \beta_N)(\beta_1 \ldots \beta_N| = \mathbb{1} \,. \tag{3.3}$$

The corresponding wave functions are given by the coordinate space projections in the natural way

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[1] Here we follow the development given in Negele and Orland, Chap 1.

$$\begin{aligned}\psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) &= (\mathbf{x}_1\ldots\mathbf{x}_N|\beta_1\ldots\beta_N) \\ &= \phi_{\beta_1}(\mathbf{x}_1)\ldots\phi_{\beta_N}(\mathbf{x}_N)\,,\end{aligned} \tag{3.4}$$

where $\phi_{\beta_i}(\mathbf{x}_j)$ is the wave function of a particle in state $|\beta_i\rangle$ at location $\mathbf{x}_j$[1].

In nature, it is found that the Hilbert space $\mathscr{H}_N$ is split into two classes: one for all wave functions symmetric under particle exchange and one for functions antisymmetric under particle exchange. Symmetric many-body wave functions correspond to bosons, or particles with integer spin, whereas the antisymmetric case describes fermions which have half integer spin. To accommodate this requirement, it is convenient to define an operator that naturally splits $\mathscr{H}_N$ into bosonic, $\mathcal{B}_N$, and fermionic, $\mathcal{F}_N$, Hilbert spaces. Hence, it is common to introduce symmetrization, $\mathcal{P}_\mathcal{B}$, and antisymmetrization, $\mathcal{P}_\mathcal{F}$, operators whose action on the base kets projects out the symmetric and antisymmetric components

$$\mathcal{P}_{\left\{\substack{\mathcal{B}\\ \mathcal{F}}\right\}}|\beta_1\ldots\beta_N) = \frac{1}{N!}\sum_{\mathcal{P}}\zeta^{\mathcal{P}}|\beta_{\mathcal{P}_1}\ldots\beta_{\mathcal{P}_N})\,. \tag{3.5}$$

For bosons $\zeta = 1$, whereas for fermions $\zeta = -1$. Additionally, the exponent $\mathcal{P}$ denotes the permutation's parity which is defined as the number of transpositions required to obtain the original $|\beta_1\ldots\beta_N)$. Finally, the sum in (3.5) is over all $N!$ such permutations with the notation $\mathcal{P}_1\ldots\mathcal{P}_N$ representing a single permutation in the set. Symbolically, the boson and fermion spaces are given by

$$\begin{aligned}\mathcal{B}_N &= \mathcal{P}_\mathcal{B}\mathscr{H}_N \\ \mathcal{F}_N &= \mathcal{P}_\mathcal{F}\mathscr{H}_N\,.\end{aligned} \tag{3.6}$$

Since the operator $\mathcal{P}$ is a projector, it can be shown that $\mathcal{P}^2 = \mathcal{P}$.

An assembly of bosons or fermions with one particle in state β_1, one in β_2, and so on is reproduced by the state with the proper symmetry

$$|\beta_1\ldots\beta_N\} = \frac{1}{\sqrt{N!}}\sum_{\mathcal{P}}\zeta^{\mathcal{P}}|\beta_{\mathcal{P}_1}\ldots\beta_{\mathcal{P}_N})\,. \tag{3.7}$$

From this construction, it is easily seen that if two fermionic particles occupy the same state ($\beta_1 = \beta_2$), then the entire vector vanishes. The inner product of two such vectors is given by

$$\begin{aligned}\{\beta'_1\ldots\beta'_N|\beta_1\ldots\beta_N\} &= \sum_{\mathcal{P}}\zeta^{\mathcal{P}}\langle\beta'_1|\beta_{\mathcal{P}_1}\rangle\ldots\langle\beta'_N|\beta_{\mathcal{P}_N}\rangle \\ &= \zeta^{\mathcal{P}}\prod_\beta n_\beta!\,,\end{aligned} \tag{3.8}$$

where we have used the fact that $\mathcal{P}^2 = \mathcal{P}$. For fermions, can only be one particle in each state, $|\beta\rangle$, reducing this result to $(-1)^{\mathcal{P}}$. On the other hand, some of the bosonic states

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[1] Note that the ordering in (3.4) is important, since $(\mathbf{x}_1\ldots\mathbf{x}_N|\beta_N\ldots\beta_1) = \phi_{\beta_N}(\mathbf{x}_1)\ldots\phi_{\beta_1}(\mathbf{x}_N)$.

may be degenerate, indicating that there is more than one boson in the state. If there are n_β bosons in each unique single particle state, $|\beta\rangle$, then there are $n_\beta!$ permutations of the particles that do not change the overall many-body state $|\beta_1 \dots \beta_N\}$. The product of each gives the sum over all permutations in (3.8). The fact that there can be many bosons in the same quantum state gives rise to the phenomenon of Bose-Einstein condensation, where a macroscopic number of particles reside in the ground state. Due to this degenerate ground state occupation, it is beneficial to define a mean field or order parameter, ψ, with the absolute square giving the density of condensed bosons.

From (3.7) and (3.8) an orthonormal basis for $\mathcal{B}_N$ or $\mathcal{F}_N$ can be constructed as

$$|\beta_1 \dots \beta_N\rangle = \frac{1}{\sqrt{N! \prod_\beta n_\beta!}} \sum_{\mathcal{P}} \zeta^{\mathcal{P}} |\beta_{\mathcal{P}_1} \dots \beta_{\mathcal{P}_N}) \,. \tag{3.9}$$

Taking two arbitrary sets of single particle states, $\{\alpha\}$ and $\{\beta\}$, it is convenient to define the overlap matrix as all inner products between the two sets:

$$M_{ij} = \langle \alpha_i | \beta_j \rangle \,. \tag{3.10}$$

Using this definition, the wave function corresponding to the state in Eq. (3.9) is given by the product

$$(\mathbf{x}_1 \dots \mathbf{x}_N | \beta_1 \dots \beta_N\rangle = \frac{1}{\sqrt{N! \prod_\beta n_\beta!}} \sum_{\mathcal{P}} \zeta^{\mathcal{P}} \phi_{\beta_{\mathcal{P}_1}}(\mathbf{x}_1) \dots \phi_{\beta_{\mathcal{P}_N}}(\mathbf{x}_N) \,. \tag{3.11}$$

For the bosons, $\zeta = +1$ with the summation being a permanent, or a sum of the products of all possible elements of M, giving the bosonic basis wave functions,

$$\begin{aligned} (\mathbf{x}_1 \dots \mathbf{x}_N | \beta_1 \dots \beta_N\rangle &= \psi_{\beta_1 \dots \beta_N}(\mathbf{x}_1, \dots \mathbf{x}_N) \\ &= \frac{1}{\sqrt{N! \prod_\beta n_\beta!}} Per\left[\phi_{\beta_i}(\mathbf{x}_j)\right] \,. \end{aligned} \tag{3.12}$$

Alternatively, the fermionic basis consists of the familiar Slater determinants,

$$\psi_{\beta_1 \dots \beta_N}(\mathbf{x}_1, \dots \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \det\left[\phi_{\beta_i}(\mathbf{x}_j)\right] \,, \tag{3.13}$$

where $n_\beta = 1$ since there is only one fermion per state.

3.2 Many-Body Operators

Now that the many-particle basis states have been described, it is possible to discuss the action of operators on these states. In most cases of interest, the Hamiltonian of the system will consist of one and two-body operators. By definition, a one-body operator acts on each particle individually, with the net effect represented as a sum over all particles. Similarly, two-body operators act on all distinct particle pairs, with the total effect being a sum on the pairs. Hence, the pseudopotentials discussed in Sec. 2.4 belong to this class of operators, for example. In general, an N-body operator acts on all distinct N-particle groups in the assembly. Although present, N-body forces are usually weak and will therefore be ignored as higher order effects. Mathematically, the typical many-body Hamiltonian has the form

$$\hat{H} = \sum_{i=1}^{N} \hat{T}_i + \sum_{i=1}^{N} \hat{U}_i + \frac{1}{2} \sum_{i \neq j=1}^{N} \hat{V}_{ij} \,. \tag{3.14}$$

As indicated, the kinetic energy, $\hat{T}_i$, and the external potential, $\hat{U}_i$, operate on individual particles, whereas the particle-particle interaction, $\hat{V}_{ij}$, operates on all distinct pairs[1]. For example, the kinetic energy operator in the momentum basis acts as[2]

$$\hat{T}|\mathbf{k}_1 \ldots \mathbf{k}_N) = \sum_{i=1}^{N} \mathbf{k}^2 |\mathbf{k}_1 \ldots \mathbf{k}_N) \,. \tag{3.15}$$

Not surprisingly, the one-body operator matrix elements are completely determined within the single particle Hilbert space,

$$(\alpha_1 \ldots \alpha_N|\hat{U}|\beta_1 \ldots \beta_N) = \sum_{i=1}^{N} \prod_{\ell \neq i} \langle \alpha_\ell|\beta_\ell\rangle \cdot \langle \alpha_i|\hat{U}|\beta_i\rangle \,. \tag{3.16}$$

Similarly, two-body operators act on particle pairs and as such are completely determined by their matrix elements in the Hilbert space of two particles, $\mathscr{H} \otimes \mathscr{H}$:

$$(\alpha_1 \ldots \alpha_N|\hat{V}|\beta_1 \ldots \beta_N) = \frac{1}{2} \sum_{i \neq j} \prod_{\ell \neq i,j} \langle \alpha_\ell|\beta_\ell\rangle \cdot (\alpha_i\, \alpha_j|\hat{V}|\beta_i\, \beta_j) \,. \tag{3.17}$$

Finally, two-body interactions are said to be local when they have the form

$$(\mathbf{x}_1\, \mathbf{x}_2|\hat{V}|\mathbf{x}_3\, \mathbf{x}_4) = \delta(\mathbf{x}_1 - \mathbf{x}_3)\delta(\mathbf{x}_2 - \mathbf{x}_4)\, V(\mathbf{x}_1 - \mathbf{x}_2) \,. \tag{3.18}$$

3.3 Fock Space and Ladder Operators

By repeated action on the vacuum state (defined as the state with no particles) the ladder operators can generate the entire Hilbert space. Additionally, these operators can be paired in ways that provide a basis for the expression of the many-body operators of the previous section. As a starting point, the destruction operator, a_λ, is defined by its action on a properly symmetrized basis state of $\mathcal{B}_N$ or $\mathcal{F}_N$. Since it is required that a_λ decrease the number of particles in state $|\lambda\rangle$ by one, the action on some state $|\beta_1 \ldots \beta_N\rangle$ can be expressed by using (3.2) and (3.7):

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[1] Since we will only be concerned with indistinguishable particles, all operators are invariant under any permutation of the particles.

[2] Recall that energy is on the scale of $\hbar^2/2m$.

$$\begin{aligned}a_\lambda|\beta_1\ldots\beta_N\} &= \frac{1}{\sqrt{N!}}\sum_{\mathcal{P}}\zeta^{\mathcal{P}} a_\lambda|\beta_{\mathcal{P}_1}\rangle\otimes|\beta_{\mathcal{P}_2}\rangle\otimes|\beta_{\mathcal{P}_3}\rangle\otimes\ldots\otimes|\beta_{\mathcal{P}_{N-1}}\rangle\otimes|\beta_{\mathcal{P}_N}\rangle\\ &= \frac{1}{\sqrt{N!}}\Bigg\{\zeta^0\sum_{\mathcal{P}}\delta_{\lambda\,\beta_{\mathcal{P}_1}}|\beta_{\mathcal{P}_2}\rangle\otimes|\beta_{\mathcal{P}_3}\rangle\ldots\otimes|\beta_{\mathcal{P}_{N-1}}\rangle|\beta_{\mathcal{P}_N}\rangle\\ &\qquad+\zeta\sum_{\mathcal{P}}\delta_{\lambda\,\beta_{\mathcal{P}_2}}|\beta_{\mathcal{P}_1}\rangle\otimes|\beta_{\mathcal{P}_3}\rangle\otimes\ldots\otimes|\beta_{\mathcal{P}_{N-1}}\rangle\otimes|\beta_{\mathcal{P}_N}\rangle\\ &\qquad+\ldots+\zeta^{N-1}\sum_{\mathcal{P}}\delta_{\lambda\,\beta_N}|\beta_{\mathcal{P}_1}\rangle\otimes|\beta_{\mathcal{P}_2}\rangle\otimes|\beta_{\mathcal{P}_3}\rangle\otimes\ldots\otimes|\beta_{\mathcal{P}_{N-1}}\rangle\Bigg\}\,.\end{aligned}$$

Using the definition of the basis states in (3.9), the summations on the right-hand side reduce to the following

$$\begin{aligned}a_\lambda|\beta_1\ldots\beta_N\} &= \zeta^0\,\delta_{\lambda\,\beta_1}|\beta_2\,\beta_3\ldots\beta_N\}+\zeta\,\delta_{\lambda\,\beta_2}|\beta_1\,\beta_3\ldots\beta_N\}+\ldots\\ &\qquad+\zeta^{N-1}\,\delta_{\lambda\,\beta_N}|\beta_1\,\beta_2\,\beta_3\ldots\beta_{N-1}\}\\ &=\sum_{i=1}^{N}\zeta^{i-1}\,\delta_{\lambda\,\beta_i}|\beta_1\ldots\beta_{i-1}\,\beta_{i+1}\ldots\beta_N\}\,.\end{aligned}\tag{3.19}$$

Similarly, for the normailized state we have

$$a_\lambda|\beta_1\ldots\beta_N\rangle = \frac{1}{\sqrt{n_\lambda}}\sum_{i=1}^{N}\zeta^{i-1}\delta_{\lambda\,\beta_i}|\beta_1\ldots\beta_{i-1}\,\beta_{i+1}\ldots\beta_N\rangle\,.\tag{3.20}$$

Because there are no particles in the vacuum state, the annihilation operator must obliterate it completely,

$$a_\lambda|0\rangle = 0\,.\tag{3.21}$$

Writing the annihilation operator as a linear combination of a coordinate and a momentum leads to the configuration space form of (3.21):

$$(\hat{x}+i\hat{k})\,|0\rangle = \Big(\mathbf{x}+\nabla_{\mathbf{x}}\Big)\psi_0(\mathbf{x}) = 0\,.\tag{3.22}$$

From this relationship, a Gaussian wave function, $\psi_0(\mathbf{x}) = (2\pi)^{-3/2}e^{-x^2/2}$, is seen to satisfy the requirements of the vacuum. This observation provides motivation for the Gaussian variational procedure as discussed in the next chapter.

The adjoint of (3.20) reveals the action of the creation operator, $a_\lambda^\dagger$, through the evaluation of the matrix element between two arbitrary states as

$$\{\beta_1\ldots\beta_n|a_\lambda^\dagger|\alpha_1\ldots\alpha_m\} = \sum_{i=1}^{N}\zeta^{i-1}\delta_{\lambda\,\beta_i}\{\beta_1\ldots\beta_{i-1}\,\beta_{i+1}\ldots\beta_n|\alpha_1\ldots\alpha_m\}\,.\tag{3.23}$$

This expression is nonzero only if $n = m + 1$, thus indicating that $a^\dagger_\lambda$ increases the number of particles in $|\alpha_1 \dots \alpha_m\}$ by one. In analogy with (3.19) and (3.20), we have

$$a^\dagger_\lambda|\beta_1 \dots \beta_N\} = |\lambda\, \beta_1 \dots \beta_N\}\,, \tag{3.24a}$$

$$a^\dagger_\lambda|\beta_1 \dots \beta_N\} = \sqrt{n_\lambda + 1}|\lambda\, \beta_1 \dots \beta_N\rangle\,. \tag{3.24b}$$

As seen from these relationships, the creation operators do not act within one space, $\mathcal{B}_N$ or $\mathcal{F}_N$, but instead take elements from $\mathcal{B}_N/\mathcal{F}_N$ to $\mathcal{B}_{N+1}/\mathcal{F}_{N+1}$. If these operators are to act within a closed vector space, then it is necessary to define the Fock space as a direct sum of the Hilbert spaces with $1, 2, 3, \dots, n, \dots$ particles, where the respective Fock spaces of bosons and fermions are

$$\mathcal{B} = \mathcal{B}_0 \oplus \mathcal{B}_1 \oplus \mathcal{B}_2 \oplus \dots = \bigoplus_{n=0}^{\infty} \mathcal{B}_n \tag{3.25a}$$

$$\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \dots = \bigoplus_{n=0}^{\infty} \mathcal{F}_n\,, \tag{3.25b}$$

where $\mathcal{B}_0 = \mathcal{F}_0 = |0\rangle$ and $\mathcal{B}_1 = \mathcal{F}_1 = \mathscr{H}$. By their action on the basis states, the ladder operators' commutation relations can be deduced. First, the product $a^\dagger_\lambda a^\dagger_\nu$ acts on an arbitrary state in the following way

$$\begin{aligned} a^\dagger_\lambda\, a^\dagger_\nu\, |\beta_1 \dots \beta_N\} &= |\lambda\, \nu\, \beta_1 \dots \beta_N\} \\ &= \zeta|\nu\, \lambda\, \beta_1 \dots \beta_N\} \\ &= \zeta a^\dagger_\nu\, a^\dagger_\lambda\, |\beta_1 \dots \beta_N\}\,. \end{aligned} \tag{3.26}$$

Being an arbitrary state, $|\beta_1 \dots \beta_N\}$, can be factored out, leaving a relationship between the operators. Because $\zeta = +1$ for bosons and -1 for fermions, (3.26) gives the respective commutator or anticommutator, which is compactly expressed by the notation

$$[a^\dagger_\lambda, a^\dagger_\nu]_{-\zeta} = a^\dagger_\lambda\, a^\dagger_\nu - \zeta\, a^\dagger_\nu\, a^\dagger_\lambda = 0\,. \tag{3.27a}$$

Taking the adjoint gives

$$[a_\lambda, a_\nu]_{-\zeta} = a_\lambda\, a_\nu - \zeta\, a_\nu\, a_\lambda = 0\,. \tag{3.27b}$$

Likewise, the application of (3.19) and (3.24) obtains the commutator and anticommutator of the product $a_\lambda\, a^\dagger_\nu$. Operating $a_\lambda\, a^\dagger_\nu$ and $a^\dagger_\nu\, a_\lambda$ on an arbitrary state, we have

$$a_\lambda\, a^\dagger_\nu\, |\beta_1 \dots \beta_N\} = \delta_{\lambda\,\nu}|\beta_1 \dots \beta_N\} + \zeta \sum_{i=1}^{N} \zeta^{i-1} \delta_{\lambda\,\beta_i}|\nu\, \beta_1 \dots \beta_{i-1}\, \beta_{i+1} \dots \beta_N\} \tag{3.28a}$$

$$a^\dagger_\nu\, a_\lambda\, |\beta_1 \dots \beta_N\} = \sum_{i=1}^{N} \zeta^{i-1} \delta_{\lambda\,\beta_i}|\nu\, \beta_1 \dots \beta_{i-1}\, \beta_{i+1} \dots \beta_N\}\,, \tag{3.28b}$$

where the combination of (3.28a) and (3.28b) completes the commutation relations for a and $a^\dagger$:

$$[a_\lambda, a_\nu^\dagger]_{-\zeta} = a_\lambda\, a_\nu^\dagger - \zeta\, a_\nu^\dagger\, a_\lambda = \delta_{\lambda\,\nu}\,. \tag{3.29}$$

Under a change of basis, the orthonormal set $\{|\beta\rangle\}$ is transformed into $\{|\tilde\beta\rangle\}$ using the relation $|\tilde\beta\rangle = \sum_\beta \langle\beta|\tilde\beta\rangle|\beta\rangle$. In this new basis it is useful to specify the action of $a_{\tilde\beta}, a_{\tilde\beta}^\dagger$ in terms of the old $a_\beta, a_\beta^\dagger$. To accomplish this, consider the action on an arbitrary state in the new basis,

$$\begin{aligned} a_{\tilde\beta}^\dagger|\tilde\beta_1\dots\tilde\beta_N\} &= |\tilde\beta\,\tilde\beta_1\dots\tilde\beta_N\} \\ &= \sum_\beta \langle\beta|\tilde\beta\rangle a_\beta^\dagger|\tilde\beta_1\dots\tilde\beta_N\}\,, \end{aligned} \tag{3.30}$$

which implies

$$a_{\tilde\beta}^\dagger = \sum_\beta \langle\beta|\tilde\beta\rangle\, a_\beta^\dagger\,, \tag{3.31a}$$

$$a_{\tilde\beta} = \sum_\beta \langle\tilde\beta|\beta\rangle\, a_\beta\,. \tag{3.31b}$$

If the transformation is canonical and the new basis is orthonormal, the commutator algebra has the same form as in (3.27) and (3.29). For example, in the coordinate basis, $\{|\mathbf{x}\rangle\}$, the creation and destruction operators are more commonly known as field operators, $\hat\psi(\mathbf{x})^\dagger$ and $\hat\psi(\mathbf{x})$[1]:

$$\hat\psi(\mathbf{x})^\dagger = \sum_\beta \langle\beta|\mathbf{x}\rangle\, a_\beta^\dagger = \sum_\beta \phi_\beta(\mathbf{x})^*\, a_\beta^\dagger\,, \tag{3.32a}$$

$$\hat\psi(\mathbf{x}) = \sum_\beta \langle\mathbf{x}|\beta\rangle\, a_\beta = \sum_\beta \phi_\beta(\mathbf{x})\, a_\beta\,. \tag{3.32b}$$

In this case, the unitary transformation matrix is composed of the set of wave functions, $\{\phi_\beta(\mathbf{x})\}$, in each of the states $\{|\beta\rangle\}$. The field operator commutators are given by

$$\begin{aligned} \big[\hat\psi(\mathbf{x})^\dagger, \hat\psi(\mathbf{y})^\dagger\big]_{-\zeta} = \big[[\hat\psi(\mathbf{x}), \hat\psi(\mathbf{y})\big]_{-\zeta} &= 0\,, \\ \big[\hat\psi(\mathbf{x}), \hat\psi(\mathbf{y})^\dagger\big]_{-\zeta} &= \delta(\mathbf{x}-\mathbf{y})\,. \end{aligned} \tag{3.33}$$

In addition to generating the entire Fock space from the vacuum state, the creation and destruction operators also provide a convenient basis from which to construct the various

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[1] Because of the generality of the subscript notation, no further distinction will be made between the ladder operators and the field operators, thus keeping the basis general unless stated otherwise.

operators acting on this space. One fundamental element of this basis is the number operator which counts the number of particles in some particular state, $|\beta\rangle$:

$$\hat{n}_\beta = a^\dagger_\beta \, a_\beta \tag{3.34}$$

Hence, the total number operator sums the numbers in each single particle state,

$$\hat{N} = \sum_\beta \hat{n}_\beta = \sum a^\dagger_\beta \, a_\beta \, . \tag{3.35}$$

When expressed in terms of the creation and annihilation operators acting on the Fock space, the operators defined in Sec. 3.2 are said to be in "second quantized" form. First consider a one-body operator, $\hat{T}$, diagonal in the orthonormal basis $\{|\beta\rangle\}$. By Eqs. (3.2) and (3.7), the action of $\hat{T}$ is given by

$$\hat{T}|\beta_1 \ldots \beta_N\} = \frac{1}{\sqrt{N!}} \sum_{\mathcal{P}} \zeta^{\mathcal{P}} \, \hat{T} \, |\beta_{\mathcal{P}_1}\rangle \otimes \ldots \otimes |\beta_{\mathcal{P}_N}\rangle \, . \tag{3.36}$$

According to (3.15), the one-body operator acts on each individual single particle state in the tensor product, resulting in a sum over the eigenvalues

$$\begin{aligned} \hat{T}|\beta_1 \ldots \beta_N\} &= \frac{1}{\sqrt{N!}} \sum_{\mathcal{P}} \zeta^{\mathcal{P}} \sum_{i=1}^{N} T_{\beta_{\mathcal{P}_i}} |\beta_{\mathcal{P}_1}\rangle \otimes \ldots \otimes |\beta_{\mathcal{P}_N}\rangle \\ &= \sum_{i=1}^{N} T_{\beta_i} |\beta_1 \ldots \beta_N\} \\ &= \sum_\beta T_\beta \, \hat{n}_\beta \, |\beta_1 \ldots \beta_N\rangle \, . \end{aligned} \tag{3.37}$$

Since $\hat{T}$ is diagonal in $\{|\beta\rangle\}$, the eigenvalues are denoted by $T_\beta = \langle\beta|\hat{T}|\beta\rangle$. In writing the last step in (3.37), use has been made of the fact that summing the eigenvalues over each particle is equivalent to a sum over states, where the number in each state gets multiplied by the corresponding eigenvalue. Thus, the diagonal representation of $\hat{T}$ is

$$\hat{T} = \sum_\beta \langle\beta|T|\beta\rangle \, a^\dagger_\beta \, a_\beta \, , \tag{3.38a}$$

from which is implied the generalization to an arbitrary basis:

$$\hat{T} = \sum_{\alpha\,\beta} \langle\alpha|T|\beta\rangle \, a^\dagger_\alpha \, a_\beta \, . \tag{3.38b}$$

In coordinate space we have

$$\begin{aligned} \hat{T} &= \int_{\mathbf{x}} \int_{\mathbf{y}} \langle\alpha|\mathbf{y}\rangle\langle\mathbf{y}|T|\mathbf{x}\rangle\langle\mathbf{x}|\beta\rangle \, a^\dagger_\alpha \, a_\beta \\ &= -\int_{\mathbf{x}} \hat{\psi}(\mathbf{x})^\dagger \, \nabla^2_{\mathbf{x}} \, \hat{\psi}(\mathbf{x}) \, , \end{aligned} \tag{3.39}$$

where we have used the fact that $\langle \mathbf{y}|T|\mathbf{x}\rangle = -\delta(\mathbf{y}-\mathbf{x})\nabla^2_{\mathbf{x}}$, in units where $\hbar^2/(2m) = 1$.

Similar steps are followed in obtaining the form of the two-body operator. In the basis, $\{|\alpha\,\beta)\}$, where $\hat{V}$ is diagonal, its action on an arbitrary state is

$$\begin{aligned}\hat{V}|\beta_1\ldots\beta_N\} &= \frac{1}{\sqrt{N!}}\sum_{\mathcal{P}}\zeta^{\mathcal{P}}\,\frac{1}{2}\sum_{i\neq j}^{N} V_{\beta_{\mathcal{P}_i}\,\beta_{\mathcal{P}_j}}|\beta_{\mathcal{P}_1}\rangle\otimes\ldots\otimes|\beta_{\mathcal{P}_N}\rangle \\ &= \frac{1}{2}\sum_{i\neq j}^{N} V_{\beta_i\,\beta_j}\,|\beta_1\ldots\beta_N\}\,.\end{aligned} \tag{3.40}$$

Unlike the one-body operator case, the summation here is over all particle pairs, with the factor of 1/2 taking account of double counting. In order to convert this to a summation over pair states, an operator must be constructed to count the number of particle pairs. If some particles are in state $|\alpha\rangle$ while others are in state $|\beta\rangle$, then between these two states, there are $n_\alpha\,n_\beta$ pairs if $\alpha\neq\beta$, but $n_\alpha\,n_\beta - 1$ pairs if $\alpha = \beta$. Therefore, the pair counting operator is given by

$$\begin{aligned}\hat{n}_\alpha\hat{n}_\beta - \delta_{\alpha\,\beta}\,\hat{n}_\alpha &= a^\dagger_\alpha\,a_\alpha\,a^\dagger_\beta\,a_\beta - \delta_{\alpha\beta}\,a^\dagger_\alpha\,a_\alpha \\ &= a^\dagger_\alpha\,\zeta\,a^\dagger_\beta\,a_\alpha\,a_\beta \\ &= a^\dagger_\alpha\,a^\dagger_\beta\,a_\beta\,a_\alpha\,,\end{aligned} \tag{3.41}$$

where use has been made of the commutators (3.27b) and (3.29). Note that the ordering is such as to include both bosonic and fermionic cases. Substitution of (3.41) into (3.40) gives the diagonal representation of the two-body operator[1]

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta}(\alpha\,\beta|V|\alpha\,\beta)\,a^\dagger_\alpha\,a^\dagger_\beta\,a_\beta\,a_\alpha\,, \tag{3.42a}$$

with the generalization

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\,\beta|V|\delta\,\gamma)\,a^\dagger_\alpha\,a^\dagger_\beta\,a_\delta\,a_\gamma\,. \tag{3.42b}$$

If the interaction is local as in (3.18), this operator has the coordinate space representation

$$\hat{V} = \frac{1}{2}\int_{\mathbf{x},\mathbf{y}} V(\mathbf{x}-\mathbf{y})\hat{\psi}(\mathbf{x})^\dagger\,\hat{\psi}(\mathbf{y})^\dagger\,\hat{\psi}(\mathbf{y})\,\hat{\psi}(\mathbf{x})\,. \tag{3.43}$$

Equations (3.38b) and (3.42b) express the one and two-body operators in terms of the particle creation and destruction operators that act on the Fock space. From these constructions, it can be seen that the procedure simply involves a sum of the products between the operator's matrix element and the combination of a and $a^\dagger$ that count the number acted upon by the operator. For example, the "second quantization" of a general

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[1] Here, $V_{\alpha\beta} = (\alpha\beta|\hat{V}|\alpha\beta)$.

n-body operator would involve the specification of the matrix element in $\mathscr{H}_N$ as well as the construction of the operator that counts all distinct n-particle groups in the assembly. In what follows, we use this formalism to express the Hamiltonian as well as other operators of interest.

3.4 Coherent States

Although permanents and Slater determinants can be used as bases for $\mathcal{B}$ or $\mathcal{F}$, coherent states provide a useful basis especially when discussing variational many-body approaches. Since the two spaces have different commutator algebra, each is discussed separately. In either case, however, a coherent state, $|\phi\rangle$, is defined as an eigenstate of the annihilation operator, a_β:

$$a_\beta|\phi\rangle = \phi_\beta|\phi\rangle \,. \tag{3.44}$$

Application of the commutator on the coherent state gives unusual properties of the eigenvalues for the fermionic case. In particular we have

$$\left[\phi_\alpha, \phi_\beta\right]_{-\zeta} = \phi_\alpha\,\phi_\beta - \zeta\,\phi_\beta\phi_\alpha = 0\,, \tag{3.45}$$

which, for fermions ($\zeta = -1$) implies that the eigenvalues are Grassmann variables instead of ordinary numbers as in the bosonic ($\zeta = +1$) case. We deal with the bosons first, then outline the appropriate analog for the fermions.

3.4.1 Bosonic Case

Boson coherent states are important for the subsequent variational formalism which relies on a coherent state trial wave functional. When discussing coherent states, the occupation number representation is most convenient to use, where $|n_{\beta_1}\,n_{\beta_2}\ldots n_{\beta_N}\rangle$ denotes a normalized, symmetrized state with n_{β_1} particles in state $|\beta_1\rangle$, n_{β_2} particles in state $|\beta_2\rangle$, and so on. In this representation, any coherent state may be expanded as

$$|\phi\rangle = \sum_{\{n_\beta\}} \phi_{n_{\beta_1}\ldots n_{\beta_p}\ldots}|n_{\beta_1}\ldots n_{\beta_p}\ldots\rangle\,, \tag{3.46}$$

where the summation is over all occupation numbers in each of the states. Application of the annihilation operator results in

$$\begin{aligned}
a_{\beta_i}|\phi\rangle &= \sum_{\{n_\beta\}} \phi_{n_{\beta_1}\ldots n_{\beta_p}\ldots}\sqrt{n_{\beta_i}}\,|n_{\beta_1}\ldots(n_{\beta_i}-1)\ldots n_{\beta_p}\ldots\rangle \\
&= \phi_{\beta_i}\sum_{\{n_\beta\}} \phi_{n_{\beta_1}\ldots n_{\beta_p}\ldots}|n_{\beta_1}\ldots n_{\beta_p}\ldots\rangle \\
&= \phi_{\beta_i}\sum_{\{n_\beta\}} \phi_{n_{\beta_1}\ldots(n_{\beta_i}-1)\ldots n_{\beta_p}\ldots}|n_{\beta_1}\ldots(n_{\beta_i}-1)\ldots n_{\beta_p}\ldots\rangle\,.
\end{aligned} \tag{3.47}$$

The last line follows from the eigenvalue equation (3.44) along with the recognition that the summation is over all occupation numbers. Repeated use of the destruction operator applied to all of the states in $|\phi\rangle$, gives the coefficient in (3.46),

$$\phi_{n_{\beta_1}\dots n_{\beta_p}\dots} = \prod_i \frac{\phi_{\beta_i}^{n_{\beta_i}}}{\sqrt{n_{\beta_i}!}} \,. \tag{3.48}$$

Noting that $|n_{\beta_1}\dots n_{\beta_p}\dots\rangle = \prod_i [(a^\dagger_{\beta_i})^{n_{\beta_i}}/\sqrt{n_{\beta_i}!}]\,|0\rangle$, the coherent state in (3.46) can be expressed as

$$\begin{aligned} |\phi\rangle &= \sum_{\{n_\beta\}} \prod_i \frac{\left(\phi_{\beta_i}\, a^\dagger_{\beta_i}\right)^{n_{\beta_i}}}{n_{\beta_i}!}\,|0\rangle \\ &= e^{\sum_\beta \phi_\beta\, a^\dagger_\beta}\,|0\rangle\,, && (3.49\text{a}) \\ \langle\phi| &= \langle 0|\, e^{\sum_\beta \phi^*_\beta\, a_\beta}\,. && (3.49\text{b}) \end{aligned}$$

Using this form, the action of the creation operator on the coherent state is given by

$$\begin{aligned} a^\dagger_\beta\,|\phi\rangle &= a^\dagger_\beta\, e^{\sum_\alpha \phi_\alpha\, a^\dagger_\alpha}\,|0\rangle \\ &= \frac{\partial}{\partial\phi_\beta}\,|\phi\rangle\,, && (3.50\text{a}) \end{aligned}$$

with the adjoint,

$$\langle\phi|\, a_\beta = \frac{\partial}{\partial\phi^*_\beta}\,\langle\phi| \tag{3.50b}$$

In addition, it is useful to calculate the overlap of two coherent states, obtaining a form dependent upon the set of eigenvalues $\{\phi_\beta\}$. Using the expansions in the occupation number representation, the inner product is

$$\langle\phi|\phi'\rangle = \sum_{\{n_\beta\}}\sum_{\{n'_\beta\}}\prod_i \frac{\left(\phi^*_{\beta_i}\right)^{n_{\beta_i}}}{\sqrt{n_{\beta_i}!}}\prod_j \frac{\left(\phi'_{\beta_j}{}^*\right)^{n_{\beta_j}}}{\sqrt{n'_{\beta_j}!}}\,\langle n_{\beta_1}\dots n_{\beta_p}\dots|n'_{\beta_1}\dots n'_{\beta_p}\dots\rangle\,. \tag{3.51}$$

Due to the orthonormality of the states $\{|\beta\rangle\}$, the scalar product reduces to $\delta_{n_{\beta_1}\,n'_{\beta_1}}\dots\delta_{n_{\beta_p}\,n'_{\beta_p}}\dots$, thus simplifying the result:

$$\langle\phi|\phi'\rangle = e^{\sum_\beta \phi^*_\beta\,\phi'_\beta}\,. \tag{3.52}$$

Such a Gaussian will be used as a trial state in the variational method discussed in Chapter 4.

Any Fock space vector may be expanded in terms of the coherent states, a fact implicit in the coherent state closure relation

$$\int \prod_\beta \frac{d\phi^*_\beta \, d\phi_\beta}{2\pi i} \, e^{-\sum_\beta \phi^*_\beta \phi_\beta} \, |\phi\rangle\langle\phi| = 1 \, . \tag{3.53}$$

Hence, the coherent state expansion of $|\Psi\rangle$ is

$$|\Psi\rangle = \int \prod_\beta \frac{d\phi^*_\beta \, d\phi_\beta}{2\pi i} \, e^{-\sum_\beta \phi^*_\beta \phi_\beta} \, \Psi(\phi^*) \, |\phi\rangle \, . \tag{3.54}$$

Just as $\langle \mathbf{x}|\psi\rangle = \psi(\mathbf{x})$ is the coordinate representation of the single particle state $|\psi\rangle$, $\langle\phi|\Psi\rangle = \Psi(\phi^*)$ is defined as the coherent state representation of the many-body state $|\Psi\rangle$. In the bosonic case, ϕ, also known as the field, is representative of the set of eigenvalues $\{\phi_\alpha\}$. In contrast, no such field exists in the fermionic case. Using the adjoint of (3.44) with (3.50b), the field dependence of the creation and destruction operators can be obtained by their action on the bras:

$$\langle\phi| \, a_\beta \, |\Psi\rangle = \frac{\partial}{\partial\phi^*_\beta} \, \Psi(\phi^*) \Rightarrow a_\beta = \frac{\partial}{\partial\phi^*_\beta} \tag{3.55a}$$

$$\langle\phi| \, a^\dagger_\beta \, |\Psi\rangle = \phi^*_\beta \, \Psi(\phi^*) \Rightarrow a^\dagger_\beta = \phi^*_\beta \tag{3.55b}$$

3.4.2 Fermionic Case

In this section, the fermionic coherent state is developed as an analog of the bosonic case. Unlike the bosons, however, the destruction operator eigenvalues anticommute, as seen from (3.45). Fortunately, the Grassmann algebra provides the theoretical scaffolding required for such numbers.

A Grassmann algebra is given by a set of generators, $\{\xi_\alpha\}$, which anticommute

$$\xi_\alpha \, \xi_\beta + \xi_\beta \, \xi_\alpha = 0 \, . \tag{3.56}$$

Consequently, the square of a generator must be zero,

$$\xi^2_\alpha = 0 \, . \tag{3.57}$$

Such an algebra has elements that are linear combinations of all distinct generator products, $\{1, \xi_\alpha, \xi_\alpha \, \xi_\beta, \ldots \xi_\alpha \, \xi_\beta \, \xi_\gamma \ldots\}$. By this construction, the Grassmann space is 2^n dimensional, given n generators. In other words, every element either contains or does not contain each of the generators.

A space with $2p$ generators is obtained by conjugation. Given p generators, $\xi_1, \xi_2, \ldots, \xi_p$, the complementary set is obtained with $\xi^*_1, \xi^*_2, \ldots, \xi^*_p$, where conjugation is defined as

$$(\xi_\alpha)^* = \xi^*_\alpha \tag{3.58a}$$

$$(\xi^*_\alpha)^* = \xi_\alpha \tag{3.58b}$$

$$(\lambda\xi_\alpha)^* = \lambda^* \, \xi^*_\alpha \qquad (\lambda \in \mathbb{C}) \tag{3.58c}$$

$$(\xi_{\alpha_1} \ldots \xi_{\alpha_n})^* = \xi^*_{\alpha_n} \ldots \xi^*_{\alpha_1} \, . \tag{3.58d}$$

As a demonstrative example, consider the algebra generated by ξ and ξ^*. Because of the anticommutative property (3.57), this space only admits functions having the linear form

$$f(\xi) = f_0 + f_1\xi\,, \tag{3.59}$$

whereas operators assume the quadratic form

$$\mathcal{O}(\xi^*, \xi) = c_0 + c_1\xi + \bar{c}_1\xi^* + c_{12}\,\xi^*\,\xi\,. \tag{3.60}$$

Grassmann algebra derivatives are performed in the usual way, except for terms involving operator products, in which case the generator being differentiated must be anticommuted through the product before the derivative can act. Thus, we have $\frac{\partial}{\partial\xi}\,\xi = 1$ and $\frac{\partial}{\partial\xi}\,\xi^*\xi = -\xi^*$. As expected, the operators $\frac{\partial}{\partial\xi}$ and $\frac{\partial}{\partial\xi^*}$ anticommute, as illustrated by their action on $\mathcal{O}$:

$$\frac{\partial}{\partial\xi}\,\mathcal{O}(\xi^*, \xi) = c_1 - c_{12}\,\xi^* \tag{3.61a}$$

$$\frac{\partial}{\partial\xi^*}\,\frac{\partial}{\partial\xi}\,\mathcal{O}(\xi^*, \xi) = -c_{12}\,. \tag{3.61b}$$

Similarly, we have

$$\begin{aligned}\frac{\partial}{\partial\xi}\,\frac{\partial}{\partial\xi^*}\,\mathcal{O}(\xi^*, \xi) &= c_{12}\\ &= -\frac{\partial}{\partial\xi^*}\,\frac{\partial}{\partial\xi}\,\mathcal{O}(\xi^*, \xi)\end{aligned} \tag{3.62}$$

Since $\mathcal{O}$ is arbitrary, this verifies the anticommutator.

Grassmann integration is defined by the following

$$\int d\xi\,1 = \int d\xi^*\,1 = 0 \tag{3.63a}$$

$$\int d\xi\,\xi = \int d\xi^*\,\xi^* = 1\,, \tag{3.63b}$$

with the caveat that $d\,\xi$ and $d\,\xi^*$ are not Grassmann numbers so they are not conjugate variables.

Another useful operator is the δ function, which can be obtained through an analog of the normal Fourier integral form:

$$\begin{aligned}\delta(\xi, \xi') &= \int d\eta\, e^{-\eta(\xi-\xi')}\\ &= \int d\eta\big[1 - \eta(\xi - \xi')\big]\\ &= -(\xi - \xi')\,.\end{aligned} \tag{3.64}$$

To test that this is indeed the Grassmann delta function, it is applied to $f(\xi')$:

$$\begin{aligned}\int d\xi'\,\delta(\xi,\xi')\,f(\xi') &= -\int d\xi'\,(\xi-\xi')\,(f_0+f_1\,\xi') \\ &= f_0+f_1\,\xi\,.\end{aligned} \tag{3.65}$$

Having reviewed these basic features of Grassmann algebra, it is now possible to apply this formalism in constructing a fermionic coherent state. Such a state does not lie in the ordinary fermionic Fock space, as it must be produced by linear combinations of ordinary Fock space states with Grassmann generators as coefficients. Consequently, a generator, ξ_α or ξ^*_α, is associated with its respective destruction, a_α, or creation, $a^\dagger_\alpha$, operator. Such an association requires a set of rules governing the products between a generator and a ladder operator. Therefore, it is natural to impose the following requirements:

$$\left[\xi_\alpha, a_\alpha\right]_+ = \left[\xi_\alpha, a^\dagger_\alpha\right]_+ = 0 \tag{3.66a}$$

$$\left[\xi_\alpha, a_\beta\right]_- = \left[\xi_\alpha, a^\dagger_\beta\right]_- = 0\,,\ \alpha\neq\beta \tag{3.66b}$$

$$(\xi\,a)^\dagger = a^\dagger\,\xi^\dagger\,. \tag{3.66c}$$

In analogy with the bosonic case (3.49), the fermionic coherent state is constructed as

$$\begin{aligned}|\xi\rangle &= e^{-\sum_\beta \xi_\beta\,a^\dagger_\beta}\,|0\rangle \\ &= \prod_\beta \left(1-\xi_\beta\,a^\dagger_\beta\right)|0\rangle\end{aligned} \tag{3.67a}$$

with the adjoint

$$\begin{aligned}\langle\xi| &= \langle 0|\,\prod_\beta\left(1-a_\beta\,\xi^*_\beta\right) \\ &= \langle 0|\,\prod_\beta\left(1+\xi^*_\beta\,a_\beta\right),\end{aligned} \tag{3.67b}$$

where we have used the linearity property (3.59) in defining the exponential in the Grassmann algebra. It must now be verified that the coherent state constructed in this way is in fact an eigenstate of the destruction operator, a_α. Along with (3.57), we use (3.67) and the commutation relations (3.29) to obtain

$$\begin{aligned}
a_\alpha \left|\xi\right\rangle &= a_\alpha \prod_{\beta\neq\alpha} \left(1-\xi_\beta\, a^\dagger_\beta\right) \left(1-\xi_\alpha\, a^\dagger_\alpha\right) \left|0\right\rangle \\
&= \prod_{\beta\neq\alpha} \left(1-\xi_\beta\, a^\dagger_\beta\right) a_\alpha \left(1-\xi_\alpha\, a^\dagger_\alpha\right) \left|0\right\rangle \\
&= \prod_{\beta\neq\alpha} \left(1-\xi_\beta\, a^\dagger_\beta\right) \xi_\alpha \left|0\right\rangle \\
&= \prod_{\beta\neq\alpha} \left(1-\xi_\beta\, a^\dagger_\beta\right) \xi_\alpha \left(1-\xi_\alpha\, a^\dagger_\alpha\right) \left|0\right\rangle \\
&= \xi_\alpha \left|\xi\right\rangle .
\end{aligned} \tag{3.68}$$

Hence, the construction (3.67) is an eigenstate of a as expected. Furthermore, the same Grassmann rules are employed in finding the action of $a^\dagger$ on the coherent state,

$$\begin{aligned}
a^\dagger_\alpha \left|\xi\right\rangle &= a^\dagger_\alpha \prod_{\beta\neq\alpha} \left(1-\xi_\beta\, a^\dagger_\beta\right)\left(1-\xi_\alpha\, a^\dagger_\alpha\right) \left|0\right\rangle \\
&= \prod_{\beta\neq\alpha} \left(1-\xi_\beta\, a^\dagger_\beta\right) a^\dagger_\alpha \left|0\right\rangle \\
&= -\frac{\partial}{\partial\xi_\alpha} \prod_{\beta} \left(1-\xi_\beta\, a^\dagger_\beta\right) \left|0\right\rangle \\
&= -\frac{\partial}{\partial\xi_\alpha} \left|\xi\right\rangle .
\end{aligned} \tag{3.69}$$

It can be directly verified from (3.67b) that the adjoint of (3.69) is

$$\left\langle\xi\right| a_\alpha = \frac{\partial}{\partial\xi^*_\alpha} \left\langle\xi\right| . \tag{3.70}$$

From the above, we construct the analogs of the bosonic results of equations (3.52), (3.53), (3.54) and (3.55). For the overlap of two fermionic coherent states we have

$$\left\langle\xi|\xi'\right\rangle = \prod_\beta \left(1+\xi^*_\beta\, \xi_\beta\right) = e^{\sum_\beta \xi^*_\beta\, \xi_\beta} . \tag{3.71}$$

Since any vector in the fermion Fock space can be expanded in coherent states, there is a closure relation given by

$$\int \prod_\beta d\xi^*_\beta\, d\xi_\beta \left(1-\xi^*_\beta\, \xi_\beta\right) \left|\xi\right\rangle\!\left\langle\xi\right| = 1 , \tag{3.72}$$

whence, the coherent state expression of any many-body fermionic state, $\left|\Psi\right\rangle$ is

$$\left|\Psi\right\rangle = \int \prod_\beta d\xi^*_\beta\, d\xi_\beta \left(1-\xi^*_\beta\, \xi_\beta\right) \Psi(\xi^*) \left|\xi\right\rangle , \tag{3.73}$$

where $\Psi(\xi^*)$ is the projection of $|\Psi\rangle$ onto the coherent space. Finally, the creation and destruction operators have the form

$$\langle\xi|a_\beta^\dagger|\Psi\rangle = \xi_\beta^*\,\Psi(\xi^*) \tag{3.74a}$$

$$\langle\xi|a_\beta|\Psi\rangle = \frac{\partial}{\partial\xi_\beta^*}\,\Psi(\xi^*) \tag{3.74b}$$

with (3.74a) following from (3.68) and (3.74b) from (3.70). Although not the emphasis in this work, the fermionic formalism has been included for completeness. Moreover, as there has been increasing interest in producing composite Bose-Fermi superfluids in atomic traps, the fermionic coherent states can be applied to further extensions of this work. Indeed, a variational form of (3.67a) has been used in the famous BCS theory of superconductivity.

Chapter 4

Variational Method

This chapter establishes the basic formalisms applied in the analysis of the model bosonic systems discussed herein. Using the coherent states of the previous chapter, it is possible to generalize the single particle variational principle to the many-body case. Section 4.1 describes a Gaussian trial wave functional which can be used to stationarize model Hamiltonians. For the special case of a static, uniform medium, Section 4.2 gives the stationary solutions that explicitly determine the unknown parameters in the trial functional. Expanding around these stationary points, the small oscillation equations of motion are developed from which the excitation spectrum may be derived. Finally, Section 4.4 discusses a more conventional perspective involving the Gross-Pitaevskii equation for the order parameter. From this analysis, it is demonstrated that the chemical potential is the phase of this parameter, which can be consistently defined in two different but equivalent ways.

4.1 Gaussian Variational Principle for Bosons

For the bosonic case, we review the variational procedure whereby a Gaussian trial functional is used in calculating the mean value of the many-body Hamiltonian[1]. Constrained by a fixed particle number, this quantity is extremized to determine the ground state of the model, which then gives the equation of state. To understand this approach, we begin by defining an effective action for the time-dependent quantum system,

$$S = \int L(t)dt = \int dt \langle \psi, t | i\partial_t - \hat{H} | \psi, t \rangle, \tag{4.1}$$

where $|\psi, t\rangle$ is the many-body quantum state and $\hat{H}$ is the Hamiltonian. For a system of bosons interacting through some two-body potential, V, the second-quantized form of the Hamiltonian is

$$\hat{H} = \sum_{\alpha\beta} \hat{\psi}^\dagger_\alpha T_{\alpha\beta} \hat{\psi}_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \hat{\psi}^\dagger_\alpha \hat{\psi}^\dagger_\beta V_{\alpha\beta;\delta\gamma} \hat{\psi}_\delta \hat{\psi}_\gamma \, , \tag{4.2}$$

where $T_{\alpha\beta}$ represents a kinetic energy operator as well as any one-body potential acting on the system. In addition, the quasiparticle creation, $\hat{\psi}^\dagger$, and destruction, $\hat{\psi}^\dagger$, operators can

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[1] The variational procedure discussed here was first put forth in A. K. Kerman and P. Tommasini (1997).

be written in terms of the field operator "coordinate", $\hat{\phi}$, and its conjugate momentum, $\hat{\pi}$, as

$$\begin{aligned}\hat{\psi}_\alpha &= \frac{1}{\sqrt{2}}\left(\hat{\phi}_\alpha + i\hat{\pi}_\alpha\right)\\ \hat{\psi}^\dagger_\alpha &= \frac{1}{\sqrt{2}}\left(\hat{\phi}_\alpha - i\hat{\pi}_\alpha\right) .\end{aligned} \tag{4.3}$$

As usual, the field operators' commutation relations are

$$\begin{aligned}\left[\hat{\phi}_\alpha, \hat{\phi}_\beta\right] = \left[\hat{\pi}_\alpha, \hat{\pi}_\beta\right] &= 0\\ \left[i\hat{\pi}_\alpha, \hat{\phi}_\beta\right] &= \delta_{\alpha\beta} ,\end{aligned} \tag{4.4}$$

which imply the following commutators for $\hat{\psi}$,

$$\begin{aligned}\left[\hat{\psi}_\alpha, \hat{\psi}_\beta\right] = \left[\hat{\psi}^\dagger_\alpha, \hat{\psi}^\dagger_\beta\right] &= 0\\ \left[\hat{\psi}_\alpha, \hat{\psi}^\dagger_\beta\right] &= \delta_{\alpha\beta} .\end{aligned} \tag{4.5}$$

In the functional Schrödinger picture, the state vector, $|\psi, t\rangle$, depends on the field ϕ'_α,

$$|\psi, t\rangle \to \psi\left[\phi', t\right] . \tag{4.6}$$

Consequently, the action of the operators $\hat{\phi}$ and $\hat{\psi}$ on this state are defined as

$$\hat{\phi}_\alpha |\psi, t\rangle \to \phi'_\alpha \psi\left[\phi', t\right] , \tag{4.7a}$$

$$\hat{\pi}_\alpha |\psi, t\rangle \to -i\frac{\delta}{\delta\phi'_\alpha}\psi\left[\phi', t\right] . \tag{4.7b}$$

To extremize the Hamiltonian of Eq. (4.2) we will employ a Gaussian trial functional that is parametrized by a width, $G^{-1}_{\alpha\beta}$, its canonical conjugate, $\Sigma_{\alpha\beta}$, and a source term;

$$\psi\left[\phi', t\right] = N\mathrm{exp}\left\{-\sum_{\alpha\beta}\delta\phi'_\alpha(t)\left[\frac{1}{4}G^{-1}_{\alpha\beta}(t) - i\Sigma_{\alpha\beta}(t)\right]\delta\phi'_\beta(t) + i\sum_\alpha \pi_\alpha(t)\delta\phi'_\alpha(t)\right\} , \tag{4.8}$$

where N is the normalization and the fluctuation is given by the field minus its mean,

$$\delta\phi'_\alpha(t) = \phi'_\alpha - \phi_\alpha(t) . \tag{4.9}$$

Containing only terms involving equal numbers of $\hat{\psi}$ and $\hat{\psi}^\dagger$, the Hamiltonian must therefore remain invariant under any phase transformation of the trial functional,

$$|\psi, t\rangle \to e^{-i\hat{N}\theta(t)}|\psi, t\rangle . \tag{4.10}$$

In other words, the invariance with respect to the phase angle, $\theta(t)$, must be intimately connected with a fixed total particle number, N. Inversely, the fixed particle constraint must induce a mode of zero energy, as the Hamiltonian is invariant under changes in the continuous variable θ. Hence, this so called Goldstone mode will be seen to be a feature of a small oscillation analysis in the Random Phase Approximation (RPA).

In this formalism, the mean of any operator, $\mathcal{O}$, is calculated from the functional integral

$$\langle\psi, t|\hat{\mathcal{O}}|\psi, t\rangle = \int \mathcal{D}\phi' \psi^* \left[\phi', t\right] \hat{\mathcal{O}} \psi \left[\phi', t\right]. \tag{4.11}$$

Since the Hamiltonian of Eq. (4.2) will involve terms of the form $< \hat{\psi}^\dagger \hat{\psi} >$ and $< \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} >$, it is useful to construct creation and destruction operators explicitly for the Gaussian of Eq. (4.8)[1]. As linear combinations of the $\hat{\phi}$ and $\hat{\pi}$, these operators are found to be

$$\begin{aligned}
\hat{c}^\dagger_\alpha(t) &= \frac{1}{\sqrt{2}} \sum_\beta G_{\alpha\beta}(t) \left\{ 2 \sum_\gamma \left[\frac{1}{4} G^{-1}_{\beta\gamma}(t) + i\Sigma_{\beta\gamma}(t) \right] \left[\hat{\phi}_\gamma(t) - \phi_\gamma(t) \right] - i \left[\hat{\pi}_\beta(t) - \pi_\beta(t) \right] \right\} \\
\hat{c}_\alpha(t) &= \frac{1}{\sqrt{2}} \sum_\beta G_{\alpha\beta}(t) \left\{ 2 \sum_\gamma \left[\frac{1}{4} G^{-1}_{\beta\gamma}(t) - i\Sigma_{\beta\gamma}(t) \right] \left[\hat{\phi}_\gamma(t) - \phi_\gamma(t) \right] + i \left[\hat{\pi}_\beta(t) - \pi_\beta(t) \right] \right\}
\end{aligned} \tag{4.12}$$

such that

$$\begin{aligned}
&\hat{c}^\dagger_\alpha(t) \left|\psi, t\right\rangle \to \frac{1}{\sqrt{2}} \delta\phi_\alpha(t) \psi \left[\phi', t\right] \\
&\hat{c}_\alpha(t) \left|\psi, t\right\rangle \to 0
\end{aligned} \tag{4.13}$$

Using the commutation relations of Eq. (4.4) we have

$$\left[\hat{c}^\dagger_\alpha(t), \hat{c}_\beta(t) \right] = -\frac{1}{2} G_{\alpha\beta}(t) \tag{4.14}$$

Inversion of Eq. (4.12) allows the quasiparticle operators to be expressed as linear combinations of $\hat{c}$ and $\hat{c}^\dagger$,

$$\begin{aligned}
\hat{\psi}_\alpha(t) = & 2 \sum_\beta \left[\frac{1}{4} G^{-1}_{\alpha\beta}(t) + i\Sigma_{\alpha\beta}(t) + \frac{1}{2} \delta_{\alpha\beta} \right] \hat{c}_\beta(t) \\
& -2 \sum_\beta \left[\frac{1}{4} G^{-1}_{\alpha\beta}(t) - i\Sigma_{\alpha\beta}(t) - \frac{1}{2} \delta_{\alpha\beta} \right] \hat{c}^\dagger_\beta(t) + \frac{1}{\sqrt{2}} \left[\phi_\alpha(t) + i\pi_\alpha(t) \right] .
\end{aligned} \tag{4.15}$$

Employing Eqs. (4.12)-(4.15), all required mean values are calculated,

$$\langle\psi, t|\hat{\psi}_\alpha(t)|\psi, t\rangle = \frac{1}{\sqrt{2}} \left[\phi_\alpha(t) + i\pi_\alpha(t) \right] = \frac{1}{\sqrt{2}} \psi_\alpha(t) \tag{4.16a}$$

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[1] A similar construction was used on the vacuum state of (3.21).

$$\langle\psi,t|\hat{\psi}_\alpha(t)\hat{\psi}_\beta(t)|\psi,t\rangle = -D_{\alpha\beta}(t) + \frac{1}{2}\psi_\alpha(t)\psi_\beta(t) \tag{4.16b}$$

$$\langle\psi,t|\hat{\psi}^\dagger_\alpha(t)\hat{\psi}_\beta(t)|\psi,t\rangle = R_{\alpha\beta}(t) + \frac{1}{2}\psi^*_\alpha(t)\psi_\beta(t) \tag{4.16c}$$

$$\begin{aligned}\langle\psi,t|\hat{\psi}^\dagger_\alpha(t)\hat{\psi}^\dagger_\beta(t)\hat{\psi}_\gamma(t)\hat{\psi}_\delta(t)|\psi,t\rangle = {}& D^*_{\alpha\beta}(t)D_{\delta\gamma}(t) - D^*_{\alpha\beta}(t)\psi_\delta(t)\psi_\gamma(t)\\ &+ R_{\beta\gamma}(t)R_{\alpha\delta}(t) + R_{\delta\beta}(t)R_{\alpha\gamma}(t)\\ &+ \psi^*_\beta(t)\psi_\delta(t)R_{\alpha\gamma}(t) + \psi^*_\beta(t)\psi_\gamma(t)R_{\alpha\gamma}(t)\\ &+ \psi^*_\alpha(t)\psi_\delta(t)R_{\beta\gamma}(t) + \psi^*_\alpha(t)\psi_\gamma(t)R_{\delta\beta}(t)\\ &- D_{\delta\gamma}(t)\psi^*_\alpha(t)\psi^*_\beta(t) + \psi_\gamma(t)\psi_\delta(t)\psi^*_\alpha(t)\psi^*_\beta(t)\end{aligned} \tag{4.16d}$$

$$\begin{aligned}\langle\psi,t|i\frac{\delta}{\delta t}|\psi,t\rangle = {}&\sum_{\alpha\beta}\Sigma_{\alpha\beta}(t)\dot{G}_{\beta\alpha}(t) + \sum_\alpha \pi_\alpha(t)\dot{\phi}_\alpha(t) + N\dot{\theta}(t)\\ &+ \text{total time derivatives},\end{aligned} \tag{4.16e}$$

where $R_{\alpha\beta}(t)$ and $D_{\alpha\beta}(t)$ are the respective fluctuations of $\langle\hat{\psi}^\dagger\hat{\psi}\rangle$ and $\langle\hat{\psi}\hat{\psi}\rangle$ about their mean-field values of $(1/2)|\psi|^2$ and $(1/2)\psi^2$. However, $R_{\alpha\beta}(t)$ and $D_{\alpha\beta}(t)$ are not independent, being related through the Gaussian width, $G_{\alpha\beta}(t)$ and its conjugate;

$$\begin{aligned}R_{\alpha\beta}(t) &= \frac{1}{2}\left[\frac{1}{4}G^{-1}_{\alpha\beta}(t) + G_{\alpha\beta}(t) - \delta_{\alpha\beta}\right] + 2\sum_{\gamma\delta}\Sigma_{\alpha\gamma}(t)G_{\gamma\delta}(t)\Sigma_{\delta\beta}(t)\\ D_{\alpha\beta}(t) &= \frac{1}{2}\left[\frac{1}{4}G^{-1}_{\alpha\beta}(t) - G_{\alpha\beta}(t)\right] + 2\sum_{\gamma\delta}\Sigma_{\alpha\gamma}(t)G_{\gamma\delta}(t)\Sigma_{\delta\beta}(t)\\ &\quad - i\sum_\gamma\left[\Sigma_{\alpha\gamma}(t)G_{\gamma\beta}(t) + G_{\alpha\gamma}(t)\Sigma_{\gamma\beta}(t)\right].\end{aligned} \tag{4.17}$$

Moreover, Eq. (4.16e) takes explicit account of the trial wave functional phase, introduced in the transformation equation (4.10). Substitution of the mean values [Eqs. (4.16)] into the action of equation (4.1) obtains

$$S = \int dt\left[\sum_\alpha \pi_\alpha(t)\dot{\phi}_\alpha(t) + \sum_{\alpha\beta}\dot{G}_{\beta\alpha}(t) + N\dot{\theta}(t) - \mathcal{H}\right], \tag{4.18}$$

where

$$\mathcal{H} = \langle\psi,t|\hat{H}|\psi,t\rangle, \tag{4.19}$$

and

$$N = \langle\psi,t|\hat{N}|\psi,t\rangle; \quad \hat{N} = \sum_\alpha \hat{\psi}^\dagger_\alpha\hat{\psi}_\alpha. \tag{4.20}$$

Since N is constant, θ must be time independent, thus allowing the association $\dot{\theta} = 0 \Rightarrow \theta = \text{const.} = \mu$. With this value for θ, we use Eq. (4.18) to write the Hamilton equations of motion

$$\dot{G}_{\alpha\beta}(t) = \frac{\delta(\mathcal{H} - \mu N)}{\delta\Sigma_{\alpha\beta}(t)} \tag{4.21a}$$

$$\dot{\Sigma}_{\alpha\beta}(t) = -\frac{\delta(\mathcal{H} - \mu N)}{\delta G_{\alpha\beta}(t)} \tag{4.21b}$$

$$\dot{\phi}_{\alpha}(t) = \frac{\delta(\mathcal{H} - \mu N)}{\delta\pi_{\alpha}(t)} \tag{4.21c}$$

$$\dot{\pi}_{\alpha}(t) = -\frac{\delta(\mathcal{H} - \mu N)}{\delta\phi_{\alpha}(t)} \tag{4.21d}$$

Thus, it can be seen that (N, θ), (π, ϕ) and (Σ, G) are canonical pairs. Using Eqs. (4.2), (4.16) and (4.20), the expectation value of the grand canonical Hamiltonian is given by

$$\begin{aligned}
\mathcal{H} - \mu N = {} & \sum_{\alpha\beta}(T_{\alpha\beta} - \mu\delta_{\alpha\beta})\left[R_{\alpha\beta}(t) + \psi^*_{\alpha}(t)\psi_{\beta}(t)\right] \\
& + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta;\gamma\delta}\left[D^*_{\alpha\beta}(t)D_{\gamma\delta}(t) - D^*_{\alpha\beta}(t)\psi_{\delta}(t)\psi_{\gamma}(t) + 2R_{\beta\gamma}(t)R_{\alpha\delta}(t)\right. \\
& \left. + 4\psi^*_{\beta}(t)\psi_{\gamma}(t)R_{\alpha\delta}(t) - D_{\gamma\delta}(t)\psi^*_{\alpha}(t)\psi^*_{\beta}(t) + \psi_{\delta}(t)\psi_{\gamma}(t)\psi^*_{\alpha}(t)\psi^*_{\beta}(t)\right] ,
\end{aligned} \tag{4.22}$$

where we have used the particle exchange symmetry property of the potential, $V_{\alpha\beta;\gamma\delta} = V_{\beta\alpha;\gamma\delta} = V_{\alpha\beta;\delta\gamma}$, to combine terms in the substitution of Eq. (4.16d). Equation (4.22) is the general form of the grand canonical Hamiltonian of a system of bosons interacting through an arbitrary potential, V. At this point, we turn to the special case of the static, uniform medium, as the insight garnered from this simplified system will prove useful when discussions of time dependence or nonuniformities arise. Hence, the time dependent description is deferred until the treatment of the random phase approximation, an analysis entailing a small oscillation expansion around a stationary point of the grand canonical Hamiltonian. In addition, nonuniformities such as trapping potentials can, in most cases, be handled with a local density approximation if the system changes "slowly" enough in density such that it may be approximated locally by a uniform profile.

4.2 Static, Uniform Solution

To avoid confusion, we clarify what is meant by the "static" and "uniform" descriptors, as it is necessary to define these properties as concretely as possible to lend clarity to the resulting discussions based on such solutions. In particular, when referring to a static solution, the meaning is in reference to an absence of all collective motion of the assembly as a whole, and in no way should be confused with the microscopic motion of the individual atoms. Thus, the collective momenta should be zero whereas the single particle momentum operators are nonzero in general. Also, uniformity means that the fields fill all of space by imparting a continuous translational symmetry.

4.2.1 Coordinate and Momentum Space Representations

In a static medium all conjugate momenta (Σ, π) will be zero. Due to the simplified form of the single particle kinetic energy operator, it is most convenient to work in the momentum basis, wherein the Gaussian trial wave functional's width assumes a diagonal form

$$G(\mathbf{k}, \mathbf{k}') = G(\mathbf{k})\delta(\mathbf{k} - \mathbf{k}')\,, \tag{4.23}$$

which, by Eqs. (4.17), is seen to give diagonal form for the fluctuations as well,

$$\begin{aligned} R(\mathbf{k}, \mathbf{k}') &= \frac{1}{2}\left[\frac{1}{4}G(\mathbf{k})^{-1} + G(\mathbf{k}) - 1\right]\delta(\mathbf{k} - \mathbf{k}') \\ &= R(\mathbf{k})\delta(\mathbf{k} - \mathbf{k}')\,, \end{aligned} \tag{4.24a}$$

$$\begin{aligned} D(\mathbf{k}, \mathbf{k}') &= \frac{1}{2}\left[\frac{1}{4}G(\mathbf{k})^{-1} - G(\mathbf{k})\right]\delta(\mathbf{k} - \mathbf{k}') \\ &= D(\mathbf{k})\delta(\mathbf{k} - \mathbf{k}')\,. \end{aligned} \tag{4.24b}$$

To understand the momentum-space representation of the uniform field, it is necessary to first notice that in coordinate space, it is simply a constant denoted by $(1/\sqrt{2})\phi$. Consequently, its counterpart is trivially obtained from a Fourier transformation[1],

$$\frac{1}{\sqrt{2}}\phi \xrightarrow{F.T.} \int\limits_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}}\frac{1}{\sqrt{2}}\phi = \frac{1}{\sqrt{2}}\phi\,\delta(\mathbf{k})\,. \tag{4.25}$$

Before arriving at the static, uniform grand canonical Hamiltonian, it is first necessary to find the momentum space matrix elements of the one-body kinetic energy operator, $T_{\alpha\beta}$ as well as the two-body potential, $V_{\alpha\beta;\gamma\delta}$. To this end, we simply transform the known coordinate space matrix elements. First, for the kinetic energy we have

$$\langle\mathbf{x}|T|\mathbf{x}'\rangle = -\delta(\mathbf{x} - \mathbf{x}')\nabla^2_{\mathbf{x}} \tag{4.26}$$

from which the momentum counterpart can be found from the completeness of the basis spanning the space [$\int_{\mathbf{k}} |\mathbf{k}\rangle\langle\mathbf{k}| = 1$],

$$\begin{aligned} \langle\mathbf{k}|T|\mathbf{k}'\rangle &= \int\limits_{\mathbf{x},\mathbf{x}'} \langle\mathbf{k}|\mathbf{x}'\rangle\langle\mathbf{x}'|T|\mathbf{x}\rangle\langle\mathbf{x}|\mathbf{k}'\rangle \\ &= \int\limits_{\mathbf{x},\mathbf{x}'} e^{-i\mathbf{k}\cdot\mathbf{x}'}[-\delta(\mathbf{x} - \mathbf{x}')\nabla^2_{\mathbf{x}}]e^{i\mathbf{k}'\cdot\mathbf{x}} \\ &= k^2\delta(\mathbf{k} - \mathbf{k}')\,, \end{aligned} \tag{4.27}$$

where the definition of the Dirac delta function,

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[1] Recall the convention used in (2.5).

$$\int_{\mathbf{x}} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} = \delta(\mathbf{k}-\mathbf{k}')\,, \tag{4.28}$$

has been used. Recall from (3.18) that a local potential, depending only on the relative coordinate between particles, $\mathbf{x}-\mathbf{x}'$, has the position representation

$$\langle \mathbf{x}\mathbf{x}'|V|\mathbf{x}''\mathbf{x}'''\rangle = \lambda V(\mathbf{x}-\mathbf{x}')\delta(\mathbf{x}-\mathbf{x}'')\delta(\mathbf{x}'-\mathbf{x}''')\,, \tag{4.29}$$

where the strength, λ, has been factored out for notational simplicity later. In momentum space, this matrix element becomes

$$\begin{aligned}\langle \mathbf{k}\mathbf{k}'|V|\mathbf{k}''\mathbf{k}'''\rangle &= \int_{\mathbf{x},\mathbf{x}',\mathbf{x}'',\mathbf{x}'''} \langle \mathbf{k}\mathbf{k}'|\mathbf{x}\mathbf{x}'\rangle\langle \mathbf{x}\mathbf{x}'|V|\mathbf{x}\mathbf{x}'\rangle\langle \mathbf{k}''\mathbf{k}'''|\mathbf{x}''\mathbf{x}'''\rangle \\ &= \lambda\int_{\mathbf{x},\mathbf{x}'} e^{-i\mathbf{k}\cdot\mathbf{x}}e^{i\mathbf{k}'\cdot\mathbf{x}'}V(\mathbf{x}-\mathbf{x}')e^{i\mathbf{k}''\cdot\mathbf{x}}e^{-i\mathbf{k}'''\cdot\mathbf{x}'}\,.\end{aligned} \tag{4.30}$$

With the variable substitutions, $\mathbf{x_1}=\mathbf{x}$ and $\mathbf{x_2}=\mathbf{x}-\mathbf{x}'$, this expression reduces to

$$\begin{aligned}\langle \mathbf{k}\mathbf{k}'|V|\mathbf{k}''\mathbf{k}'''\rangle &= \lambda\int_{\mathbf{x_1}} e^{-i(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')\cdot\mathbf{x_1}}\int_{\mathbf{x_2}} e^{i(\mathbf{k}''-\mathbf{k})\cdot\mathbf{x_2}}V(\mathbf{x_2}) \\ &= \lambda\delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')V(\mathbf{k}-\mathbf{k}'')\,,\end{aligned} \tag{4.31}$$

where $V(\mathbf{k}-\mathbf{k}'')$ is the Fourier transform of $V(\mathbf{x}-\mathbf{x}')$.

As discussed in Section 2.4.2, the separable potential may be written as

$$\langle \mathbf{x}\mathbf{x}'|V|\mathbf{x}''\mathbf{x}'''\rangle = \lambda v(\mathbf{x}-\mathbf{x}')v(\mathbf{x}''-\mathbf{x}''')\delta(\mathbf{x}+\mathbf{x}'-\mathbf{x}''-\mathbf{x}''')\,, \tag{4.32}$$

which in momentum space is

$$\langle \mathbf{k}\mathbf{k}'|V|\mathbf{k}''\mathbf{k}'''\rangle = \lambda\int_{\mathbf{x},\mathbf{x}',\mathbf{x}'',\mathbf{x}'''} e^{-i\mathbf{k}\cdot\mathbf{x}}e^{i\mathbf{k}'\cdot\mathbf{x}'}v(\mathbf{x}-\mathbf{x}')v(\mathbf{x}''-\mathbf{x}''')\delta(\mathbf{x}+\mathbf{x}'-\mathbf{x}''-\mathbf{x}''')e^{i\mathbf{k}''\cdot\mathbf{x}''}e^{-i\mathbf{k}'''\cdot\mathbf{x}'''}\,. \tag{4.33}$$

Defining

$$\begin{aligned}\mathbf{r} &= \mathbf{x}-\mathbf{x}'\,, & \mathbf{r}' &= \mathbf{x}''-\mathbf{x}''' \\ \mathbf{R} &= \frac{1}{2}(\mathbf{x}+\mathbf{x}')\,, & \mathbf{R}' &= \frac{1}{2}(\mathbf{x}''+\mathbf{x}''')\,,\end{aligned} \tag{4.34}$$

the Fourier integral of Eq. (4.33) becomes

$$\langle \mathbf{k}\mathbf{k}'|V|\mathbf{k}''\mathbf{k}'''\rangle = \lambda \int\limits_{\mathbf{r},\mathbf{R},\mathbf{r}',\mathbf{R}'} e^{-i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}/2)}\, e^{i\mathbf{k}'\cdot(\mathbf{R}-\mathbf{r}/2)} v(\mathbf{r})v(\mathbf{r}')$$

$$\times\, \delta(\mathbf{R}-\mathbf{R}')e^{i\mathbf{k}''\cdot(\mathbf{R}'+\mathbf{r}'/2)}\, e^{-i\mathbf{k}'''\cdot(\mathbf{R}'-\mathbf{r}'/2)} \tag{4.35}$$

$$= \lambda\delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')v\left(\frac{\mathbf{k}+\mathbf{k}'}{2}\right)v\left(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\right),$$

where $v(\mathbf{k}/2+\mathbf{k}'/2)$ is the Fourier transform of $v(\mathbf{r})$:

$$v\left(\frac{\mathbf{k}+\mathbf{k}'}{2}\right) = \int\limits_{\mathbf{r}} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}/2}\, v(\mathbf{r})\,. \tag{4.36}$$

Some care must be exercised when using these forms in the grand canonical Hamiltonian (4.22), for the delta function products inside the integrals are limit operations that must be performed in the appropriate order. Therefore, the integral representation of the delta function, given by Eq. (4.28), will be employed in this regard. Consider first the kinetic-plus-constraint piece of the Hamiltonian,

$$\int\limits_{\mathbf{k},\mathbf{k}'}{}' (k^2-\mu)\delta(\mathbf{k}-\mathbf{k}')\left[R(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}')+\frac{1}{2}|\phi|^2\delta(\mathbf{k})\delta(\mathbf{k}')\right], \tag{4.37}$$

where we have used Eqs. (4.23)-(4.25) and (4.27) in the first summation of Eq. (4.22). As the integrand involves a product of the same delta function, Eq. (4.28) is used to express this as

$$\int\limits_{\mathbf{k},\mathbf{k}'}{}' (k^2-\mu)\delta(\mathbf{k}-\mathbf{k}')R(\mathbf{k})\int\limits_{\mathbf{x}} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} - \mu\int\limits_{\mathbf{k},\mathbf{k}'}{}'\int\limits_{\mathbf{x}} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}\frac{1}{2}|\phi|^2\delta(\mathbf{k})\delta(\mathbf{k}')$$

$$= \mathcal{V}\left[\int\limits_{\mathbf{k}}{}' (k^2-\mu)R(\mathbf{k}) - \frac{1}{2}\,\mu\,|\phi|^2\right], \tag{4.38}$$

where $\mathcal{V} = \int\limits_{\mathbf{x}}$ is the volume of the space. Similarly, the interaction terms not involving $R(\mathbf{k},\mathbf{k}')$ are given by

$$\int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \frac{\lambda}{2}\delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')V(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')\Big[D^*(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}')D(\mathbf{k}'')\delta(\mathbf{k}''-\mathbf{k}''')$$
$$- D^*(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}')\,\frac{1}{2}\phi^2\delta(\mathbf{k}'')\delta(\mathbf{k}''') - D(\mathbf{k}'')\delta(\mathbf{k}''-\mathbf{k}''')\,\frac{1}{2}\phi^{*2}\delta(\mathbf{k})\delta(\mathbf{k}')$$
$$+\frac{1}{4}\,|\phi|^4\delta(\mathbf{k})\delta(\mathbf{k}')\delta(\mathbf{k}'')\delta(\mathbf{k}''')\Big]$$
$$= \mathcal{V}\,\frac{\lambda}{2}\Bigg\{\int'_{\mathbf{k},\mathbf{k}'} V(\mathbf{k},\mathbf{k},\mathbf{k}',\mathbf{k}')D^*(\mathbf{k})D(\mathbf{k}') + \frac{1}{4}V(0)|\phi|^4$$
$$- \int'_{\mathbf{k}} V(\mathbf{k},\mathbf{k},0,0)\Big[D^*(\mathbf{k})\frac{1}{2}\phi^2 + D(\mathbf{k})\frac{1}{2}\phi^{*2}\Big]\Bigg\}\,, \quad (4.39)$$

where $V(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')$ represents either the term in (4.31) or the separable form, $v(\mathbf{k}/2+\mathbf{k}'/2)\,v(\mathbf{k}''/2+\mathbf{k}'''/2)$, of Eq. (4.35). In arriving at expression (4.39), use has been made of the symmetry properties of these functions under particle exchange, i.e. $V(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''') = V(\mathbf{k}'',\mathbf{k}''',\mathbf{k},\mathbf{k}')$.

Finally, the terms in the potential involving the pair correlation R are given as

$$\int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')\lambda V(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')\,\big[R(\mathbf{k}')\delta(\mathbf{k}'-\mathbf{k}'')R(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}''')$$
$$+R(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}''')\,|\phi|^2\delta(\mathbf{k}')\delta(\mathbf{k}'')\big]\,. \quad (4.40)$$

At first glance, it does not appear that this integral can be factored in the same way as (4.38). However, making the change of variables $\mathbf{k}' \to -\mathbf{k}', \mathbf{k}''' \to -\mathbf{k}'''$ in Eqs. (4.30)-(4.35) enables (4.40) to be written as

$$\mathcal{V}\frac{\lambda}{2}\Bigg\{\int'_{\mathbf{k},\mathbf{k}'} V(\mathbf{k},\mathbf{k}',\mathbf{k}',\mathbf{k})2R(\mathbf{k})R(\mathbf{k}') + \int'_{\mathbf{k}} V(\mathbf{k},0,0,\mathbf{k})2|\phi|^2R(\mathbf{k})\Bigg\}\,. \quad (4.41)$$

Taking all quantities to be real, substitution of Eqs. (4.38), (4.39) and (4.41) into the grand canonical Hamiltonian obtains

$$-P = \frac{1}{\mathcal{V}}(\mathcal{H}-\mu N)$$
$$= \int'_{\mathbf{k}}(k^2-\mu)R(\mathbf{k}) + \frac{\lambda}{2}\int'_{\mathbf{k},\mathbf{k}'}\big[V(\mathbf{k},\mathbf{k},\mathbf{k}',\mathbf{k}')D(\mathbf{k})D(\mathbf{k}') + 2V(\mathbf{k},\mathbf{k}',\mathbf{k}',\mathbf{k})R(\mathbf{k})R(\mathbf{k}')\big]$$
$$+\frac{\lambda}{2}\phi^2\int'_{\mathbf{k}}\,[2V(\mathbf{k},0,0,\mathbf{k})R(\mathbf{k}) - V(\mathbf{k},\mathbf{k},0,0)D(\mathbf{k})] - \mu\frac{1}{2}\phi^2 + \lambda V(0)\frac{1}{8}\phi^4\,, \quad (4.42)$$

where we have made the association of $(\mathcal{H} - \mu N)/\mathcal{V}$ with the negative of the pressure, P, an identity which follows from the First Law of thermodynamics at zero temperature:

$$dE = -P d\mathcal{V} + \mu dN \,. \tag{4.43}$$

For a uniform system, $dE/d\mathcal{V} = \mathcal{H}/\mathcal{V}$ and $dN/d\mathcal{V} = N/\mathcal{V} = \rho$, thus giving the required pressure relationship used in Eq. (4.42). Lastly, the uniform number density, ρ, is given by a sum of the respective pair and condensate components, $\int R(\mathbf{k})$ and $\phi^2/2$:

$$\rho = \langle \psi, t | \hat{\psi}^\dagger \hat{\psi} | \psi, t \rangle = \int_{\mathbf{k}}^{\prime} R(\mathbf{k}) + \frac{1}{2}\phi^2 \,. \tag{4.44}$$

Given a $G(\mathbf{k})$ and a ϕ, Eqs. (4.24), (4.42) and (4.44) are sufficient to completely describe the uniform, static system. Obtaining this solution requires stationarizing Eq. (4.42) with respect to these variable parameters.

4.2.2 Stationary Points

In order to find $G(\mathbf{k})$ and ϕ, we seek the solution that minimizes Eq. (4.42) in both $G(\mathbf{k})$ and ϕ. A necessary, but not sufficient, condition for the minimum is that the first variation vanish, whereas a true minimum would only be assured with a second-order analysis. Thus, the procedure here will be referred to simply as an "stationarization" of the grand canonical energy density, a quantity equivalent to the negative of the pressure. Due to the implicit dependence of the pressure on $G(\mathbf{k})$, the variations of the fluctuations, $R(\mathbf{k})$ and $D(\mathbf{k})$, must first be calculated using their definitions in Eqs. (4.24a) and (4.24b), respectively[1],

$$\frac{\delta R(\mathbf{k})}{\delta G(\mathbf{k}')} = \frac{1}{2}\left[1 - \frac{1}{4}G(\mathbf{k})^{-2}\right]\delta(\mathbf{k} - \mathbf{k}') \,, \tag{4.45a}$$

$$\frac{\delta D(\mathbf{k})}{\delta G(\mathbf{k}')} = -\frac{1}{2}\left[1 + \frac{1}{4}G(\mathbf{k})^{-2}\right]\delta(\mathbf{k} - \mathbf{k}') \,. \tag{4.45b}$$

Using Eqs. (4.45) in extremizing the pressure, we obtain, after some algebraic manipulation,

$$\frac{\delta P}{\delta G(\mathbf{k})} = 0 \Rightarrow G(\mathbf{k}) = \frac{1}{2}\sqrt{\frac{k^2 + \gamma(\mathbf{k})^2 + \xi(\mathbf{k})}{k^2 + \gamma(\mathbf{k})^2 - \xi(\mathbf{k})}} \,, \tag{4.46a}$$

$$\frac{\delta P}{\delta \phi} = 0 \Rightarrow \phi \left\{ \lambda \int_{\mathbf{k}}^{\prime} \left[2V(\mathbf{k},0,0,\mathbf{k})R(\mathbf{k}) - V(\mathbf{k},\mathbf{k},0,0)D(\mathbf{k})\right] - \mu + \frac{1}{2}\lambda V(0)\phi^2 \right\} \,, \tag{4.46b}$$

where we have defined

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[1] Note that the delta functions arise due to the variations, hence should not be confused with those due to the diagonal forms of R and D.

$$\gamma(\mathbf{k})^2 = -\mu + 2\lambda \int_{\mathbf{k}'}' V(\mathbf{k}, \mathbf{k}', \mathbf{k}', \mathbf{k}) R(\mathbf{k}') + \lambda \phi^2 V(\mathbf{k}, 0, 0, \mathbf{k})\,, \tag{4.47a}$$

$$\xi(\mathbf{k}) = \lambda \int_{\mathbf{k}'}' V(\mathbf{k}, \mathbf{k}, \mathbf{k}', \mathbf{k}') D(\mathbf{k}') - \frac{\lambda}{2} \phi^2 V(\mathbf{k}, \mathbf{k}, 0, 0)\,. \tag{4.47b}$$

Note that since $G(\mathbf{k})$ must always be real, we must have $\gamma(\mathbf{k})^2 \geq \xi(\mathbf{k})$ [see Eq. (4.46a)], which implies that an attractive, zero-range potential leads to a negative chemical potential, as can be seen from the definition of γ^2 in Eq. (4.47a) and the fact that $\lambda \to 0^-$ in this limit. Given some potential V, the self-consistent solution of Eqs. (4.46) and (4.47), subject to the constraint (4.44), completely specify the state of the static, uniform system. Time dependence as well as density nonuniformities can be described by expanding all quantities around their stationary values in the small oscillation regime.

4.3 Small Oscillations: Generalized Random Phase Approximation (RPA)

4.3.1 General Expansion

To find the RPA equations of small oscillation, we expand all stationary quantities around their equilibrium values,

$$G(\mathbf{k}, \mathbf{k}', t) = G(\mathbf{k}) \delta(\mathbf{k} - \mathbf{k}') + \delta G(\mathbf{k}, \mathbf{k}', t) \tag{4.48a}$$

$$\Sigma(\mathbf{k}, \mathbf{k}', t) = \delta \Sigma(\mathbf{k}, \mathbf{k}', t) \tag{4.48b}$$

$$\phi(\mathbf{k}, t) = \phi \delta(\mathbf{k}) + \delta \phi(\mathbf{k}, t) \tag{4.48c}$$

$$\pi(\mathbf{k}, t) = \delta \pi(\mathbf{k}, t)\,. \tag{4.48d}$$

It will prove convenient to define new coordinates such that

$$\mathbf{P} = \mathbf{k} - \mathbf{k}' \tag{4.49a}$$

$$\mathbf{q} = \frac{1}{2} \left(\mathbf{k} + \mathbf{k}' \right)\,, \tag{4.49b}$$

where $\mathbf{P}$ and $\mathbf{q}$ are interpreted as the respective total and relative momenta of a pair of quasi-particles. To illustrate the relationship between the variations when transformed to these new coordinates, consider the expression for the inverse of $G(\mathbf{k}, \mathbf{k}', t)$, which is, to second order in δG,

$$G^{-1}(\mathbf{k}, \mathbf{k}', t) = G(\mathbf{k})^{-1} \delta(\mathbf{k} - \mathbf{k}') + \delta G^{-1}(\mathbf{k}, \mathbf{k}', t) + \frac{1}{2} \delta G^{-2}(\mathbf{k}, \mathbf{k}', t)\,. \tag{4.50}$$

By using the identity $\int_{\mathbf{k}''}' G(\mathbf{k},\mathbf{k}'',t)G^{-1}(\mathbf{k}'',\mathbf{k}',t) = \delta(\mathbf{k}-\mathbf{k}')$, it follows that

$$\delta G^{-1}(\mathbf{k},\mathbf{k}',t) = -G(\mathbf{k})^{-1}\delta G(\mathbf{k},\mathbf{k}',t)G(\mathbf{k}')^{-1} \tag{4.51a}$$

$$\delta G^{-2}(\mathbf{k},\mathbf{k}',t) = 2G(\mathbf{k})^{-1}\int_{\mathbf{k}''}' \delta G(\mathbf{k},\mathbf{k}'',t)G(\mathbf{k}'')^{-1}\delta G(\mathbf{k}'',\mathbf{k}',t)G(\mathbf{k}')^{-1}\,. \tag{4.51b}$$

Constructing inner products requires the Hermitian conjugation operation: $\delta G(\mathbf{k},\mathbf{k}',t)^\dagger = \delta G^*(\mathbf{k}',\mathbf{k},t)$. In promoting all quantities to the new variables $(\mathbf{P},\mathbf{q})$, it is seen that

$$\delta G(\mathbf{k},\mathbf{k}',t) \to \delta G(\mathbf{q},\mathbf{P},t) \Leftrightarrow \delta G^*(\mathbf{k}',\mathbf{k},t) \to \delta G^*(\mathbf{q},-\mathbf{P},t)\,, \tag{4.52}$$

which, by the definition of $\mathbf{P}$ given in Eq. (4.49a), follows from the interchange of $\mathbf{k}$ and $\mathbf{k}'$.

To employ the RPA, the mean grand canonical Hamiltonian, $K = \langle \hat{H} - \mu\hat{N}\rangle$, must be expanded to second order in the small deviations of Eqs. (4.48),

$$K = K^{(0)} + \delta K\delta\mathcal{P} + \frac{1}{2}\delta\mathcal{P}^\dagger\,\mathfrak{A}\,\delta\mathcal{P} + \frac{1}{2}\delta\mathcal{Q}^\dagger\,\mathfrak{B}\,\delta\mathcal{Q}\,, \tag{4.53}$$

where the vectors $\delta\mathcal{Q}$ and its canonical conjugate $\delta\mathcal{P}$ are given as

$$\begin{aligned}\delta\mathcal{Q}^\dagger(\mathbf{q},\mathbf{P},t) &= [\delta\Sigma(\mathbf{q},-\mathbf{P},t)\,,\delta\pi(-\mathbf{P},t)]\\ \delta\mathcal{P}^\dagger(\mathbf{q},\mathbf{P},t) &= [\delta G(\mathbf{q},-\mathbf{P},t)\,,\delta\phi(-\mathbf{P},t)]\,.\end{aligned} \tag{4.54}$$

In expression (4.53), the zero-order constant term, $K^{(0)}$, is the static, uniform piece that can be dropped as it merely represents a constant energy shift, having no effect on any ensuing dynamics. Also, the first variation, δK, is zero at the stationary points given by (4.46), thus leaving a quadratic Hamiltonian in $\delta\mathcal{Q}$ and $\delta\mathcal{P}$. As the second derivatives with respect to these vectors, $\mathfrak{A}$ and $\mathfrak{B}$ can be seen as the "spring" and "mass" matrices of the theory from which the spectrum of the product $\mathfrak{A}\cdot\mathfrak{B}$ determines the quasi-particle excitations of the system.

Deriving the $\mathfrak{A}$ and $\mathfrak{B}$ matrices requires an expansion of K to second order in the variations given in Eqs. (4.48). For the case of the separable potential of (4.35), this expansion has been carried out explicitly in Appendix A. The quadratic RPA Hamiltonian is

$$K_{RPA}(\mathbf{P},t) = \frac{1}{2}\delta\mathcal{P}^\dagger(\mathbf{q},\mathbf{P},t)\,\mathfrak{A}(\mathbf{q},\mathbf{q}',\mathbf{P})\delta\mathcal{P}(\mathbf{q}',\mathbf{P},t) + \frac{1}{2}\delta\mathcal{Q}^\dagger(\mathbf{q},\mathbf{P},t)\mathfrak{B}(\mathbf{q},\mathbf{q}',\mathbf{P})\delta\mathcal{Q}(\mathbf{q}',\mathbf{P},t)\,, \tag{4.55}$$

where the integrations over $\mathbf{q}$ and $\mathbf{q}'$ are understood. Also, the $\mathfrak{A}$ and $\mathfrak{B}$ matrices can be written as

$$\mathfrak{A}(\mathbf{q},\mathbf{q}',\mathbf{P}) = \begin{bmatrix} S_K(\mathbf{q},\mathbf{q}',\mathbf{P}) + s_K(\mathbf{q},\mathbf{P})\delta(\mathbf{q}-\mathbf{q}') & c_K(\mathbf{q},\mathbf{P}) \\ c_K(\mathbf{q}',\mathbf{P}) & A(\mathbf{P}) \end{bmatrix} \tag{4.56a}$$

$$\mathfrak{B}(\mathbf{q},\mathbf{q}',\mathbf{P}) = \begin{bmatrix} S_M(\mathbf{q},\mathbf{q}',\mathbf{P}) + s_M(\mathbf{q},\mathbf{P})\delta(\mathbf{q}-\mathbf{q}') & c_M(\mathbf{q},\mathbf{P}) \\ c_M(\mathbf{q}',\mathbf{P}) & B(\mathbf{P}) \end{bmatrix}\,. \tag{4.56b}$$

where the elements can be found in Sec. A.4.

4.3.2 Quasi-Boson Interpretation

As seen from (4.56), it is natural to separate the diagonal or noninteracting part of K_{RPA} from the off-diagonal piece so that

$$K_{RPA} = K_0 + K_{int}\,, \tag{4.57}$$

with

$$K_0 = \frac{1}{2}\begin{pmatrix}\delta\Sigma^* & \delta\pi^*\end{pmatrix}\begin{pmatrix}s_K & 0\\ 0 & A\end{pmatrix}\begin{pmatrix}\delta\Sigma\\ \delta\pi\end{pmatrix} + \frac{1}{2}\begin{pmatrix}\delta G^* & \delta\phi^*\end{pmatrix}\begin{pmatrix}s_M & 0\\ 0 & B\end{pmatrix}\begin{pmatrix}\delta G\\ \delta\phi\end{pmatrix} \tag{4.58a}$$

$$K_{int} = \frac{1}{2}\begin{pmatrix}\delta\Sigma^* & \delta\pi^*\end{pmatrix}\begin{pmatrix}S_K & c_K\\ c_K & 0\end{pmatrix}\begin{pmatrix}\delta\Sigma\\ \delta\pi\end{pmatrix} + \frac{1}{2}\begin{pmatrix}\delta G^* & \delta\phi^*\end{pmatrix}\begin{pmatrix}S_M & c_M\\ c_M & 0\end{pmatrix}\begin{pmatrix}\delta G\\ \delta\phi\end{pmatrix}\,. \tag{4.58b}$$

Much insight may be gleaned by first considering the noninteracting case involving only K_0. Introducing the multiplicative canonical transformation

$$\begin{aligned}\begin{pmatrix}\delta\Sigma\\ \delta\pi\end{pmatrix} &\to \begin{pmatrix}\delta\Sigma\\ \delta\pi\end{pmatrix}' = \begin{pmatrix}\delta\Sigma\sqrt{s_M}\\ \delta\pi\sqrt{B}\end{pmatrix}\\ \begin{pmatrix}\delta G\\ \delta\phi\end{pmatrix} &\to \begin{pmatrix}\delta G\\ \delta\phi\end{pmatrix}' = \begin{pmatrix}\frac{\delta G}{\sqrt{s_M}}\\ \frac{\delta\phi}{\sqrt{B}}\end{pmatrix}\,,\end{aligned} \tag{4.59}$$

results in

$$K_0 = \frac{1}{2}\begin{pmatrix}\delta\Sigma^* & \delta\pi^*\end{pmatrix}'\begin{pmatrix}\Omega_2^2 & 0\\ 0 & \omega^2\end{pmatrix}\begin{pmatrix}\delta\Sigma\\ \delta\pi\end{pmatrix}' + \frac{1}{2}\begin{pmatrix}\delta G^* & \delta\phi^*\end{pmatrix}'\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\delta G\\ \delta\phi\end{pmatrix}'\,, \tag{4.60}$$

where

$$\omega(\mathbf{P}) = \sqrt{A(\mathbf{P})B(\mathbf{P})} \tag{4.61a}$$

$$\Omega_2(\mathbf{q},\mathbf{P}) = \sqrt{s_K(\mathbf{q},\mathbf{P})\,s_M(\mathbf{q},\mathbf{P})}\,. \tag{4.61b}$$

As given by Eqs. (A.38a) and (A.44a) of the appendix, we have

$$s_K(\mathbf{q},\mathbf{P}) = \frac{1}{8}G_+^{-2}G_-^{-1}(q_+^2+\gamma_+^2-\xi_+) + \frac{1}{8}G_-^{-2}G_+^{-1}(q_-^2+\gamma_-^2-\xi_-) \tag{4.62a}$$

$$s_M(\mathbf{q},\mathbf{P}) = 2(q_+^2+\gamma_+^2-\xi_+)G_- + 2(q_-^2+\gamma_-^2-\xi_-)G_+\,, \tag{4.62b}$$

with γ^2 and ξ given by Eqs. (4.47), whereas the ± subscripts are defined by the coordinate shifts of $\pm\mathbf{P}/2$ as $f_\pm = f(\mathbf{q}\pm\mathbf{P}/2)$. To simplify these expressions, we use Eq. (4.46a) to write the explicit definition of $G_\pm^{-1}$,

$$G_\pm^{-1} = 2\sqrt{\frac{q_\pm^2+\gamma_\pm^2+\xi_\pm}{q_\pm^2+\gamma_\pm^2-\xi_\pm}}\,. \tag{4.63}$$

Substitution of Eqs. (4.62) into (4.61b), then using the result of (4.63) obtains

$$
\begin{aligned}
\sqrt{s_K s_M} &= \left[(q_+^2+\gamma_+^2)^2 - \xi_+^2 + 2\sqrt{(q_+^2+\gamma_+^2)^2 - \xi_+^2}\sqrt{(q_-^2+\gamma_-^2)^2 - \xi_-^2} + (q_-^2+\gamma_-^2)^2 - \xi_-^2\right]^{1/2} \\
&= \sqrt{(q_+^2+\gamma_+^2)^2 - \xi_+^2} + \sqrt{(q_-^2+\gamma_-^2)^2 - \xi_-^2} \\
&= \sqrt{A_+B_+} + \sqrt{A_-B_-}\,,
\end{aligned}
\tag{4.64}
$$

with the last line following from (A.40) and (A.46) of Appendix A. Finally, we have the result

$$
\Omega_2(\mathbf{q},\mathbf{P}) = \omega(\mathbf{k}) + \omega(\mathbf{k}')\,, \tag{4.65}
$$

thereby leading to the interpretation of $\omega(\mathbf{P})$ and $\Omega_2(\mathbf{q},\mathbf{P})$ as the one and two free quasi-boson energies, respectively. Extending this observation to the general interacting case of the full RPA Hamiltonian, it can be seen that the oscillations of the $\delta\phi, \delta\pi$ pair are the quasi-boson modes whereas the $\delta G, \delta\Sigma$ oscillations comprise an interacting pair of these same quasi-bosons.

4.3.3 Equations of Motion and Stability

Using Eqs. (4.21), the equations of motion for K_{RPA} can be written in matrix form as

$$
\begin{aligned}
\delta\dot{\mathcal{P}} &= \mathfrak{B}\,\delta\mathcal{Q} \\
\delta\dot{\mathcal{Q}} &= -\mathfrak{A}\,\delta\mathcal{P}\,,
\end{aligned}
\tag{4.66}
$$

which can be cast as second order equations

$$
\delta\ddot{\mathcal{P}} = -\mathfrak{B}\mathfrak{A}\,\delta\mathcal{P} \tag{4.67a}
$$

$$
\delta\ddot{\mathcal{Q}} = -\mathfrak{A}\mathfrak{B}\,\delta\mathcal{Q}\,, \tag{4.67b}
$$

Defining

$$
\begin{aligned}
\mathfrak{S}_K(\mathbf{q},\mathbf{q}',\mathbf{P}) &= S_K(\mathbf{q},\mathbf{q}',\mathbf{P}) + s_K(\mathbf{q},\mathbf{P})\delta(\mathbf{q}-\mathbf{q}') \\
\mathfrak{S}_M(\mathbf{q},\mathbf{q}',\mathbf{P}) &= S_M(\mathbf{q},\mathbf{q}',\mathbf{P}) + s_M(\mathbf{q},\mathbf{P})\delta(\mathbf{q}-\mathbf{q}')\,,
\end{aligned}
\tag{4.68}
$$

we can use the definitions of $\mathfrak{A}$ and $\mathfrak{B}$ given in (4.56) to express (4.67b) explicitly as

$$
\begin{aligned}
\delta\ddot{G}(\mathbf{q},\mathbf{P},t) &+ \int'_{\mathbf{q}',\mathbf{q}''} \mathfrak{S}_K(\mathbf{q},\mathbf{q}',\mathbf{P})\mathfrak{S}_M(\mathbf{q}',\mathbf{q}'',\mathbf{P})\delta G(\mathbf{q}'',\mathbf{P},t) + c_K(\mathbf{q},\mathbf{P})\int_{\mathbf{q}'} c_M(\mathbf{q}',\mathbf{P})\delta G(\mathbf{q}',\mathbf{P},t) \\
&= -\left[B(\mathbf{P})c_K(\mathbf{q},\mathbf{P}) + \int'_{\mathbf{q}'} \mathfrak{S}_K(\mathbf{q},\mathbf{q}',\mathbf{P})c_M(\mathbf{q}',\mathbf{P})\right]\delta\phi(\mathbf{P},t)
\end{aligned}
\tag{4.69}
$$

$$
\begin{aligned}
&\delta\ddot{\phi}(\mathbf{P},t) + \left[A(\mathbf{P})B(\mathbf{P}) + \int'_{\mathbf{q}'} c_K(\mathbf{q}',\mathbf{P})c_M(\mathbf{q}',\mathbf{P})\right]\delta\phi(\mathbf{P},t) \\
&\qquad = -A(\mathbf{P})\int'_{\mathbf{q}'} c_M(\mathbf{q}',\mathbf{P})\delta G(\mathbf{q}',\mathbf{P},t) - \int'_{\mathbf{q}',\mathbf{q}''} c_K(\mathbf{q}',\mathbf{P})\mathfrak{S}_M(\mathbf{q}',\mathbf{q}'',\mathbf{P})\delta G(\mathbf{q}'',\mathbf{P},t)\,.
\end{aligned}
\tag{4.70}
$$

Looking for oscillatory, time-dependent solutions of the form

$$\delta G(\mathbf{q},\mathbf{P},t) = \delta G(\mathbf{q},\mathbf{P})e^{i\Omega t} \tag{4.71a}$$

$$\delta\Sigma(\mathbf{q},\mathbf{P},t) = \delta\Sigma(\mathbf{q},\mathbf{P})e^{i\Omega t} \tag{4.71b}$$

$$\delta\pi(\mathbf{P},t) = \delta\pi(\mathbf{P})e^{i\Omega t} \tag{4.71c}$$

$$\delta\phi(\mathbf{P},t) = \delta\phi(\mathbf{P})e^{i\Omega t}\,, \tag{4.71d}$$

equations (4.69) and (4.70) may be written compactly as

$$\left(\Omega^2 - h_2\right)\delta G = \left(c_K B + \int \mathfrak{S}_K c_M\right)\delta\phi \tag{4.72a}$$

$$\left(\Omega^2 - h_1\right)\delta\phi = \left(A\int c_M + \int c_K\mathfrak{S}_M\right)\delta G\,, \tag{4.72b}$$

where we have defined

$$h_1(\mathbf{P}) = A(\mathbf{P})B(\mathbf{P}) + \int'_{\mathbf{q}'} c_K(\mathbf{q}',\mathbf{P})c_M(\mathbf{q}',\mathbf{P}) \tag{4.73a}$$

$$h_2(\mathbf{q},\mathbf{q}',\mathbf{P}) = \int'_{\mathbf{q}''} \mathfrak{S}_K(\mathbf{q},\mathbf{q}'',\mathbf{P})\mathfrak{S}_M(\mathbf{q}'',\mathbf{q}',\mathbf{P}) + c_K(\mathbf{q},\mathbf{P})c_M(\mathbf{q}',\mathbf{P})\,. \tag{4.73b}$$

Alternatively, h_1 and h_2 may be expressed in terms of the free quasi-boson energies defined in (4.61),

$$h_1(\mathbf{P}) = \omega(\mathbf{P})^2 + \int'_{\mathbf{q}} c_K(\mathbf{q},\mathbf{P})c_M(\mathbf{q},\mathbf{P}) \tag{4.74a}$$

$$
\begin{aligned}
h_2(\mathbf{q},\mathbf{q}',\mathbf{P}) = \Omega_2^2(\mathbf{q},\mathbf{q}',\mathbf{P}) &+ \int'_{\mathbf{q}''} S_K(\mathbf{q},\mathbf{q}'',\mathbf{P})S_M(\mathbf{q}'',\mathbf{q}',\mathbf{P}) \\
&+ s_K(\mathbf{q},\mathbf{P})S_M(\mathbf{q},\mathbf{q}',\mathbf{P}) + S_K(\mathbf{q},\mathbf{q}',\mathbf{P})s_M(\mathbf{q}',\mathbf{P})\,.
\end{aligned}
\tag{4.74b}
$$

Elimination of $\delta\phi$ from Eqs. (4.72) obtains a single equation for the mode frequencies, Ω,

$$
\begin{aligned}
\int'_{\mathbf{q}'}\Bigg\{&\left[\Omega^2\delta(\mathbf{q}-\mathbf{q}') - h_2(\mathbf{q},\mathbf{q}',\mathbf{P})\right] - \left[c_K(\mathbf{q},\mathbf{P})B(\mathbf{P}) + \int'_{\mathbf{q}''}\mathfrak{S}_K(\mathbf{q},\mathbf{q}'',\mathbf{P})c_M(\mathbf{q}'',\mathbf{P})\right] \\
&\times\frac{1}{\Omega^2 - h_1(\mathbf{P})}\left[A(\mathbf{P})c_M(\mathbf{q}',\mathbf{P}) + \int'_{\mathbf{q}''} c_K(\mathbf{q}'',\mathbf{P})\mathfrak{S}_M(\mathbf{q}'',\mathbf{q}',\mathbf{P})\right]\Bigg\}\delta G(\mathbf{q}',\mathbf{P}) = 0\,.
\end{aligned}
\tag{4.75}
$$

Thus, it can be seen that the eigenvalue spectrum of the operator product $\mathfrak{A}\cdot\mathfrak{B}$ is found from the values of Ω^2 for which the operator between the curly braces has no inverse. In general, this spectrum will consist of discrete values, or elements of the point spectrum, and continuous values which are elements of the continuous spectrum. From the continuous phase symmetry exhibited by the Hamiltonian, we expect to always find a zero (Goldstone) mode at zero total momentum ($\mathbf{P} = 0$). Finally, by the time dependence in Eqs. (4.71), it follows that $\Omega^2 \leq 0$ results in instability of the system.

4.4 Order Parameters and the Gross-Pitaevskii Equation

For comparative purposes, it is helpful to describe the more conventional formalism commonly used in treating bosonic systems. This standard approach has at its root the fact that at zero temperature, bosons are highly degenerate as they are capable of occupying the same quantum state. When all particles are in the ground state, the system is called a Bose-Einstein condensate which can be viewed as a macroscopic quantum state. As such, this collective must be associated with a mean field or order parameter which is a measure of the ground state occupation. Explicitly, the mean field, ϕ, can be defined as the expectation value of the field operator, $\hat{\psi}$:

$$\langle \hat{\psi}(\mathbf{x},t)\rangle = \phi(\mathbf{x},t)\,. \tag{4.76}$$

This identification of the mean field suggests a decomposition of the field operator in terms of the macroscopically populated mean field, plus a fluctuation operator, $\delta\hat{\phi}'(\mathbf{x})$:

$$\hat{\psi}(\mathbf{x},t) = \phi(\mathbf{x},t) + \delta\hat{\phi}'(\mathbf{x})\,. \tag{4.77}$$

Given by the mean field, the ground state can be associated with a "vacuum" that has an indefinite number of particles. This association will become more apparent in the discussion of creation and annihilation operators for the Gaussian trial functional. As seen in Sec. 3.3, the number density at location $\mathbf{x}$ is $\rho = \langle\hat{\psi}(\mathbf{x})^\dagger\hat{\psi}(\mathbf{x})\rangle$, where the generalization is given by the density matrix,

$$\rho(\mathbf{x},\mathbf{y}) = \langle\hat{\psi}(\mathbf{x})^\dagger\hat{\psi}(\mathbf{y})\rangle\,. \tag{4.78}$$

If almost all particles are in the condensate, then the density is dominated by the mean field, $\rho(\mathbf{x}) = |\phi(\mathbf{x})|^2$. As it governs the evolution of the mean field, the Gross-Pitaevskii equation or the non-linear Schrödinger equation (NLSE) can be developed through the Heisenberg time dependence of the field operator. By the results of Sec. 3.3, the Hamiltonian is most conveniently expressed in terms of the field operators. Taking a general two-body interaction potential $V(\mathbf{x},\mathbf{y})$, we have

$$\hat{H} = \int\limits_{\mathbf{x}} \hat{\psi}(\mathbf{x})^\dagger\, h(\mathbf{x})\,\hat{\psi}(\mathbf{x}) + \frac{1}{2}\int\limits_{\mathbf{x}\mathbf{y}} \hat{\psi}(\mathbf{x})^\dagger\,\hat{\psi}(\mathbf{y})^\dagger\,V(\mathbf{x},\mathbf{y})\,\hat{\psi}(\mathbf{y})\,\hat{\psi}(\mathbf{x})\,. \tag{4.79}$$

Here, $h(\mathbf{x})$ represents all one-body operators, including the kinetic energy, $-\nabla^2$, and any external trapping potential, $U(\mathbf{x})$. In the low temperature regime, the interactions are completely described by the low-energy s-waves, which can be modeled as elastic hard sphere collisions. Hence, it is believed that the interaction potential is well-approximated by the delta function form of Eq. (2.106)[1]:

$$V(\mathbf{x},\mathbf{y}) = 8\pi a\,\delta(\mathbf{x}-\mathbf{y})\,. \tag{4.80}$$

By approximating V in this way, it is evident that the Gross-Pitaevskii equation should only give valid results at low density, in which the interparticle separation is much larger than the range of the potential. In this model, attractive or repulsive interactions are determined from the sign of the scattering length, but by the discussion of Sec. 2.4, this association is not always true.

Inserting (4.80) into (4.79) results in the effective Hamiltonian

$$\hat{H} = \int\limits_{\mathbf{x}} \hat{\psi}(\mathbf{x})^\dagger\, h(\mathbf{x})\,\hat{\psi}(\mathbf{x}) + 4\pi a \int\limits_{\mathbf{x}\,\mathbf{y}} \hat{\psi}(\mathbf{x})^\dagger\,\hat{\psi}(\mathbf{y})^\dagger\,\delta(\mathbf{x}-\mathbf{y})\,\hat{\psi}(\mathbf{y})\,\hat{\psi}(\mathbf{x})\,, \tag{4.81}$$

which is repeatedly used in most contemporary many-body treatments of condensate physics. Using the commutators of Eqs. (3.33), the time evolution of the field operator is found from the Heisenberg equation of motion,

$$\begin{aligned} i\hbar\,\partial_t\hat{\psi}(\mathbf{x}',t) &= \left[\hat{\psi}(\mathbf{x}',t),\hat{H}\right] \\ &= \hat{\psi}(\mathbf{x}',t)\,\hat{H} - \int\limits_{\mathbf{x}} \hat{\psi}(\mathbf{x},t)^\dagger\,h(\mathbf{x})\,\hat{\psi}(\mathbf{x},t)\,\hat{\psi}(\mathbf{x}',t) \\ &\qquad - 4\pi a \int\limits_{\mathbf{x}} \hat{\psi}(\mathbf{x},t)^\dagger\,\hat{\psi}(\mathbf{x},t)^\dagger\,\hat{\psi}(\mathbf{x},t)\,\hat{\psi}(\mathbf{x}',t) \\ &= h(\mathbf{x}')\,\hat{\psi}(\mathbf{x}',t) + 8\pi a\,\hat{\psi}(\mathbf{x}',t)^\dagger\,\hat{\psi}(\mathbf{x}',t)\,\hat{\psi}(\mathbf{x}',t)\,. \end{aligned} \tag{4.82}$$

Substituting the decomposition (4.77) into this expression, then ignoring all terms involving quantum fluctuations, results in the time dependent Gross-Pitaevskii equation for the order parameter $\phi(\mathbf{x},t)$:

$$i\hbar\,\frac{\partial\phi}{\partial t} = \left[-\nabla^2_{\mathbf{x}} + U(\mathbf{x}) + 8\pi a\,|\phi|^2\right]\phi\,, \tag{4.83}$$

where $h(\mathbf{x})$ is explicitly written as $-\nabla^2 + U(\mathbf{x})$. This equation is also called the non-linear Schrödinger equation, with the nonlinearity arising from the interparticle interactions.

Neglecting the terms involving the fluctuation operator amounts to ignoring the quantum depletion. Put another way, the correlated but non-condensed atom pairs are not included in this description. Taking the order parameter to be stationary in energy, its time dependence is given by $e^{-i\mu t/\hbar}$, thus leading to the time independent Gross-Pitaevskii equation:

$$\mu\,\phi = \left[-\nabla^2_{\mathbf{x}} + V_{ext}(\mathbf{x}) + 8\pi a\,|\phi|^2\right]\phi\,. \tag{4.84}$$

Given $N_0 = \int\limits_{\mathbf{x}} \phi^*\phi$ particles in the condensate, we multiply (4.84) by ϕ^* then integrate over the volume, resulting in

---

[1] We remind the reader that energy is expressed on the scale of $\hbar^2/(2m)$

$$\mu N_0 = \langle \hat{H} \rangle_{N_0} \,. \tag{4.85}$$

Thus $\delta \langle \hat{H} \rangle / \delta N = \mu$, and we see that the phase of the order parameter is equal to the chemical potential of the particles in the system[1].

Another definition of the order parameter arises from the single particle ground state wave function, $\varphi_0(\mathbf{x}, t)$, or the quantum state in which all particles coalesce. Apart from its normalization to the total number of particles, N_0, the order parameter, $\phi(\mathbf{x}, t)$, can be identified as

$$\phi(\mathbf{x}, t) = \sqrt{N_0}\varphi_0(\mathbf{x}, t) \,. \tag{4.86}$$

This definition of the mean field provides an alternate route to the Gross-Pitaevskii equation. Consider the N-particle ground state, $\Psi_N(\mathbf{x}_1, \dots \mathbf{x}_N, t)$, constructed as a product of single particle wave functions

$$\Psi_N(\mathbf{x}_1, \dots \mathbf{x}_N, t) = \prod_{i=1}^{N} \varphi_0(\mathbf{x_i}, t) \,. \tag{4.87}$$

Using this ansatz, the expectation value of the energy is calculated with the Hamiltonian of (4.79). When calculating the mean, it is more convenient to express each contribution as a sum. The one-body terms are calculated as

$$\begin{aligned} \langle \hat{\psi}^\dagger \, h \, \hat{\psi} \rangle &= \int\limits_{\mathbf{x}_1} \dots \int\limits_{\mathbf{x}_N} \prod_{i=1}^{N} \varphi_0(\mathbf{x_i})^* \sum_{k\,\ell} \delta_{k\,\ell} \, \hat{\psi}(\mathbf{x}_k)^\dagger \, h(\mathbf{x}_k, \mathbf{x}_\ell) \, \hat{\psi}(\mathbf{x}_\ell) \prod_{j=1}^{N} \varphi_0(\mathbf{x}_j) \\ &= \sum_{k\,\ell} \delta_{k\,\ell} \int\limits_{\mathbf{x}_1} \dots \int\limits_{\mathbf{x}_N} \prod_{i=1}^{N} \varphi_0(\mathbf{x_i})^* \, h(\mathbf{x}_k, \mathbf{x}_\ell) \, \hat{\psi}(\mathbf{x}_k)^\dagger \, \hat{\psi}(\mathbf{x}_\ell) \prod_{j=1}^{N} \varphi_0(\mathbf{x}_j) \,, \end{aligned} \tag{4.88}$$

where the explicit time dependence has been dropped for convenience. The action of the number operator, $\hat{\psi}(\mathbf{x}_k)^\dagger \, \hat{\psi}(\mathbf{x}_\ell)$, gives the number ($= 1$) in the state at $\mathbf{x}_k = \mathbf{x}_\ell$, resulting in the sum

$$\langle \hat{\psi}^\dagger \, h \, \hat{\psi} \rangle = \sum_{i=1}^{N} \int\limits_{\mathbf{x}_i} \varphi_0^*(\mathbf{x}_i) \, h(\mathbf{x}_i, \mathbf{x}_i) \varphi_0(\mathbf{x}_i) \prod_{j \neq i}^{N} \int\limits_{\mathbf{x}_j} |\varphi_0(\mathbf{x}_j)|^2 \,. \tag{4.89}$$

Since the single-particle states are normalized to unity, this reduces to

$$\begin{aligned} \langle \hat{\psi}^\dagger \, h \, \hat{\psi} \rangle &= N \int\limits_{\mathbf{x}} \varphi_0^*(\mathbf{x}) \, h(\mathbf{x}) \, \varphi_0(\mathbf{x}) \\ &= N \int\limits_{\mathbf{x}} \Big\{ |\nabla_{\mathbf{x}} \, \varphi_0(\mathbf{x})|^2 + U(\mathbf{x}) |\varphi_0(\mathbf{x})|^2 \Big\} \,. \end{aligned} \tag{4.90}$$

---

[1] This identification follows from the statistical mechanics definition of the chemical potential as $\delta \langle \hat{H} \rangle / \delta N$.

For the two-body term we have

$$
\begin{aligned}
\langle \hat\psi^\dagger\, \hat\psi^\dagger\, \hat\psi\, \hat\psi \rangle &= \frac{1}{2} \int\limits_{\mathbf{x}_1} \cdots \int\limits_{\mathbf{x}_N} \prod_{i=1}^{N} \varphi_0^*(\mathbf{x}_i) \sum_{k\,\ell} \hat\psi(\mathbf{x}_k)^\dagger\, \hat\psi(\mathbf{x}_\ell)^\dagger\, V(\mathbf{x}_k, \mathbf{x}_\ell)\, \hat\psi(\mathbf{x}_\ell)\, \hat\psi(\mathbf{x}_k) \prod_{j=1}^{N} \varphi_0(\mathbf{x}_j) \\
&= \frac{1}{2} \sum_{k\,\ell} \int\limits_{\mathbf{x}_1} \cdots \int\limits_{\mathbf{x}_N} \prod_{i=1}^{N} \varphi_0^*(\mathbf{x}_i) \hat\psi(\mathbf{x}_\ell)^\dagger\, \hat\psi(\mathbf{x}_\ell)\, V(\mathbf{x}_k, \mathbf{x}_\ell) \\
&\qquad\qquad \times \left[\hat\psi(\mathbf{x}_k)^\dagger\, \hat\psi(\mathbf{x}_k) - \delta_{k,\ell} \right] \prod_{j=1}^{N} \varphi_0(\mathbf{x}_j) \\
&= \frac{1}{2} \sum_{k\,\ell} \int\limits_{\mathbf{x}_k} \int\limits_{\mathbf{x}_\ell} V(\mathbf{x}_k, \mathbf{x}_\ell)\, |\varphi_0(\mathbf{x}_\ell)|^2 \left[|\varphi_0(\mathbf{x}_k)|^2 - \varphi_0(\mathbf{x}_k)\, \delta_{k,\ell}\, \varphi_0(\mathbf{x}_\ell) \right] \\
&\qquad\qquad \times \prod_{j \neq k,\ell} \int\limits_{\mathbf{x}_j} |\varphi_0(\mathbf{x}_j)|^2 \,.
\end{aligned}
\tag{4.91}
$$

Since there are N values of $\mathbf{x}_\ell$ for each of the N $\mathbf{x}_k$'s, there are N^2 terms in the product $|\varphi_0(\mathbf{x}_\ell)|^2 |\varphi_0(\mathbf{x}_k)|^2$. On the far right of (4.91), the product of integrals is unity, thus simplifying the two-body contribution to

$$
\begin{aligned}
\langle \hat\psi^\dagger\, \hat\psi^\dagger\, \hat\psi\, \hat\psi \rangle &= \frac{1}{2} N^2 \int\limits_{\mathbf{x}\,\mathbf{y}} V(\mathbf{x}, \mathbf{y})\, |\varphi_0(\mathbf{x})|^2\, |\varphi_0(\mathbf{y})|^2 - \frac{1}{2} N \int\limits_{\mathbf{x}} V(\mathbf{x}, \mathbf{x}) |\varphi_0(\mathbf{x})|^4 \\
&= 4\pi a\, N(N-1) \int\limits_{\mathbf{x}} |\varphi_0(\mathbf{x})|^4 \,.
\end{aligned}
\tag{4.92}
$$

It must be emphasized that the form of the potential given by (4.80) can only be substituted in at the final step in order to maintain the appropriate ordering of the limits. Additionally, $V(\mathbf{x}, \mathbf{x})$ must be interpreted as the diagonal coefficient of the matrix, without the delta function.

Adding the results (4.90) and (4.92) gives the total mean energy

$$
\langle \hat H \rangle_N = N \int\limits_{\mathbf{x}} \left\{ |\nabla \varphi_0(\mathbf{x}, t)|^2 + U(\mathbf{x})\, |\varphi_0(\mathbf{x}, t)|^2 \right\} + 4\pi a\, N^2 \int\limits_{\mathbf{x}} |\varphi_0(\mathbf{x}, t)|^4 \,. \tag{4.93}
$$

Because N is large, it is appropriate to make the approximation $N(N-1) \sim N^2$. The dynamical equation for the order parameter is obtained from an effective action which is defined as

$$\begin{aligned} S &= \int\limits_{\mathbf{x}_1} \dots \int\limits_{\mathbf{x}_N} dt\, \Psi_N^*(\mathbf{x}_1, \dots \mathbf{x}_N, t)\, (i\hbar\, \partial_t - \hat{H})\, \Psi_N(\mathbf{x}_1, \dots \mathbf{x}_N, t) \\ &= N \int\limits_{\mathbf{x}} \varphi_0^*(\mathbf{x}, t)\, i\hbar \frac{\partial \varphi_0}{\partial t} - \langle \hat{H} \rangle_N \,. \end{aligned} \tag{4.94}$$

Extremizing the action with respect to φ_0^*, then dividing the result by $\sqrt{N}$ obtains the Gross-Pitaevskii equation for the order parameter in (4.86):

$$\frac{\delta S}{\delta \varphi_0^*(\mathbf{x}, t)} = 0 \quad \Rightarrow \quad i\hbar \frac{\partial \phi}{\partial t} = \left[-\nabla^2 + U(\mathbf{x}) + 8\pi a\, |\phi|^2 \right] \phi \,. \tag{4.95}$$

This is the same equation as (4.83), but obtained through a different definition of the order parameter. From the latter definition of the order parameter, there emerge many quantifiers of superfluid behavior.

4.5 Superfluidity

Some further corollaries follow directly from the order parameter of (4.86)[1]. In particular, we can define a superfluid velocity, $v_s(\mathbf{x}, t)$, as the phase gradient of the condensate wave function, $\varphi_0(\mathbf{x}, t) = |\varphi_0(\mathbf{x}, t)| \exp\{i\theta(\mathbf{x}, t)\}$:

$$\mathbf{v}_s(\mathbf{x}, t) = \frac{\hbar}{m} \nabla_{\mathbf{x}}\, \theta(\mathbf{x}, t) \,. \tag{4.96}$$

It is this quantity that is of primary interest when discussing BEC vortices. From the definition, the superfluid velocity satisfies the condition of irrotationality

$$\nabla \times \mathbf{v}_s(\mathbf{x}, t) = 0 \,, \tag{4.97a}$$

and the quantization condition

$$\oint \mathbf{v}_s(\mathbf{x}, t) \cdot d\ell = \frac{nh}{m} \qquad (n = 0, 1, 2, \dots) \,. \tag{4.97b}$$

From the latter condition, quantized vortices may arise for $n \neq 0$. More importantly, (4.97) are conditions that reflect the superfluidity of the condensate. In contrast, the hydrodynamic velocity, $\mathbf{v}_h(\mathbf{x}, t) = \mathbf{j}(\mathbf{x}, t)/\rho(\mathbf{x}, t)$, is a classical construction which averages over the quasi-continuum of the excited many-particle states. As such, $\mathbf{v}_h$ fails in general to satisfy (4.97).

---

[1] See Leggett (2001), p. 317.

Chapter 5

Coherent Decay in Zero-Range Systems

At equilibrium, the alkali elements exist as crystalline solids. Therefore, when in dilute vapor form, they should exhibit a natural tendency toward collapse, indicating that the BEC must be in a metastable state. The purpose of this chapter is to arrive at a fundamental description of this metastablity by incorporating it into the many-body model.

For dilute samples, the initial impetus will be molecule formation, implying that a molecular coupling term should be included into the Hamiltonian. Here we consider a special case of the zero-range attractive interaction ($\lambda \to 0^-$), deferring the more general model to the following chapter. This analysis is particularly well suited to the case of ^{85}Rb which has a tendency towards collapse due to its innately negative scattering length. However, by using the Feshbach bound state, the scattering length may be tuned to positive values, thereby yielding what is thought to be a stable condensate.

After establishing the model Hamiltonian in Sec. 5.1, the variational solution is obtained in 5.2. Because the zero-range limit allows a diagonalization of the Hamiltonian, Sec. 5.3 uses the standard oscillator modes in arriving at the expression for the ground state energy per particle, thus confirming the variational results. Next, it is found that the solutions reveal a two-piece collapsing ground state, where the first is comprised of a molecular condensate and correlated pairs, having no atomic condensate component ($\psi = 0$)[1]. This piece terminates at some critical density where it is met by the $\psi \neq 0$ solution, thus completing the energy per particle curve. In spite of being in the positive scattering length regime, this solution indicates an imploding BEC, which directly contradicts experimental observations. In resolving this contradiction, Section 5.6 demonstrates that the usual low-density solution is obtained as an excited state associated with a complex chemical potential[2]. Finally, the last section derives an RPA expansion from which emerges the continuum of excitations for the lower collapsing state. Because the excited state lies within this spectrum, the imaginary part of the chemical potential corresponds to the decay rate into collective excitations of the lower solution. Hence, this model provides a fundamental account of the vapor's instability due to its propensity to form a solid.

---

[1] Chapter 7 discusses this solution in the context of macroscopic quantum tunneling of attractive condensates.

[2] This perspective can also be found in G. E. Cragg and A. K. Kerman (2005).

5.1 Hamiltonian of the Coupled System

With a fixed particle number, we work in the grand canonical ensemble where the model Hamiltonian is given by[1]

$$\begin{aligned}\hat{K} = \hat{H} - \mu\hat{N} = \sum_{\alpha\beta} \hat{\psi}^{\dagger}_{\alpha} \left(T_{\alpha\beta} - \mu\,\delta_{\alpha\beta}\right) \hat{\psi}_{\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \hat{\psi}^{\dagger}_{\alpha}\hat{\psi}^{\dagger}_{\beta} V_{\alpha\beta;\delta\gamma} \hat{\psi}_{\delta}\hat{\psi}_{\gamma} \\ + (\epsilon - 2\mu) \sum_{\alpha} \hat{\phi}^{\dagger}_{\alpha}\hat{\phi}_{\alpha} + \frac{\lambda\alpha}{\sqrt{2}} \sum_{\alpha\beta\gamma} \hat{\phi}^{\dagger}_{\alpha} F_{\alpha;\beta\gamma} \hat{\psi}_{\alpha}\hat{\psi}_{\beta} + \text{H.c.}\,.\end{aligned} \tag{5.1}$$

In this expression, the Lagrange multiplier, μ, is identified as the chemical potential. Also, the first two terms are the same as those in Eq. (4.2), whereas the third term is the contribution from the molecular component, which is seen by noticing that it comprises the molecular density multiplied by the detuning, ϵ, defined by Eq. (2.133). Finally, the last term is the coupling energy, with $\lambda\alpha$ as the coupling constant and F the molecular form factor.

Before using the variational approach described in Sec. 4.1, it is advantageous to attempt a simplification of the above model by exploiting the observation in Sec. 2.6.4. Accordingly, an appropriate detuning, $\varepsilon = 2/\lambda^2$, and a coupling, $g = \sqrt{-2/\lambda}$ are defined such that $-g^2/\varepsilon$ is equal to the original interaction strength, λ. Going to the limit of zero range, $\lambda \to 0$, it is seen that this choice automatically fulfills the requirement that $|\varepsilon| \gg |E|$. Under this approach, the two-body potential can be replaced by a second coupling to an auxiliary molecular field, $\hat{\chi}$. Finally, the simplified model is obtained by replacing the potential with another pair of coupling terms, having the same form as the last two in Eq. (5.1), resulting in a Hamiltonian given by[2]

$$\begin{aligned}\hat{K} = \sum_{\alpha\beta} \hat{\psi}^{\dagger}_{\alpha} \left(T_{\alpha\beta} - \mu\,\delta_{\alpha\beta}\right) \hat{\psi}_{\beta} + (\epsilon - 2\mu) \sum_{\alpha} \hat{\phi}^{\dagger}_{\alpha}\hat{\phi}_{\alpha} + (\varepsilon - 2\mu) \sum_{\alpha} \hat{\chi}^{\dagger}_{\alpha}\hat{\chi}_{\alpha} \\ + \frac{\lambda\alpha}{\sqrt{2}} \sum_{\alpha\beta\gamma} \hat{\phi}^{\dagger}_{\alpha} F_{\alpha;\beta\gamma} \hat{\psi}_{\alpha}\hat{\psi}_{\beta} + \text{H.c.} + \frac{g}{\sqrt{2}} \sum_{\alpha\beta\gamma} \hat{\chi}^{\dagger}_{\alpha} F_{\alpha;\beta\gamma} \hat{\psi}_{\alpha}\hat{\psi}_{\beta} + \text{H.c.}\,.\end{aligned} \tag{5.2}$$

5.2 Variational Analysis

In arriving at Eq. (5.2), we have gone from a form quartic in the atomic field operators, to one which is quadratic, thereby suggesting a simplification in terms of oscillator modes. Deferring the oscillator analysis to Sec. 5.3, we first use the variational approach, as it is somewhat more axiomatic allowing an extension to time dependent small oscillations (RPA). In analogy with the single field case, we begin by constructing a trial functional composed of a product of three decoupled Gaussians:

---

[1] Timmermans (1999) was the first to propose the Feshbach coupling to the molecular state. See also Kokkelmans, Milstein *et al.* (2002)

[2] This is analogous to the Hubbard-Stratonovich transformation as discussed in Weinberg (1995), p. 461.

$$
\begin{aligned}
\psi\left[\psi',\phi',\chi',t\right] = N_\psi \mathrm{exp}&\left\{-\sum_{\alpha\beta}\delta\psi'_\alpha(t)\left[\frac{1}{4}G^{-1}_{\alpha\beta}(t)-i\Sigma_{\alpha\beta}(t)\right]\delta\psi'_\beta(t)+i\sum_\alpha \pi_\alpha(t)\delta\psi'_\alpha(t)\right\}\\
&\cdot N_\phi \mathrm{exp}\left\{-\sum_\alpha\left[\frac{1}{4}\delta\phi'_\alpha(t)^2+i\omega_\alpha(t)\delta\phi'_\alpha(t)\right]\right\}\\
&\cdot N_\chi \mathrm{exp}\left\{-\sum_\alpha\left[\frac{1}{4}\delta\chi'_\alpha(t)^2+i\nu_\alpha(t)\delta\chi'_\alpha(t)\right]\right\}\,,
\end{aligned}
\tag{5.3}
$$

where the atomic part is the same as that of Eq. (4.8), but it is multiplied by two molecular Gaussian functionals representing the effects of the two fields, $\hat{\phi}$ and $\hat{\chi}$. In the same manner as the single field case, the fluctuations $\delta\phi'$ and $\delta\chi'$ are given by the value of the field minus its mean [see Eq. (4.9)], while ω and ν are their respective dynamical conjugates. Compared to the atomic piece, the molecular functionals are chosen such that their widths are constant, equal to $\frac{1}{2}$. Although a more general form could have been used, variation on the molecular widths would simply give back the form of (5.3). Without performing the full calculation, this can be seen by observing that (5.2) contains only density-like ($\hat{\phi}^\dagger\hat{\phi}$) terms in the molecular fields, whereas the atomic field appears in both types of correlation functions, $\hat{\psi}^\dagger\hat{\psi}$ and $\hat{\psi}\hat{\psi}$. Consequently, the presence of both kinds of terms in (5.2) gives rise to a non-constant atomic functional width, G^{-1}.

Employing Eq. (4.11) with Eqs. (4.16), we use the trial functional (5.3) to calculate the expectation of (5.2), thus resulting in the following form for the pressure[1],

$$
\begin{aligned}
-P = \frac{1}{\mathcal{V}}\langle\hat{K}\rangle = \int_{\mathbf{k}}' \left(k^2-\mu\right)R(\mathbf{k}) + \xi\int_{\mathbf{k}}' D(\mathbf{k}) - (\xi-\mu)\,\frac{1}{2}\psi^2\\
+\left(\frac{1}{2}\epsilon-\mu\right)\left(\frac{\xi+\eta}{2\lambda\alpha}\right)^2+\left(\frac{1}{2}\varepsilon-\mu\right)\left(\frac{\xi-\eta}{2g}\right)^2\,,
\end{aligned}
\tag{5.4}
$$

By first studying the uniform case (see Sec. 4.2), we have accordingly normalized by the volume factor, $\mathcal{V}$, when going to momentum space. In arriving at this expression, the molecular form factors, F, are set equal to unity since the limit of zero range is to be taken, as discussed in Sec. 2.3. The parameters ξ and η are defined in terms of linear combinations of the molecular fields,

$$\xi = \lambda\alpha\phi + g\chi \tag{5.5a}$$

$$\eta = \lambda\alpha\phi - g\chi\,. \tag{5.5b}$$

Extremizing the pressure results in the following set of variational equations

---

[1] The sign in front of the fluctuation $D(\mathbf{k})$ is unimportant, as it can be absorbed into the yet undetermined parameter ξ. Compare with (4.42).

$$\frac{\delta P}{\delta G} = 0 \quad \Rightarrow \quad G(\mathbf{k}) = \frac{1}{2}\sqrt{\frac{k^2-\mu+\xi}{k^2-\mu-\xi}} \tag{5.6a}$$

$$\frac{\delta P}{\delta \psi} = (\xi - \mu)\,\psi = 0 \tag{5.6b}$$

$$\frac{\delta P}{\delta \eta} = 0 \quad \Rightarrow \quad \eta = \xi\frac{\tau-\sigma}{\tau+\sigma} \tag{5.6c}$$

$$\frac{\delta P}{\delta \xi} = 0 \quad \Rightarrow \quad \xi\,(\sigma+\tau) + \eta\,(\sigma-\tau) + \int'_{\mathbf{k}} D(\mathbf{k}) + \frac{1}{2}\psi^2 = 0\,, \tag{5.6d}$$

where we have defined $\sigma = (\epsilon - 2\mu)/(2\lambda\alpha)^2$ and $\tau = (\varepsilon - 2\mu)/(2g)^2$. Substitution of (5.6c) into (5.6d) gives

$$\frac{4\xi\tau\sigma}{\tau+\sigma} + \int'_{\mathbf{k}} D(\mathbf{k}) + \frac{1}{2}\psi^2 = 0\,. \tag{5.7}$$

For a step function form factor, the momentum cutoff, $K\left(\int'_{\mathbf{k}} \frac{1}{k^2} \equiv \frac{1}{4\pi^2}\int_0^K dk\right)$, is inversely proportional to the effective range, $b \propto 4\pi^2/K$, hence, it can be seen that the zero-range limit corresponds to $K \to \infty$ and $\lambda \to 0^-$. In this limit, the appropriate quantities are expanded to the required order in λ, giving

$$\frac{\tau\sigma}{\tau+\sigma} \quad \to \quad -\frac{1}{4\lambda} - \frac{1}{4}\,\frac{\alpha^2}{\epsilon-2\mu} \tag{5.8a}$$

$$\phi = \frac{\xi+\eta}{2\lambda\alpha} \quad \to \quad -\frac{\xi\alpha}{\epsilon-2\mu} \tag{5.8b}$$

$$\chi = \frac{\xi-\eta}{2g} \quad \to \quad -\frac{1}{2}\,\lambda\,\xi^2 - \lambda^2\,\frac{\alpha^2\xi^2}{\epsilon-2\mu}\,. \tag{5.8c}$$

With the help of Eqs. (5.8) and (5.6c), (5.6d) and (5.4) become

$$-\frac{\xi}{\lambda} - \frac{\xi\alpha^2}{\epsilon-2\mu} + \int'_{\mathbf{k}} D(\mathbf{k}) + \frac{1}{2}\psi^2 = 0\,, \tag{5.9}$$

$$-P = \int'_{\mathbf{k}} \left(k^2-\mu\right) R(\mathbf{k}) + (\xi-\mu)\,\frac{1}{2}\psi^2 - \frac{1}{2}\,\frac{\xi^2\alpha^2}{\epsilon-2\mu} - \frac{1}{2\lambda}\,\xi^2 + \xi\int'_{\mathbf{k}} D(\mathbf{k})\,, \tag{5.10}$$

respectively. Thus, Eqs. (2.110), (4.24), (5.6a), (5.6b), (5.9) and (5.10) comprise a complete set in which everything is expressible in terms of the scattering length and the density, ρ, where

$$\begin{aligned}\rho &= \int_{\mathbf{k}}' R(\mathbf{k}) + \frac{1}{2}\psi^2 + \phi^2 + \chi^2 \\ &= \int_{\mathbf{k}}' R(\mathbf{k}) + \frac{1}{2}\psi^2 + \frac{\xi^2\alpha^2}{(\epsilon - 2\mu)^2}\,.\end{aligned} \tag{5.11}$$

It is helpful to arrange this set into more illustrative equations for analysis and interpretation. First, the integrals involving R and D are written out explicitly, resulting in forms that can be expressed in terms of the complete elliptic integrals of the first and second kind, denoted as F and E, respectively[1]:

$$\begin{aligned}\int_{\mathbf{k}}' k^2 R(\mathbf{k}) &= \frac{1}{4\pi^2}\int_0^K k^4\left[\frac{k^2+\gamma^2}{\sqrt{\left(k^2+\gamma^2\right)^2-\xi^2}} - 1\right]dk \\ &= \frac{\sqrt{\gamma^2+|\xi|}}{20\pi^2}\left[-\left(3\xi^2+\gamma^4\right)E\left(\sqrt{\frac{2|\xi|}{|\xi|+\gamma^2}}\right) + \gamma^2\left(\gamma^2-|\xi|\right)F\left(\sqrt{\frac{2|\xi|}{|\xi|+\gamma^2}}\right)\right] + \frac{\xi^2}{2b}\,,\end{aligned} \tag{5.12a}$$

$$\begin{aligned}\int_{\mathbf{k}}' R(\mathbf{k}) &= \frac{1}{4\pi^2}\int_0^K k^2\left[\frac{k^2+\gamma^2}{\sqrt{\left(k^2+\gamma^2\right)^2-\xi^2}} - 1\right]dk \\ &= \frac{\sqrt{\gamma^2+|\xi|}}{12\pi^2}\left[\gamma^2 E\left(\sqrt{\frac{2|\xi|}{|\xi|+\gamma^2}}\right) - \left(\gamma^2-|\xi|\right)F\left(\sqrt{\frac{2|\xi|}{|\xi|+\gamma^2}}\right)\right],\end{aligned} \tag{5.12b}$$

$$\begin{aligned}\int_{\mathbf{k}}' D(\mathbf{k}) &= -\frac{\xi}{4\pi^2}\int_0^K \frac{k^2}{\sqrt{\left(k^2+\gamma^2\right)^2-\xi^2}}dk \\ &= \frac{|\xi|}{4\pi^2}\sqrt{|\xi|+\gamma^2}\,E\left(\sqrt{\frac{2|\xi|}{|\xi|+\gamma^2}}\right) - \frac{|\xi|}{b}\,,\end{aligned} \tag{5.12c}$$

where we use the definitions

$$\begin{aligned}F(r) &\equiv \int_0^{\pi/2}\frac{d\alpha}{\sqrt{1-r^2\sin^2\alpha}} \\ E(r) &\equiv \int_0^{\pi/2}\sqrt{1-r^2\sin^2\alpha}\,d\alpha\end{aligned} \tag{5.13}$$

---

[1] The expression in terms of elliptic integrals can be found in Gradshteyn and Ryzhik (2000), p.276-9.

$$\mu \equiv -\gamma^2 \,. \tag{5.14}$$

The complete solution to the $\psi = 0$ case is given by

$$-P = \int_{\mathbf{k}}' (k^2 + \gamma^2) R(\mathbf{k}) + \frac{1}{2}\frac{\xi^2\alpha^2}{\epsilon + 2\gamma^2} + \frac{\xi^2}{16\pi a} - \frac{\xi^2}{2b} \,, \tag{5.15}$$

$$\rho = \int_{\mathbf{k}}' R(\mathbf{k}) + \frac{\xi^2\alpha^2}{(\epsilon + 2\gamma^2)^2} \,, \tag{5.16}$$

where Eq. (5.9) is substituted into Eq. (5.10), thereby obtaining the simplified form for the pressure. It is desirable to express all quantities in terms of the density, which is itself dependent upon ξ and γ. With $\psi = 0$, Eq. (5.9) relates ξ to γ,

$$\frac{\xi}{8\pi a} - \frac{\xi}{b} + \frac{\xi\alpha^2}{\epsilon + 2\gamma^2} - \int_{\mathbf{k}}' D(\mathbf{k}) = 0 \,, \tag{5.17}$$

thereby allowing the density to be obtained in terms of a single parameter. Subsequently, the density equation can be inverted, giving all quantities in terms of ρ.

5.3 Solution in Harmonic Oscillator Modes

The fact that the Hamiltonian of Eq. (5.2) is quadratic in the atomic field suggests that there should be a suitable approximation from which it becomes possibles to diagonalize in terms of ordinary harmonic oscillator modes. Implicit in the Gaussian trial functional (5.3) is that we are in fact extremizing on an oscillator ground state. Therefore, it will be attempted to arrive at the solutions by this direct diagonalization method. Assuming a decoupled expectation for the product of atomic and molecular fields, we take $\langle\hat{\phi}^\dagger\hat{\psi}\hat{\psi}\rangle = \langle\hat{\phi}^\dagger\rangle\langle\hat{\psi}\hat{\psi}\rangle$. Replacing the molecular fields by their mean values, the Hamiltonian becomes

$$\begin{aligned}
-\hat{P} = &\int_{\mathbf{k}}' (k^2 - \mu)\hat{\psi}^\dagger(\mathbf{k})\hat{\psi}(\mathbf{k}) + (\xi - \mu)\frac{1}{2}\psi^2 + \Big(\frac{1}{2}\,\epsilon - \mu\Big)\Big(\frac{\xi + \eta}{2\lambda\alpha}\Big)^2 \\
&+ \Big(\frac{1}{2}\,\varepsilon - \mu\Big)\Big(\frac{\xi - \eta}{2g}\Big)^2 + \frac{\xi}{2}\int_{\mathbf{k}}' \big[\hat{\psi}(\mathbf{k})\hat{\psi}(\mathbf{k}) + \hat{\psi}^\dagger(\mathbf{k})\hat{\psi}^\dagger(\mathbf{k})\big] \,,
\end{aligned} \tag{5.18}$$

where we have used Eqs. (5.5) in rewriting the mean molecular fields. Because the center three terms are already the same as those found in (5.4), the attention will be confined to the terms involving the atomic field operator, $\hat{\psi}$, which can be expressed in terms of canonical coordinates and momenta:

$$\begin{aligned}
\hat{\psi}(\mathbf{k}) &= \frac{1}{\sqrt{2}}\big[\hat{\varphi}(\mathbf{k}) + i\hat{\pi}(\mathbf{k})\big] \,, \\
\hat{\psi}^\dagger(\mathbf{k}) &= \frac{1}{\sqrt{2}}\big[\hat{\varphi}(\mathbf{k}) - i\hat{\pi}(\mathbf{k})\big] \,.
\end{aligned} \tag{5.19}$$

From this change of basis, we arrive at the following products:

$$\hat{\psi}^\dagger\hat{\psi} = \frac{1}{2}\left(\hat{\varphi}^2 + \hat{\pi}^2 - 1\right), \tag{5.20a}$$

$$\frac{1}{2}\left(\hat{\psi}\hat{\psi} + \hat{\psi}^\dagger\hat{\psi}^\dagger\right) = \frac{1}{2}\left(\hat{\varphi}^2 - \hat{\pi}^2\right), \tag{5.20b}$$

which, when substituted into the first and last terms of (5.18), leads to

$$-\hat{\tilde{P}} = \frac{1}{2}\int_{\mathbf{k}}' \left[(k^2-\mu+\xi)\hat{\varphi}(\mathbf{k})^2 + (k^2-\mu-\xi)\hat{\pi}(\mathbf{k})^2 - (k^2-\mu)\right], \tag{5.21}$$

where the tilde indicates that the middle three terms are left out. To each momentum, **k**, there is associated an oscillator mode described by an effective hamiltonian

$$\hat{h}(\mathbf{k}) \equiv \frac{\hat{\pi}(\mathbf{k})^2}{2m(\mathbf{k})} + \frac{1}{2}m(\mathbf{k})\,\omega(\mathbf{k})^2\,\hat{\varphi}(\mathbf{k})^2\,. \tag{5.22}$$

A comparison with Eq. (5.21) indicates that the momentum-dependent "mass" and "frequency" are identified by

$$\frac{1}{m(\mathbf{k})} = k^2 - \mu - \xi\,, \tag{5.23a}$$

$$m(\mathbf{k})\,\omega(\mathbf{k})^2 = k^2 - \mu + \xi\,. \tag{5.23b}$$

To complete this analysis, the coordinates and momenta are written in terms of the ladder operators in the usual way:

$$\hat{\varphi}(\mathbf{k}) = \sqrt{\frac{1}{2m(\mathbf{k})\,\omega(\mathbf{k})}}\left[\hat{a}(\mathbf{k}) + \hat{a}^\dagger(\mathbf{k})\right], \tag{5.24a}$$

$$\hat{\pi}(\mathbf{k}) = i\sqrt{\frac{m(\mathbf{k})\,\omega(\mathbf{k})}{2}}\left[\hat{a}^\dagger(\mathbf{k}) - \hat{a}(\mathbf{k})\right]. \tag{5.24b}$$

Thus, the system can be interpreted as an infinite collection of oscillators, one for each momentum, **k**. In the ground state, the expectation values of $\hat{\varphi}^2$ and $\hat{\pi}^2$ are

$$\begin{aligned}\langle\hat{\varphi}(\mathbf{k})^2\rangle = \frac{1}{2m(\mathbf{k})\,\omega(\mathbf{k})} &= \frac{1}{2}\sqrt{\frac{k^2-\mu-\xi}{k^2-\mu+\xi}} \\ &= \frac{1}{4}G(\mathbf{k})^{-1}\end{aligned} \tag{5.25}$$

$$\begin{aligned}\langle\hat{\pi}(\mathbf{k})^2\rangle = \frac{1}{2}m(\mathbf{k})\,\omega(\mathbf{k}) &= \frac{1}{2}\sqrt{\frac{k^2-\mu+\xi}{k^2-\mu-\xi}} \\ &= G(\mathbf{k})\,.\end{aligned} \tag{5.26}$$

Equation (5.25) shows that the mean square of the “position” operator, $\hat{\varphi}$, is nothing more than the Gaussian width (5.6a), as it should be. Substitution of these expressions into $\tilde{P} = \langle \hat{\tilde{P}} \rangle$ gives

$$-\tilde{P} = \int'_{\mathbf{k}} \frac{1}{2}\left[\sqrt{(k^2-\mu)^2-\xi^2}-(k^2-\mu)\right]\,, \tag{5.27}$$

which is simply a sum over quasiparticel energies. The corresponding terms in Eq. (5.10) are given by $\int (k^2-\mu)R(\mathbf{k}) + \xi \int D(\mathbf{k})$, which is identical to (5.27), after the application of the integral forms in (5.12). Finally, the condition (5.17) relating ξ to μ can be arrived at by an extremization on ξ. Thus, we have confirmed the equivalence of the variational procedure to the somewhat more direct oscillator approach.

5.4 Low-Density Behavior

Because we are always in the $\rho a^3 \ll 1$ regime, it is useful to explore the low-density behavior of the solution for $\psi = 0$. In addition, the corresponding expansions lead to a much more wieldy form from an analytic perspective. By Eqs.(4.24a) and (5.6a), it can be seen that zero density corresponds to $\xi \to 0$. Thus, the low-density limit can be obtained by expanding all quantities for small ξ.

Along with the integral identity[1],

$$\int_0^\infty \frac{dk}{(k^2+\gamma^2)^m} = \frac{\pi}{2}\frac{(2m-3)!!}{(m-1)!2^{m-1}}\gamma^{1-2m} \qquad m \neq 0\,, \tag{5.28}$$

we use the series,

$$\frac{1}{\sqrt{(k^2+\gamma^2)^2-\xi^2}} = \frac{1}{k^2+\gamma^2}\sum_{n=0}^{\infty}\frac{(2n-1)!!}{2^n n!}\frac{\xi^{2n}}{(k^2+\gamma^2)^{2n}}\,, \tag{5.29}$$

to cast all quantities in terms of ξ. Substitution of (5.28) and (5.29) into Eqs. (5.12) gives

$$\int'_{\mathbf{k}} (k^2+\gamma^2)R(\mathbf{k}) = \frac{\xi^2}{2b} - \frac{\xi^2\gamma}{16\pi} + \frac{\xi^4}{256\pi}\frac{1}{\gamma^3}\sum_{n=0}^{\infty}\frac{(2n+3)!!(4n+1)!!}{(2n+1)!(n+2)!\,2^{3n}}\frac{1}{n+1}\frac{\xi^{2n}}{\gamma^{4n}}\,, \tag{5.30a}$$

$$\int'_{\mathbf{k}} R(\mathbf{k}) = \frac{\xi^2}{32\pi}\frac{1}{\gamma}\sum_{n=0}^{\infty}\frac{(2n+1)!!(4n-1)!!}{(2n)!(n+1)!\,2^{3n}}\frac{1}{2n+1}\frac{\xi^{2n}}{\gamma^{4n}}\,, \tag{5.30b}$$

$$\int'_{\mathbf{k}} D(\mathbf{k}) = -\frac{\xi}{b} + \frac{\xi\gamma}{8\pi} - \frac{\xi^3}{128\pi}\frac{1}{\gamma^3}\sum_{n=0}^{\infty}\frac{(4n+1)!!}{(n+1)!(2n)!!\,2^{3n}}\frac{1}{n+1}\frac{\xi^{2n}}{\gamma^{4n}}\,. \tag{5.30c}$$

When (5.30c) is substituted into (5.17) we obtain

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[1] These expansions use the convention $(-1)!! \equiv 1$.

$$\frac{\xi}{8\pi a} - \frac{\xi\gamma}{8\pi} + \frac{\xi\alpha^2}{\epsilon + 2\gamma^2} + \frac{\xi^3}{128\pi}\frac{1}{\gamma^3}\sum_{n=0}^{\infty}\frac{(4n+1)!!}{(n+1)!(2n)!!}\,\frac{1}{2^{3n}}\frac{1}{n+1}\frac{\xi^{2n}}{\gamma^{4n}} = 0\,. \tag{5.31}$$

In the low-density limit where $\xi \to 0$, there emerges an equation for $\gamma_0 = \gamma|_{\xi\to 0}$:

$$\frac{1}{8\pi a} + \frac{\alpha^2}{\epsilon + 2\gamma_0^2} - \frac{\gamma_0}{8\pi} = 0\,. \tag{5.32}$$

Comparing this with Eq. (2.146), it is seen that $2\gamma_0^2$ is the molecular binding energy. Using Eqs. (5.30), the pressure and density become

$$-P = \frac{\xi^4}{256\pi}\frac{1}{\gamma^3}\sum_{n=0}^{\infty}\frac{(4n+1)!!}{(2n)!!(n+1)!\,2^{3n}}\frac{1}{n+2}\frac{\xi^{2n}}{\gamma^{4n}}\,, \tag{5.33}$$

$$\rho = \frac{\xi^2}{32\pi}\frac{1}{\gamma}\sum_{n=0}^{\infty}\frac{(2n+1)!!(4n-1)!!}{(2n)!(n+1)!\,2^{3n}}\,\frac{1}{2n+1}\frac{\xi^{2n}}{\gamma^{4n}} + \frac{\xi^2\alpha^2}{(\epsilon + 2\gamma^2)^2}\,. \tag{5.34}$$

At low density, the pressure reduces to

$$-P = \frac{1}{512\pi}\frac{1}{\gamma_0^3}\Big[\frac{1}{32\pi\gamma_0} + \frac{\alpha^2}{(\epsilon + 2\gamma_0^2)^2}\Big]^{-2}\rho^2\,, \tag{5.35}$$

thus implying a collapsing solution. To obtain the energy per particle, e, we start from its definition as the energy density divided by the number density, $e = u/\rho$. Differentiation of this results in $de/d\rho = (1/\rho)du/d\rho - u/\rho^2$. One property of the stationary solution is the vanishing of the variation with respect to the constrained quantity. In this case, this means that $dP/d\rho = du/d\rho - \mu = 0$. Setting $\mu = du/d\rho$ gives $\rho^2 de/d\rho = \mu\rho - u \equiv P$. Hence, the energy per particle is obtained as an integral of P, $e = \int P/\rho^2 d\rho + \text{const.}$, where the constant is half the molecular binding energy, thus giving

$$e = -\frac{1}{512\pi}\frac{1}{\gamma_0^3}\Big[\frac{1}{32\pi\gamma_0} + \frac{\alpha^2}{\epsilon + 2\gamma_0^2)^2}\Big]^{-2}\rho - \gamma_0^2\,. \tag{5.36}$$

Setting the constant to half the molecular binding energy makes physical sense because at zero density, only the molecular state remains. To confirm this intuition, the constant in Eq. (5.36) can be verified by a direct calculation of $e = u/\rho$.

5.5 The Critical Point

Establishing the range of validity of the $\psi = 0$ solution requires a closer inspection of the relationship between ξ and γ, as given in Eq. (5.17). After canceling a factor of ξ, this condition reads

$$\frac{1}{8\pi a_{bg}} + \frac{\alpha^2}{\epsilon + 2\gamma^2} + \frac{1}{4\pi^2}\int_0^K\left[\frac{k^2}{\sqrt{(k^2+\gamma^2)^2 - \xi^2}} - 1\right]dk = 0\,. \tag{5.37}$$

As seen from the integrand, the range of ξ is from $-\gamma^2$ to zero. The density expression (5.34) indicates that $d\rho/d\xi^2 > 0$, thus implying an increasing density with increasing ξ^2. When $\xi = -\gamma^2$, a critical density is reached since Eq. (5.37) no longer admits a solution. However, it is seen from variational expression (5.6b) that $\xi = \mu = -\gamma^2$ corresponds to a different solution for which the atomic field, ψ, is nonzero in general. This solution of Eq. (5.6b), permits explicit evaluation of the integrals involving R and D:

$$\int_{\mathbf{k}}' k^2 R(\mathbf{k}) = \frac{\gamma^4}{2b} - \frac{\sqrt{2}}{5\pi^2}\gamma^5 \,, \tag{5.38a}$$

$$\int_{\mathbf{k}}' R(\mathbf{k}) = \frac{\sqrt{2}}{12\pi^2}\gamma^3 \,, \tag{5.38b}$$

$$\int_{\mathbf{k}}' D(\mathbf{k}) = \frac{\gamma^2}{b} - \frac{\sqrt{2}}{4\pi^2}\gamma^3 \,. \tag{5.38c}$$

In addition, Eq. (5.9) is solved for $\frac{1}{2}\psi^2$:

$$\frac{1}{2}\psi^2 = -\frac{\gamma^2}{8\pi a} - \frac{\gamma^2\alpha^2}{\epsilon + 2\gamma^2} + \frac{\sqrt{2}}{4\pi^2}\gamma^3 \,. \tag{5.39}$$

As a result, both the energy density and the number density are parametrized in γ:

$$u = \Big[\frac{1}{16\pi a_{bg}} + \frac{1}{2}\frac{\epsilon\alpha^2}{(\epsilon + 2\gamma^2)^2}\Big]\gamma^4 - \frac{\sqrt{2}}{5\pi^2}\gamma^5 \,, \tag{5.40}$$

$$\rho = -\frac{1}{8\pi a(\epsilon + 2\gamma^2)}\gamma^2 + \frac{\sqrt{2}}{3\pi^2}\gamma^3 + \frac{\alpha^2}{(\epsilon + 2\gamma^2)^2}\gamma^4 \,, \tag{5.41}$$

where the full scattering length expression, Eq. (2.147), is used in defining $a(\epsilon + 2\gamma^2)$. Using the ^{85}Rb parameters from table (2.1), Figure (5.1) shows the energy per perticle of the two-piece solution, indicating the critical point where the sections meet[1]. Due to its persistently negative slope, we refer to this solution as the collapsing ground state of the model Hamiltonian of Eq. (5.1)[2]. Of particular importance is that this collapsing behavior is seen to persist even if the full scattering length is tuned to positive values, a regime thought to be stable against collapse.

5.6 A Complex Chemical Potential

Having an innately negative scattering length, the background interactions in ^{85}Rb are attractive, resulting in an ensemble that tends toward collapse as quantum degeneracy is approached. As such, this particular isotope cannot form a condensate containing more atoms than some critical number[3]. However, by exploiting a Feshbach resonance, the ap-

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[1] This critical point marks a quantum phase transition as discussed by M. W. J. Romans (2004).

[2] It is interesting to contrast this ground state with that discussed by E. H. Lieb and J. Yngvason (1998).

[3] For a complete discussion of this critical number, refer to Chapter 7.

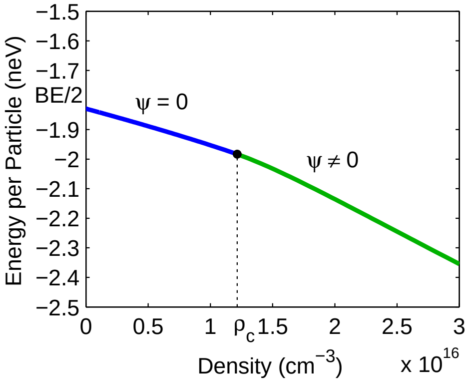

Figure 5.1: Figure showing the two-piece collapsing ground state for the case of ^{85}Rb at a magnetic field of 162.3 G. This corresponds to a critical density, ρ_c, of $1.22 \times 10^{16}\text{cm}^{-3}$ with a full scattering length of 193 Bohr radii. In the limit of zero density, the energy per particle simply reduces to half the molecular binding energy, BE/2 $\sim$ 1.85neV.

pearance of the molecular state allows the effective scattering length to be tuned to positive values, as indicated in Fig. 2.9(a)[1]. By tuning to positive values, a stable condensate has been experimentally observed in which the low-density energy per particle is found to have the usual behavior, $e \sim 4\pi a\rho$, where a is the full scattering length[2]. This observation is in agreement with the δ-function pseudopotential model.

5.6.1 Uniform Case

Despite the positive scattering length, our previous solutions predict that a uniform assembly should still tend toward collapse. Hence, we are confronted with the dilemma that using a more general potential somehow does not capture the correct physics of the system. To resolve this issue, it is necessary to reexamine the solutions obtained in the collapsing case. Since the experiments have observed the formation of an atomic condensate, we look at the solution for $\psi \neq 0$. In particular, we explore the consequences of extending this solution to zero density. To do so, the density equation (5.41) is inverted, thereby obtaining μ as an expansion in $\sqrt{\rho}$:

$$-\gamma^2 = \mu = 8\pi a(\epsilon)\rho - i\frac{\sqrt{\pi}}{3}\,256\,a(\epsilon)^{5/2}\rho^{3/2} - \left(\frac{64\,a(\epsilon)^2}{3\pi^2} + 8\pi a(\epsilon)\frac{\alpha^2}{\epsilon^2}\right)64\,\pi^2 a(\epsilon)^2\rho^2 - \dots . \tag{5.42}$$

When this expansion is substituted into (5.40), the usual low-density energy dependence, $e = u/\rho \sim 4\pi a\rho$, is obtained. Although this does give the appropriate low-density dependence, the chemical potential becomes complex at higher order. At first it may seem that

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[1] The negativity of the scattering length may be used to control the collapse, as in Roberts (2001).

[2] The experiments corresponding to the statics can be found in Cornish (2000). Theoretical investigations of the dynamics can be found in Holland (2000) and Kokkelmans and Holland (2002). However, only the latter investigation is in close agreement with the experiments reported in Donley (2002).

this situation simply cannot be valid, but upon further consideration it is recognized as a signature of an instability that is inherent in the original model of the system. With the Hamiltonian given by Eq. (5.1), consider the Heisenberg equation of motion for the atomic field operator $\hat{\psi}_\tau$: $i\hbar\,\dot{\hat{\psi}}^\dagger_\tau = [\hat{\psi}^\dagger_\tau, \hat{H}]$. Using the commutators $[\hat{\psi}_\alpha, \hat{\psi}^\dagger_\beta] = \delta_{\alpha\beta}$, $[\hat{\psi}^\dagger_\tau, \hat{\psi}^\dagger_\alpha\hat{\psi}_\beta] = -\delta_{\tau\beta}\,\hat{\psi}^\dagger_\alpha$ and $[\hat{\psi}^\dagger_\tau, \hat{\psi}_\gamma\hat{\psi}_\beta] = -\delta_{\tau\gamma}\,\hat{\psi}_\beta - \delta_{\tau\beta}\,\hat{\psi}_\gamma$, the right-hand side can be readily evaluated. Taking the expectation value using the trial functional of Eq. (5.3) gives

$$i\hbar\,\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\xi^*\psi\,. \tag{5.43}$$

We seek to add a phase to the mean fields such that (5.43) is consistent with the variational equations (5.6). If we let

$$\psi = \psi_0\,\mathrm{e}^{i\mu t/\hbar}\,, \tag{5.44a}$$

$$\xi = \xi_0\,\mathrm{e}^{2i\mu t/\hbar}\,, \tag{5.44b}$$

then the (5.43) gives back (5.6b). Thus, it is reasonable to interpret the chemical potential as the phase of the mean fields, from which the imaginary part of μ leads to a decay rate given by

$$\Gamma = \frac{\hbar}{2m}\frac{\sqrt{\pi}}{3}\,512\,a(\epsilon)^{5/2}\rho^{3/2}\,. \tag{5.45}$$

This decay rate has unique dependencies on both the scattering length ($\sim a(\epsilon)^{5/2}$) and the density ($\sim \rho^{3/2}$), both of which can be tested by experiment. Under the conditions of the ^{85}Rb experiment, there were 10^4 atoms within a cloud of radius $25\,\mu$m when the scattering length was tuned to $193a_0$ (a_0 = Bohr radius). These parameters yield a decay time, $\tau \sim 1/\Gamma$, of 14.3 seconds, which is in qualitative agreement with the observed lifetime of 10 seconds[1].

Because all quantities depend on μ, which is in general complex, it follows that the various other thermodynamic functions will assume a complex character as well. This is not unphysical, since the imaginary parts should simply be regarded as signatures of the coherent decay whereas the real parts assume their usual physical interpretations. Through this analysis, it has been shown that it is plausible to expect a coherent many-body decay process, brought about through the existence of a bound state in the system[2].

5.6.2 Decay in the Nonuniform Case

In this section it is shown that the complexity of μ persists even in the general static, nonuniform case. Thus far, only the uniform solutions have been discussed since it has been assumed that any nonuniformity can be accommodated using a local density approximation. Therefore, it might be conjectured that a chemical potential assuming a complex value is simply an artifact arising because the uniform solution is too restrictive to capture the

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[1] This lifetime was observed in Cornish (2000).

[2] The decay here is analogous to that found in the context of QED, where the instability of the electric field emerges through a complex action. See Schwinger (1951).

physics observed in experiment.

To address this concern, the origin of the complex μ must be identified. First, it must be recognized that the solution of interest has an equation of state associated with a positive chemical potential. This can be demonstrated in the following way. At low density, the energy per particle and its derivative satisfy $e \sim 4\pi a\rho > 0$ and $de/d\rho > 0$, respectively. By the definition of e as u/ρ, it follows that $de/d\rho = (\mu - e)/\rho$. The positivity of e and ρ thus implies the same for μ. From (5.6a), it is seen that for positive μ, G becomes imaginary for sufficiently small values of k. To the converse, note that in the full time-dependent form of the Gaussian trial functional (5.3), the width has a real part, G^{-1}, and an imaginary part Σ, that are canonically conjugate quantities. Since Σ is zero in static solutions, it follows that if the equation of state is associated with an imaginary G then the system is inherently unstable, which manifests as a complex chemical potential.

The ranging of G into imaginary values provides an indicator for the occurrence of this instability. Accordingly, this provides a convenient test in the nonuniform case, where a full analytic expression for μ is not possible. In the static, nonuniform case, the expectation value of the Hamiltonian in (5.2) is given by

$$\begin{aligned}\mathcal{H} - \mu\mathcal{N} = \sum_{\alpha\,\beta} h_{\alpha\,\beta}\Big(R_{\alpha\,\beta} + \frac{1}{2}\,\psi^*_\alpha\,\psi_\beta\Big) + \Big(\frac{1}{2}\,\epsilon - \mu\Big)\sum_\alpha \phi^*_\alpha\,\phi_\alpha + \Big(\frac{1}{2}\,\varepsilon - \mu\Big)\sum_\alpha \chi^*_\alpha\,\chi_\alpha \\ + \frac{1}{2}\sum_{\alpha\,\beta\,\gamma}\Big(\lambda\alpha\,\phi^*_\alpha + g\,\chi^*_\alpha\Big)F_{\alpha;\beta\gamma}\Big(D_{\gamma\,\beta} + \frac{1}{2}\,\psi_\alpha\,\psi_\beta\Big) + \text{H. c.}\end{aligned} \tag{5.46}$$

where, $h_{\alpha\beta} = T_{\alpha\beta} - \mu\,\delta_{\alpha\beta}$. The fluctuation terms are given by the static form of (4.17):

$$R_{\alpha\beta} = \frac{1}{2}\Big(\frac{1}{4}G^{-1}_{\alpha\beta} + G_{\alpha\beta} - \delta_{\alpha\beta}\Big) \tag{5.47a}$$

$$D_{\alpha\beta} = \frac{1}{2}\Big(\frac{1}{4}G^{-1}_{\alpha\beta} - G_{\alpha\beta}\Big) \tag{5.47b}$$

The derivatives of the fluctuations with respect to $G_{\rho\sigma}$ are given as[1]

$$\frac{\delta R_{\alpha\beta}}{\delta G_{\rho\sigma}} = \frac{1}{2}\Big(-\frac{1}{4}G^{-1}_{\alpha\rho}G^{-1}_{\sigma\beta} + \delta_{\alpha\rho}\,\delta_{\beta\sigma}\Big) \tag{5.48a}$$

$$\frac{\delta D_{\alpha\beta}}{\delta G_{\rho\sigma}} = \frac{1}{2}\Big(-\frac{1}{4}G^{-1}_{\alpha\rho}G^{-1}_{\sigma\beta} - \delta_{\alpha\rho}\,\delta_{\beta\sigma}\Big) \tag{5.48b}$$

Using the fluctuation derivatives, the Hamiltonian in (5.46) can be extremized on the width

$$\frac{\delta(\mathcal{H} - \mu\mathcal{N})}{\delta G_{\rho\sigma}} = -\frac{1}{4}\sum_{\alpha\beta} G^{-1}_{\rho\alpha}\,\big(h_{\alpha\beta} + \tilde{F}_{\alpha\beta}\big)\,G^{-1}_{\beta\sigma} + \sum_{\alpha\beta}\delta_{\rho\alpha}\big(h_{\alpha\beta} - \tilde{F}_{\alpha\beta}\big)\,\delta_{\beta\sigma} = 0 \tag{5.49}$$

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[1] Differentiating the identity $\sum_\gamma G_{\alpha\gamma}\,G^{-1}_{\gamma\beta} = \delta_{\alpha\beta}$, gives $\delta G^{-1}_{\alpha\beta}/\delta G_{\rho\sigma} = -G^{-1}_{\alpha\rho}\,G^{-1}_{\sigma\beta}$.

where $\tilde{F}$ is related to the form factor F by

$$\tilde{F}_{\alpha\beta} = \sum_{\gamma} \mathrm{Re}\{\alpha\, \phi_\tau + g\, \chi_\tau\}\, F_{\tau;\alpha\beta}\,. \tag{5.50}$$

By defining new matrices A and B as

$$A_{\alpha\beta} = h_{\alpha\beta} + \tilde{F}_{\alpha\beta} \tag{5.51a}$$

$$B_{\alpha\beta} = h_{\alpha\beta} - \tilde{F}_{\alpha\beta}\,, \tag{5.51b}$$

the variational equation (5.49) can be put into the compact matrix form

$$-\frac{1}{4}\, G^{-1}\, A\, G^{-1} + B = 0\,. \tag{5.52}$$

To obtain a symmetric solution for G^{-1}, we first multiply $\sqrt{A}$ on the right and on the left,

$$-\frac{1}{4}\sqrt{A}\, G^{-1}\, \sqrt{A}\, \sqrt{A}\, G^{-1}\, \sqrt{A} + \sqrt{A}\, B\, \sqrt{A} = 0\,. \tag{5.53}$$

By moving the first term to the right-hand side, then taking the square root, G^{-1} is seen to be[1]

$$G^{-1} = 2\, \frac{1}{\sqrt{A}}\, \sqrt{\sqrt{A}\, B\, \sqrt{A}}\, \frac{1}{\sqrt{A}}\,. \tag{5.54}$$

Likewise, the symmetric form of G is most easily obtained by multiplying (5.52) on the left and right by G, then following the same steps ending with[2]

$$G = \frac{1}{2}\, \frac{1}{\sqrt{B}}\, \sqrt{\sqrt{B}\, A\, \sqrt{B}}\, \frac{1}{\sqrt{B}}\,. \tag{5.55}$$

In momentum space, the operator h is given by $h(\mathbf{k}, \mathbf{k}') = (k^2 - \mu)\delta(\mathbf{k} - \mathbf{k}')$. For $k^2 = \mu$, $h = 0$. At such values of $\mathbf{k}$, Eqs. (5.51) show that $A = -B = \tilde{F}$, thus giving

$$\begin{aligned} G\Big|_{k^2=\mu} &= \frac{1}{2}\sqrt{\frac{1}{\sqrt{-\tilde{F}}}\, \tilde{F}\, \frac{1}{\sqrt{-\tilde{F}}}} \\ &= \pm\frac{i}{2}\,, \end{aligned} \tag{5.56}$$

indicating that G is in general complex. By our earlier observations, it follows that the coherent decay is present even in the general nonuniform case.

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[1] This series of manipulations obtains the required symmetric form for G^{-1}. In general, however, this is not a unique solution since multiplying (5.52) on the right by A, then taking the square root results in $G^{-1} = 2\sqrt{BA}\, A^{-1}$, which is different than the solution in (5.55)

[2] If the symmetric solutions for G and G^{-1} are unique, then it must be that $G\, G^{-1} = 1$. Thus far, I have been unable to prove this using (5.54) and (5.55).

5.7 Spectrum of $\mathfrak{A} \cdot \mathfrak{B}$

In order to better understand the meaning of the decay found in the previous section, it is helpful to examine the excitations of the solutions obtained. After expanding the Hamiltonian around the stationary solutions, we treat the simpler problem of finding the spectrum of $\mathfrak{A}$, which is seen to have a zero mode that persists into the product of $\mathfrak{A} \cdot \mathfrak{B}$. With this analysis as a template, we perform the full matrix multiplication for the general description of the excitations. From general arguments, the continuous spectrum arises from the form of the inverse of this product. When applied to the lower, collapsing solution, it is found that the excited state lies inside the continuum of excitations, thus providing a natural interpretation for the coherent decay as a transition from the excited state into collective phonon excitations of the lower state.

5.7.1 Small Oscillations

First, the Hamiltonian must be expanded around the stationary solutions. The analysis proceeds in the same way as that of Sec. (4.3), with the exception of a slight change in notation. Here, the atomic field is denoted by ψ whereas the molecular fields are ϕ and χ. Introducing the new molecular variables to Equations (4.48) results in the set

$$G(\mathbf{k},\mathbf{k}',t) = G(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}') + \delta G(\mathbf{k},\mathbf{k}',t) \tag{5.57a}$$

$$\Sigma(\mathbf{k},\mathbf{k}',t) = \delta\Sigma(\mathbf{k},\mathbf{k}',t) \tag{5.57b}$$

$$\psi(\mathbf{k},t) = \psi\delta(\mathbf{k}) + \delta\psi(\mathbf{k},t) \tag{5.57c}$$

$$\pi(\mathbf{k},t) = \delta\pi(\mathbf{k},t) \tag{5.57d}$$

$$\phi(\mathbf{k},t) = \phi\delta(\mathbf{k}) + \delta\phi(\mathbf{k},t) \tag{5.57e}$$

$$\omega(\mathbf{k},t) = \delta\omega(\mathbf{k},t) \tag{5.57f}$$

$$\chi(\mathbf{k},t) = \chi\delta(\mathbf{k}) + \delta\chi(\mathbf{k},t) \tag{5.57g}$$

$$\nu(\mathbf{k},t) = \delta\nu(\mathbf{k},t) \tag{5.57h}$$

$$\xi(\mathbf{k},t) = \xi\delta(\mathbf{k}) + \delta\xi(\mathbf{k},t)\,, \tag{5.57i}$$

where the last equation is introduced as a convenient linear combination of the mean molecular fields, $\xi = \lambda\alpha\phi + g\chi$.

With Eqs. (5.57) it is possible to expand the Hamiltonian to second order in the fluctuations, as illustrated by (4.53). In this notation, the two molecular fields yield a 4×4 matrix structure, instead of 2×2. In this case, the vectors δQ and δP are given as

$$\begin{aligned} \delta\mathcal{Q}^\dagger(\mathbf{q},\mathbf{P},t) &= [\delta\Sigma(\mathbf{q},-\mathbf{P},t), \delta\pi(-\mathbf{P},t), \delta\omega(-\mathbf{P},t), \delta\nu(-\mathbf{P},t)]\,, \\ \delta\mathcal{P}^\dagger(\mathbf{q},\mathbf{P},t) &= [\delta G(\mathbf{q},-\mathbf{P},t), \delta\psi(-\mathbf{P},t), \delta\phi(-\mathbf{P},t), \delta\chi(-\mathbf{P},t)]\,. \end{aligned} \tag{5.58}$$

This leads to exactly the same form as (4.55):

$$K_{RPA}(\mathbf{P},t) = \frac{1}{2}\delta\mathcal{P}^\dagger(\mathbf{q},\mathbf{P},t)\,\mathfrak{A}(\mathbf{q},\mathbf{q}',\mathbf{P})\delta\mathcal{P}(\mathbf{q}',\mathbf{P},t) + \frac{1}{2}\delta\mathcal{Q}^\dagger(\mathbf{q},\mathbf{P},t)\mathfrak{B}(\mathbf{q},\mathbf{q}',\mathbf{P})\delta\mathcal{Q}(\mathbf{q}',\mathbf{P},t)\,. \tag{5.59}$$

However, the $\mathfrak{A}$ and $\mathfrak{B}$ matrices are now given by

$$\mathfrak{A}(\mathbf{q},\mathbf{q}',t) = \begin{bmatrix} s_K(\mathbf{q},\mathbf{P})\delta(\mathbf{q}-\mathbf{q}') & c_K(\mathbf{q},\mathbf{P}) \\ c_K(\mathbf{q}',\mathbf{P}) & A(\mathbf{P}) \end{bmatrix} \tag{5.60a}$$

$$\mathfrak{B}(\mathbf{q},\mathbf{q}',t) = \begin{bmatrix} s_M(\mathbf{q},\mathbf{P})\delta(\mathbf{q}-\mathbf{q}') & c_M(\mathbf{q},\mathbf{P}) \\ c_M(\mathbf{q}',\mathbf{P}) & B(\mathbf{P}) \end{bmatrix}, \tag{5.60b}$$

where the off diagonal terms are

$$c_K(\mathbf{q},\mathbf{P}) = \begin{bmatrix}\mathfrak{A}_{G\psi}(\mathbf{q},\mathbf{P}) & \mathfrak{A}_{G\phi}(\mathbf{q},\mathbf{P}) & \mathfrak{A}_{G\chi}(\mathbf{q},\mathbf{P})\end{bmatrix} \tag{5.61a}$$

$$c_M(\mathbf{q},\mathbf{P}) = \begin{bmatrix}\mathfrak{B}_{\Sigma\pi}(\mathbf{q},\mathbf{P}) & \mathfrak{B}_{\Sigma\omega}(\mathbf{q},\mathbf{P}) & \mathfrak{B}_{\Sigma\nu}(\mathbf{q},\mathbf{P})\end{bmatrix}\,. \tag{5.61b}$$

In contrast to the case represented in Eqs. (4.56), $A(\mathbf{P})$ and $B(\mathbf{P})$ now have rank 3:

$$A(\mathbf{P}) = \begin{bmatrix} \mathfrak{A}_{\psi\psi}(\mathbf{P}) & \mathfrak{A}_{\psi\phi}(\mathbf{P}) & \mathfrak{A}_{\psi\chi}(\mathbf{P}) \\ \mathfrak{A}_{\phi\psi}(\mathbf{P}) & \mathfrak{A}_{\phi\phi}(\mathbf{P}) & \mathfrak{A}_{\phi\chi}(\mathbf{P}) \\ \mathfrak{A}_{\chi\psi}(\mathbf{P}) & \mathfrak{A}_{\chi\phi}(\mathbf{P}) & \mathfrak{A}_{\chi\chi}(\mathbf{P}) \end{bmatrix} \tag{5.62a}$$

$$B(\mathbf{P}) = \begin{bmatrix} \mathfrak{B}_{\pi\pi}(\mathbf{P}) & \mathfrak{B}_{\pi\omega}(\mathbf{P}) & \mathfrak{B}_{\pi\nu}(\mathbf{P}) \\ \mathfrak{B}_{\omega\pi}(\mathbf{P}) & \mathfrak{B}_{\omega\omega}(\mathbf{P}) & \mathfrak{B}_{\omega\nu}(\mathbf{P}) \\ \mathfrak{B}_{\nu\pi}(\mathbf{P}) & \mathfrak{B}_{\nu\omega}(\mathbf{P}) & \mathfrak{B}_{\nu\nu}(\mathbf{P}) \end{bmatrix}\,. \tag{5.62b}$$

All matrix elements in (5.59)–(5.62) have been calculated explicitly in Appendix B.

5.7.2 The Goldstone Mode

Finding the complete spectrum requires a multiplication of $\mathfrak{A}$ and $\mathfrak{B}$. Due to the complexity of the result, the full solution is quite difficult to obtain analytically. However, a full frontal analysis may be unnecessary, since some information may be obtained simply by finding the spectra of $\mathfrak{A}$ or $\mathfrak{B}$ individually. It will be seen that finding the spectrum in such simplified cases lends insight into the more general procedure.

As a check of the analysis performed thus far, the product must contain a zero mode as discussed at the end of Sec. (4.3.3). Although these matrices cannot be simultaneously diagonalized, a zero mode of either will nonetheless be present in the product. To illustrate this fact, discretize the space and suppose that $\mathfrak{A}$ contains the zero eigenvalue. Upon transformation to a basis that renders $\mathfrak{A}$ diagonal, this zero will lie along the diagonal. Subsequent multiplication with $\mathfrak{B}$ reveals a product having an all-zero row, thus proving the persistence of the zero mode. Accordingly, it is expected that the Goldstone mode will arise in either $\mathfrak{A}$ or $\mathfrak{B}$.

Before starting straight with the eigenvalue problem to be solved, it is convenient to employ a canonical transformation similar to the one used in Eqs. (4.59),

$$
\begin{aligned}
&\begin{pmatrix}\delta\Sigma\\ \delta\pi\\ \delta\omega\\ \delta\nu\end{pmatrix} \to \begin{pmatrix}\delta\Sigma\\ \delta\pi\\ \delta\omega\\ \delta\nu\end{pmatrix}' = \begin{pmatrix}\delta\Sigma\sqrt{s_K}\\ \delta\pi\sqrt{\mathfrak{A}_{\psi\psi}}\\ \delta\omega\sqrt{\mathfrak{A}_{\phi\phi}}\\ \delta\nu\sqrt{\mathfrak{A}_{\nu\nu}}\end{pmatrix}\\
&\begin{pmatrix}\delta G\\ \delta\psi\\ \delta\phi\\ \delta\chi\end{pmatrix} \to \begin{pmatrix}\delta G\\ \delta\psi\\ \delta\phi\\ \delta\chi\end{pmatrix}' = \begin{pmatrix}\frac{\delta G}{\sqrt{s_K}}\\ \frac{\delta\psi}{\sqrt{\mathfrak{A}_{\psi\psi}}}\\ \frac{\delta\phi}{\sqrt{\mathfrak{A}_{\phi\phi}}}\\ \frac{\delta\chi}{\sqrt{\mathfrak{A}_{\chi\chi}}}\end{pmatrix}.
\end{aligned}
\tag{5.63}
$$

This change of basis leads to new $\mathfrak{A}$ and $\mathfrak{B}$ matrices, denoted as $\mathfrak{A}'$ and $\mathfrak{B}'$, respectively. Using the original $\mathfrak{A}$ matrix calculated in B.5.1 of the appendix, the elements of $\mathfrak{A}'$ are straightforward:

$$
\begin{aligned}
\mathfrak{A}'_{GG}(\mathbf{q},\mathbf{q}',\mathbf{P}) &= \frac{\mathfrak{A}_{GG}(\mathbf{q},\mathbf{q}',\mathbf{P})}{\sqrt{s_K(\mathbf{q},\mathbf{P})s_K(\mathbf{q}',\mathbf{P})}}\\
&= \delta(\mathbf{q}-\mathbf{q}')
\end{aligned}
\tag{5.64}
$$

$$
\mathfrak{A}'_{G\psi}(\mathbf{q},\mathbf{P}) = \mathfrak{A}'_{\psi G}(\mathbf{q},\mathbf{P}) = 0 \tag{5.65}
$$

$$
\begin{aligned}
\mathfrak{A}'_{G\phi}(\mathbf{q},\mathbf{P}) = \mathfrak{A}'_{\phi G}(\mathbf{q},\mathbf{P}) &= \frac{\mathfrak{A}_{G\phi}(\mathbf{q},\mathbf{P})}{\sqrt{s_K(\mathbf{q},\mathbf{P})\mathfrak{A}_{\phi\phi}(\mathbf{P})}}\\
&= -\frac{\lambda\alpha}{2}\frac{\frac{1}{4}G_+^{-1}G_-^{-1}+1}{\sqrt{s_K(\mathbf{q},\mathbf{P})(\epsilon-2\mu)}}
\end{aligned}
\tag{5.66}
$$

$$
\begin{aligned}
\mathfrak{A}'_{G\chi}(\mathbf{q},\mathbf{P}) = \mathfrak{A}'_{\chi G}(\mathbf{q},\mathbf{P}) &= \frac{\mathfrak{A}_{G\chi}(\mathbf{q},\mathbf{P})}{\sqrt{s_K(\mathbf{q},\mathbf{P})\mathfrak{A}_{\chi\chi}(\mathbf{P})}}\\
&= -\frac{g}{2}\frac{\frac{1}{4}G_+^{-1}G_-^{-1}+1}{\sqrt{s_K(\mathbf{q},\mathbf{P})(\varepsilon-2\mu)}}
\end{aligned}
\tag{5.67}
$$

$$
\mathfrak{A}'_{\psi\psi}(\mathbf{P}) = \mathfrak{A}'_{\phi\phi}(\mathbf{P}) = \mathfrak{A}'_{\chi\chi}(\mathbf{P}) = 1 \tag{5.68}
$$

$$\begin{aligned}\mathfrak{A}'_{\psi\phi}(\mathbf{P}) = \mathfrak{A}'_{\phi\psi}(\mathbf{P}) &= \frac{\mathfrak{A}_{\psi\phi}(\mathbf{P})}{\sqrt{\mathfrak{A}_{\psi\psi}(\mathbf{P})\mathfrak{A}_{\phi\phi}(\mathbf{P})}} \\ &= \frac{\lambda\alpha\psi}{\sqrt{(P^2-\mu+\xi)(\epsilon-2\mu)}}\end{aligned} \tag{5.69}$$

$$\begin{aligned}\mathfrak{A}'_{\psi\chi}(\mathbf{P}) = \mathfrak{A}'_{\chi\psi}(\mathbf{P}) &= \frac{\mathfrak{A}_{\psi\chi}(\mathbf{P})}{\sqrt{\mathfrak{A}_{\psi\psi}(\mathbf{P})\mathfrak{A}_{\chi\chi}(\mathbf{P})}} \\ &= \frac{g\psi}{\sqrt{(P^2-\mu+\xi)(\varepsilon-2\mu)}}\end{aligned} \tag{5.70}$$

$$\mathfrak{A}'_{\phi\chi}(\mathbf{P}) = \mathfrak{A}'_{\chi\phi}(\mathbf{P}) = 0\,. \tag{5.71}$$

Due to the unitarity of this transformation, $\mathfrak{A}'\cdot\mathfrak{B}' = \mathfrak{A}\cdot\mathfrak{B}$. To find the point spectrum of $\mathfrak{A}'$, we begin with the eigenvalue equation

$$\mathfrak{A}'\delta P' = \Omega^2\delta P'\,. \tag{5.72}$$

Using the appropriate analogs of Eqs. (5.58), (5.60a), (5.61a) and (5.62a), this can be written as four linearly independent equations in the transformed variables $\delta G'$, $\delta\psi'$, $\delta\phi'$, and $\delta\chi'$:

$$\int'_{\mathbf{q}'}\delta(\mathbf{q}-\mathbf{q}')\delta G'(\mathbf{q}') + \mathfrak{A}'_{G\phi}(\mathbf{q})\delta\phi' + \mathfrak{A}'_{G\chi}(\mathbf{q})\delta\chi' = \Omega^2\delta G'(\mathbf{q}) \tag{5.73a}$$

$$\mathfrak{A}'_{\psi\psi}\delta\psi' = \Omega^2\delta\psi' \tag{5.73b}$$

$$\int'_{\mathbf{q}'}\mathfrak{A}'_{G\phi}(\mathbf{q}')\delta G'(\mathbf{q}') + \mathfrak{A}'_{\phi\phi}\delta\phi' = \Omega^2\delta\phi' \tag{5.73c}$$

$$\int'_{\mathbf{q}'}\mathfrak{A}'_{G\chi}(\mathbf{q}')\delta G'(\mathbf{q}') + \mathfrak{A}'_{\chi\chi}\delta\chi' = \Omega^2\delta\chi'\,. \tag{5.73d}$$

In writing these down, we have dropped the $\mathbf{P}$ dependencies in addition to using the fact that $\psi = 0$ for the case under consideration. Elimination of the fluctuations $\delta\phi'$ and $\delta\chi'$ leads to a single equation in $\delta G'(\mathbf{q})$,

$$\int'_{\mathbf{q}'}\left[(1-\Omega^2)\delta(\mathbf{q}-\mathbf{q}') + V(\mathbf{q},\mathbf{q}')\right]\delta G'(\mathbf{q}') = 0\,, \tag{5.74}$$

where we have identified

$$V(\mathbf{q},\mathbf{q}') = \frac{1}{\Omega^2-\mathfrak{A}'_{\phi\phi}}\mathfrak{A}'_{G\phi}(\mathbf{q})\mathfrak{A}'_{G\phi}(\mathbf{q}') + \frac{1}{\Omega^2-\mathfrak{A}'_{\chi\chi}}\mathfrak{A}'_{G\chi}(\mathbf{q})\mathfrak{A}'_{G\chi}(\mathbf{q}')\,. \tag{5.75}$$

Using the expressions for $\mathfrak{A}'_{\phi\phi}$, $\mathfrak{A}'_{\chi\chi}$, $\mathfrak{A}'_{G\phi}$ and $\mathfrak{A}'_{G\chi}$ found above, $V(\mathbf{q}, \mathbf{q}')$ simplifies to the separable form

$$V(\mathbf{q}, \mathbf{q}') = \frac{\sigma}{\Omega^2 - 1} \mathfrak{v}(\mathbf{q}) \mathfrak{v}(\mathbf{q}')\,, \tag{5.76}$$

where we have defined

$$\sigma = \frac{\lambda^2 \alpha^2}{\epsilon - 2\mu} + \frac{g^2}{\varepsilon - 2\mu}\,, \tag{5.77}$$

$$\mathfrak{v}(\mathbf{q}) = \frac{1}{\sqrt{2}} \frac{q^2 - \mu}{[(q^2 - \mu)^2 - \xi^2]^{3/4}}\,. \tag{5.78}$$

In arriving at these results, the form of G obtained in Eq. (5.6a) has been used to explicitly show the dependence on $\mathbf{q}$.

Identifying the operator in (5.74) as $\mathcal{O}(\mathbf{q}, \mathbf{q}') = (1 - \Omega^2)\delta(\mathbf{q} - \mathbf{q}') + V(\mathbf{q}, \mathbf{q}')$, the spectrum is obtained by solving for the values of Ω at which an inverse, $\mathcal{O}^{-1}$, does not exist. Without loss of generality, it may be assumed that $\mathcal{O}^{-1}$ has the form

$$\mathcal{O}^{-1}(\mathbf{q}'', \mathbf{q}') = \frac{1}{1 - \Omega^2}\, \delta(\mathbf{q}'' - \mathbf{q}') + \mathcal{S}(\mathbf{q}'', \mathbf{q}')\,, \tag{5.79}$$

where $\mathcal{S}(\mathbf{q}'', \mathbf{q}')$ is obtained through the requirement $\int \mathcal{O}(\mathbf{q}, \mathbf{q}'')\mathcal{O}^{-1}(\mathbf{q}'', \mathbf{q}') = \delta(\mathbf{q} - \mathbf{q}')$. Performing the necessary multiplications, this condition is met only if

$$(1 - \Omega^2)\, \mathcal{S}(\mathbf{q}, \mathbf{q}') + \frac{1}{1 - \Omega^2}\, V(\mathbf{q}, \mathbf{q}') + \int'_{\mathbf{q}''} \mathcal{S}(\mathbf{q}'', \mathbf{q}') = 0\,. \tag{5.80}$$

Defining

$$T(\mathbf{q}, \mathbf{q}') = (1 - \Omega^2)\mathcal{S}(\mathbf{q}, \mathbf{q}')(1 - \Omega^2)\,, \tag{5.81}$$

gives the Lippman-Schwinger equation used in the scattering theory of Chapter 2:

$$T(\mathbf{q}, \mathbf{q}') + \int'_{\mathbf{q}''} V(\mathbf{q}, \mathbf{q}'') \frac{1}{1 - \Omega^2}\, T(\mathbf{q}'', \mathbf{q}') = -V(\mathbf{q}, \mathbf{q}')\,. \tag{5.82}$$

Because this condition must be satisfied in order to invert the operator in (5.74), we seek values of Ω^2 for which (5.82) has no solution. At such values, it is assured that $\mathcal{O}^{-1}$ does not exist. According to a theorem in the spectral theory of operators, one of two conditions must be satisfied: (i) Eq. (5.82) has a non-trivial solution or (ii) there must be a solution to its homogeneous counterpart,

$$T(\mathbf{q}, \mathbf{q}') + \int'_{\mathbf{q}''} V(\mathbf{q}, \mathbf{q}'') \frac{1}{1 - \Omega^2}\, T(\mathbf{q}'', \mathbf{q}') = 0\,. \tag{5.83}$$

Known as the Fredholm Alternative, all possibilities are contained in a solution to either (5.82) or (5.83)[1]. Thus, the problem of finding the spectrum has been reduced to finding

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[1] Porter & Stirling (1990), p. 61.

the $\{\Omega\}$ that satisfy (5.83). As was done in the two-body case, a solution is attempted by taking a separable form for the T-matrix,

$$T(\mathbf{q},\mathbf{q}') = t\,\mathfrak{v}(\mathbf{q})\,\mathfrak{v}(\mathbf{q}')\,. \tag{5.84}$$

Substitution of this form into (5.83) gives

$$1 - \frac{\sigma}{(1-\Omega^2)^2}\int_{\mathbf{q}}' \mathfrak{v}(\mathbf{q})^2 = 0\,. \tag{5.85}$$

In accordance with the discussion following Eq. (5.1), we pick $g = \sqrt{-2/\lambda}$ and $\varepsilon = 2/\lambda^2$ to reproduce the background interactions in the assembly. Taking $\lambda \to 0^-$ and $K \to \infty$ in the limit of zero range, it is found that

$$\sigma \xrightarrow[\lambda\to 0^-]{} -\lambda \tag{5.86}$$

Likewise, using (5.78) for $\mathfrak{v}(\mathbf{q})$, then relating the range, $b = 4\pi^2/K$, to λ, we find

$$\int_{\mathbf{q}}' \mathfrak{v}(\mathbf{q})^2 \xrightarrow[\lambda\to 0^-]{} -\frac{1}{\lambda}\,, \tag{5.87}$$

thus leading to the final result

$$\left(1-\Omega^2\right)^2 - 1 = 0\,. \tag{5.88}$$

Hence, it is shown that $\Omega = 0, \pm\sqrt{2}$ belong to the point spectrum of $\mathfrak{A}'$. By the construction of the inverse in (5.79), it is seen that ± 1 completes the spectrum of $\mathfrak{A}'$ which is discrete. As previously shown, the $\Omega = 0$ solution implies the existence of the Goldstone mode for $\mathfrak{A}\cdot\mathfrak{B}$ in the case for $\psi = 0$, thus fulfilling expectations based on the particle number symmetry of the original Hamiltonian, discussed in the conclusion of Sec. 4.3.3.

5.7.3 Complete Spectrum of $\mathfrak{A}\cdot\mathfrak{B}$

In this section, the aim is to calculate the spectrum of $\mathfrak{A}\cdot\mathfrak{B}$. In principle, this can be carried out analytically, but it will be seen that much progress can be achieved by considering the form of the solution rather than carrying out the calculation to the end. Before proceeding in an analogous manner as was done in the preceding section for $\mathfrak{A}$, it is necessary to obtain the matrix product, which, by using the definitions (5.60), is

$$\begin{aligned}
&\mathfrak{A}\cdot\mathfrak{B}\,(\mathbf{q},\mathbf{q}',\mathbf{P}) = \mathfrak{M}(\mathbf{q},\mathbf{q}',\mathbf{P})\\
&= \begin{bmatrix} s_K(\mathbf{q},\mathbf{P})s_M(\mathbf{q}',\mathbf{P})\delta(\mathbf{q}-\mathbf{q}') + c_K(\mathbf{q},\mathbf{P})\,c_M(\mathbf{q}',\mathbf{P}) & s_K(\mathbf{q},\mathbf{P})\,c_M(\mathbf{q},\mathbf{P}) + c_K(\mathbf{q},\mathbf{P})B(\mathbf{P}) \\ c_K(\mathbf{q}',\mathbf{P})\,s_M(\mathbf{q}',\mathbf{P}) + A(\mathbf{P})c_M(\mathbf{q}',\mathbf{P}) & \displaystyle\int_{\mathbf{q}''}' c_K(\mathbf{q}'',\mathbf{P})c_M(\mathbf{q}'',\mathbf{P}) + A(\mathbf{P})\cdot B(\mathbf{P}) \end{bmatrix}.
\end{aligned} \tag{5.89}$$

By writing the product in this form, care must be taken in keeping the proper ordering of the entries, since terms like $s_K(\mathbf{q},\mathbf{P})\,c_M(\mathbf{q},\mathbf{P})$ represent the multiplication of an $\infty\times 1$ and a $3\times\infty$ matrix. As an illustration of this hidden structure, we write out the form of the term occupying the upper right quadrant, keeping the $\mathbf{P}$ dependence implicit,

$$\begin{aligned}
s_K(\mathbf{q})\,c_M(\mathbf{q}) + c_K(\mathbf{q})\,B = {} & [s_K(\mathbf{q})\mathfrak{B}_{\Sigma\pi}(\mathbf{q}) + \mathfrak{A}_{G\psi}(\mathbf{q})B_{\pi\pi} + \mathfrak{A}_{G\phi}(\mathbf{q})B_{\omega\pi} + \mathfrak{A}_{G\chi}(\mathbf{q})B_{\nu\pi}, \\
& s_K(\mathbf{q})\mathfrak{B}_{\Sigma\omega}(\mathbf{q}) + \mathfrak{A}_{G\psi}(\mathbf{q})B_{\pi\omega} + \mathfrak{A}_{G\phi}(\mathbf{q})B_{\omega\omega} + \mathfrak{A}_{G\chi}(\mathbf{q})B_{\nu\omega}, \\
& s_K(\mathbf{q})\mathfrak{B}_{\Sigma\nu}(\mathbf{q}) + \mathfrak{A}_{G\psi}(\mathbf{q})B_{\pi\nu} + \mathfrak{A}_{G\phi}(\mathbf{q})B_{\omega\nu} + \mathfrak{A}_{G\chi}(\mathbf{q})B_{\nu\nu}] \\
= {} & \Big[-\frac{1}{2}(\lambda^2\alpha^2 + g^2)\Big(\frac{1}{4}G_+^{-1}G_-^{-1} + 1\Big)\psi, \\
& - 2s_K(\mathbf{q})\lambda\alpha(G_+ + G_-) - \lambda\alpha\Big(\frac{1}{4}G_+^{-1}G_-^{-1} + 1\Big)\Big(\frac{1}{2}\epsilon - \mu\Big), \\
& -2s_K(\mathbf{q})g(G_+ + G_-) - g\Big(\frac{1}{4}G_+^{-1}G_-^{-1} + 1\Big)\Big(\frac{1}{2}\varepsilon - \mu\Big)\Big]\,. \qquad (5.90)
\end{aligned}$$

The remaining elements shown in (5.89) are calculated in analogous ways, resulting in a matrix having the same form as $\mathfrak{A}$ and $\mathfrak{B}$:

$$\mathfrak{M}(\mathbf{q},\mathbf{q}',\mathbf{P}) = \begin{bmatrix} \mathfrak{M}_{GG}(\mathbf{q},\mathbf{q}',\mathbf{P}) & \mathfrak{M}_{G\psi}(\mathbf{q},\mathbf{P}) & \mathfrak{M}_{G\phi}(\mathbf{q},\mathbf{P}) & \mathfrak{M}_{G\chi}(\mathbf{q},\mathbf{P}) \\ \mathfrak{M}_{\psi G}(\mathbf{q}',\mathbf{P}) & \mathfrak{M}_{\psi\psi}(\mathbf{P}) & \mathfrak{M}_{\psi\phi}(\mathbf{P}) & \mathfrak{M}_{\psi\chi}(\mathbf{P}) \\ \mathfrak{M}_{\phi G}(\mathbf{q}',\mathbf{P}) & \mathfrak{M}_{\phi\psi}(\mathbf{P}) & \mathfrak{M}_{\phi\phi}(\mathbf{P}) & \mathfrak{M}_{\phi\chi}(\mathbf{P}) \\ \mathfrak{M}_{\chi G}(\mathbf{q}',\mathbf{P}) & \mathfrak{M}_{\chi\psi}(\mathbf{P}) & \mathfrak{M}_{\chi\phi}(\mathbf{P}) & \mathfrak{M}_{\chi\chi}(\mathbf{P}) \end{bmatrix}\,. \qquad (5.91)$$

With $\mathbf{P} = \mathbf{P}'$, we use Eqs. (A.12) and (5.6a) along with the following identifications

$$\omega_\pm \equiv \sqrt{(q_\pm^2 - \mu)^2 - \xi^2}\,, \qquad (5.92\text{a})$$

$$\mathfrak{w}(\mathbf{q}) \equiv \frac{1}{2}\Big(\frac{1}{4}G_+^{-1}G_-^{-1} + 1\Big)\,, \qquad (5.92\text{b})$$

$$f_\pm \equiv q_\pm^2 - \mu + \xi \qquad (5.92\text{c})$$

$$I_1 \equiv \frac{1}{2}\int_{\mathbf{q}''}^{\prime} w(\mathbf{q}'')(G_+'' + G_-'')\,, \qquad (5.92\text{d})$$

thus permitting the matrix elements to be explicitly expressed as

$$\mathfrak{M}_{GG}(\mathbf{q},\mathbf{q}') = (\omega_+ + \omega_-)^2\delta(\mathbf{q}-\mathbf{q}') + (\lambda^2\alpha^2 + g^2)\mathfrak{w}(\mathbf{q})(G'_+ + G'_-) \tag{5.93a}$$

$$\mathfrak{M}_{G\psi}(\mathbf{q}) = -(\lambda^2\alpha^2 + g^2)\mathfrak{w}(\mathbf{q})\psi \tag{5.93b}$$

$$\mathfrak{M}_{G\phi}(\mathbf{q}) = -\frac{\lambda\alpha}{8}(f_+G_+^{-2}G_-^{-1} + f_-G_-^{-2}G_+^{-1})(G_+ + G_-) - \lambda\alpha\,\mathfrak{w}(\mathbf{q})(\epsilon - 2\mu) \tag{5.93c}$$

$$\mathfrak{M}_{G\chi}(\mathbf{q}) = -\frac{g}{8}(f_+G_+^{-2}G_-^{-1} + f_-G_-^{-2}G_+^{-1})(G_+ + G_-) - g\,\mathfrak{w}(\mathbf{q})(\varepsilon - 2\mu) \tag{5.93d}$$

$$\mathfrak{M}_{\psi G}(\mathbf{q}') = -(\lambda^2\alpha^2 + g^2)(G'_+ + G'_-)\psi \tag{5.93e}$$

$$\mathfrak{M}_{\phi G}(\mathbf{q}') = -2\,\lambda\alpha\,\mathfrak{w}(\mathbf{q}')(f'_+G'_- + f'_-G'_+) - \lambda\alpha\,(G'_+ + G'_-)(\epsilon - 2\mu) \tag{5.93f}$$

$$\mathfrak{M}_{\chi G}(\mathbf{q}') = -2\,g\,\mathfrak{w}(\mathbf{q}')(f'_+G'_- + f'_-G'_+) - g\,(G'_+ + G'_-)(\varepsilon - 2\mu) \tag{5.93g}$$

$$\mathfrak{M}_{\psi\psi} = (P^2 - \mu)^2 - \xi^2 + (\lambda^2\alpha^2 + g^2)\psi^2 \tag{5.93h}$$

$$\mathfrak{M}_{\psi\phi} = \lambda\alpha\,\psi(P^2 - 3\mu + \xi + \epsilon) \tag{5.93i}$$

$$\mathfrak{M}_{\psi\chi} = g\,\psi\,(P^2 - 3\mu + \xi + \varepsilon) \tag{5.93j}$$

$$\mathfrak{M}_{\phi\psi} = \lambda\alpha\,\psi\,(P^2 - 3\mu - \xi + \epsilon) \tag{5.93k}$$

$$\mathfrak{M}_{\phi\phi} = \lambda^2\alpha^2\,(2I_1 + \psi^2) + (\epsilon - 2\mu)^2 \tag{5.93l}$$

$$\mathfrak{M}_{\phi\chi} = \mathfrak{M}_{\chi\phi} = \lambda\alpha g\,(2I_1 + \psi^2\Big) \tag{5.93m}$$

$$\mathfrak{M}_{\chi\psi} = g\,\psi(P^2 - 3\mu - \xi + \varepsilon) \tag{5.93n}$$

$$\mathfrak{M}_{\chi\chi} = g^2(2I_1 + \psi^2) + (\varepsilon - 2\mu)^2\,. \tag{5.93o}$$

These elements are used in the set of equations arising from the eigenvalue problem, $\mathfrak{M}\,\delta P = \Omega^2\delta P$:

$$\int'_{\mathbf{q}''} M_{GG}(\mathbf{q},\mathbf{q}'')\,\delta G(\mathbf{q}'') + M_{G\psi}(\mathbf{q})\,\delta\psi + M_{G\phi}(\mathbf{q})\,\delta\phi + M_{G\chi}(\mathbf{q})\,\delta\chi = \Omega^2\delta G(\mathbf{q}) \tag{5.94a}$$

$$\int'_{\mathbf{q}''} M_{\psi G}(\mathbf{q}'')\,\delta G(\mathbf{q}'') + M_{\psi\psi}\,\delta\psi + M_{\psi\phi}\,\delta\phi + M_{\psi\chi}\,\delta\chi = \Omega^2\delta\psi \tag{5.94b}$$

$$\int'_{\mathbf{q}''} M_{\phi G}(\mathbf{q}'')\,\delta G(\mathbf{q}'') + M_{\phi\psi}\,\delta\psi + M_{\phi\phi}\,\delta\phi + M_{\phi\chi}\,\delta\chi = \Omega^2\delta\phi \tag{5.94c}$$

$$\int'_{\mathbf{q}''} M_{\chi G}(\mathbf{q}'')\,\delta G(\mathbf{q}'') + M_{\chi\psi}\,\delta\psi + M_{\chi\phi}\,\delta\phi + M_{\chi\chi}\,\delta\chi = \Omega^2\delta\chi\,, \tag{5.94d}$$

where the explicit dependence on the total momentum, $\mathbf{P}$, has been dropped for notational convenience.

Thus far, the equations are general, describing the excitation spectrum for any stationary solution to the Hamiltonian in Eq. (5.2). In the simplest case, $\psi = 0$, thus giving $\mathfrak{M}_{G\psi} = \mathfrak{M}_{\psi\phi} = \mathfrak{M}_{\phi\psi} = \mathfrak{M}_{\psi G} = \mathfrak{M}_{\psi\chi} = \mathfrak{M}_{\phi\psi} = \mathfrak{M}_{\chi\psi} = 0$, thereby reducing the above system to only three independent equations. Additionally, we will be solving for the case of zero total momentum, $\mathbf{P} = 0$. Using these simplifications, the molecular field displacements are expressed in terms of δG:

$$\delta\phi = \frac{1}{d} \int'_{\mathbf{q}''} \big[(\Omega^2 - \mathfrak{M}_{\chi\chi})\, \mathfrak{M}_{\phi G}(\mathbf{q}'') + \mathfrak{M}_{\phi\chi}\, \mathfrak{M}_{\chi G}(\mathbf{q}'')\big]\, \delta G(\mathbf{q}'') \tag{5.95a}$$

$$\delta\chi = \frac{1}{d} \int'_{\mathbf{q}''} \big[(\Omega^2 - \mathfrak{M}_{\phi\phi})\, \mathfrak{M}_{\chi G}(\mathbf{q}'') + \mathfrak{M}_{\chi\phi}\, \mathfrak{M}_{\phi G}(\mathbf{q}'')\big]\, \delta G(\mathbf{q}'')\,, \tag{5.95b}$$

where

$$d = (\Omega^2 - \mathfrak{M}_{\chi\chi})(\Omega^2 - \mathfrak{M}_{\phi\phi}) - \mathfrak{M}_{\chi\phi}\mathfrak{M}_{\phi\chi}\,. \tag{5.96}$$

Substitution of (5.95) into (5.94a) gives an effective matrix equation for δG,

$$\int'_{\mathbf{q}''} \big[h(\mathbf{q})\, \delta(\mathbf{q} - \mathbf{q}'') + \mathfrak{w}(\mathbf{q})\, s(\mathbf{q}'') + f(\mathbf{q})\, r(\mathbf{q}'')\big]\, \delta G(\mathbf{q}'')\,. \tag{5.97}$$

In addition to (5.92b) and (5.92c), the terms appearing in this expression are identified by the following:

$$h(\mathbf{q}) = \omega(\mathbf{q})^2 - \Omega^2\,, \tag{5.98a}$$

$$\begin{aligned} r(\mathbf{q}'') = \frac{1}{2}\Big\{&[C1\,(\epsilon - 2\mu) + C2\,(\varepsilon - 2\mu)]\, G(\mathbf{q}'') \\ &+ (C1 + C2)\,({\mathbf{q}''}^2 - \mu + \xi)\Big[\frac{1}{4} G(\mathbf{q}'')^{-1} + G(\mathbf{q}'')\Big]\Big\}\,, \end{aligned} \tag{5.98b}$$

$$s(\mathbf{q}'') = \frac{1}{2}(\lambda^2\alpha^2 + g^2) G(\mathbf{q}'') + r(\mathbf{q}'')\,, \tag{5.98c}$$

with

$$C1 = \frac{\lambda\alpha}{2d}\,[\lambda\,\alpha\,(\Omega^2 - \mathfrak{M}_{\chi\chi}) + g\,\mathfrak{M}_{\phi\chi}]\,, \tag{5.99a}$$

$$C2 = \frac{g}{2d}\,[g\,(\Omega^2 - \mathfrak{M}_{\phi\phi}) + \lambda\,\alpha\,\mathfrak{M}_{\phi\chi}]\,. \tag{5.99b}$$

The problem to be solved is to find all Ω such that Eq. (5.97) has no solution except the trivial case $\delta G = 0$. Henceforth, we illustrate the general solution method without delving too deeply into numerical specifics. It will be seen that a full calculation may be unwarranted as the continuum emerges simply from the general structure of the solution. Proceeding in analogy with the previous method used for $\mathfrak{A}$, the operator in Eq. (5.97) can be written as

$$\mathcal{O}(\mathbf{q}, \mathbf{q}'') = h(\mathbf{q})\, \delta(\mathbf{q} - \mathbf{q}'') + \begin{bmatrix}\mathfrak{w}(\mathbf{q}) & f(\mathbf{q})\end{bmatrix} \mathcal{I} \begin{bmatrix} s(\mathbf{q}'') \\ r(\mathbf{q}'') \end{bmatrix}, \tag{5.100}$$

where $\mathcal{I}$ is the identity matrix. If it exists, the inverse, $\mathcal{O}^{-1}$, has the form

$$\mathcal{O}^{-1}(\mathbf{q}'',\mathbf{q}') = \frac{1}{h(\mathbf{q}'')}\,\delta(\mathbf{q}''-\mathbf{q}') + \begin{bmatrix}\mathfrak{w}(\mathbf{q}'') & f(\mathbf{q}'')\end{bmatrix}\mathcal{N}\begin{bmatrix}s(\mathbf{q}')\\ r(\mathbf{q}')\end{bmatrix}\,, \tag{5.101}$$

where $\mathcal{N}$ is some $2{\times}2$ matrix, yet to be determined. From the definition, $\int_{\mathbf{q}''}\mathcal{O}(\mathbf{q},\mathbf{q}'')\,\mathcal{O}^{-1}(\mathbf{q}'',\mathbf{q}') = \delta(\mathbf{q}-\mathbf{q}')$, we have

$$\begin{bmatrix}\mathfrak{w}(\mathbf{q}) & f(\mathbf{q})\end{bmatrix}\left\{\mathcal{T}+\mathcal{I}+\mathcal{I}\begin{bmatrix}\displaystyle\int'_{\mathbf{q}''}\frac{s(\mathbf{q}'')\mathfrak{w}(\mathbf{q}'')}{h(\mathbf{q}'')} & \displaystyle\int'_{\mathbf{q}''}\frac{s(\mathbf{q}'')f(\mathbf{q}'')}{h(\mathbf{q}'')}\\[2ex] \displaystyle\int'_{\mathbf{q}''}\frac{r(\mathbf{q}'')\mathfrak{w}(\mathbf{q}'')}{h(\mathbf{q}'')} & \displaystyle\int'_{\mathbf{q}''}\frac{r(\mathbf{q}'')f(\mathbf{q}'')}{h(\mathbf{q}'')}\end{bmatrix}\mathcal{T}\right\}\begin{bmatrix}s(\mathbf{q}')\\ r(\mathbf{q}')\end{bmatrix} = 0\,. \tag{5.102}$$

In writing this expression, we have defined a new matrix, $\mathcal{T} \equiv h(\mathbf{q})\mathcal{N}h(\mathbf{q}')$. According to the Fredholm alternative, (5.102) will not have a solution if

$$\int'_{\mathbf{q}''}\frac{s(\mathbf{q}'')\mathfrak{w}(\mathbf{q}'')}{h(\mathbf{q}'')} = \int'_{\mathbf{q}''}\frac{r(\mathbf{q}'')f(\mathbf{q}'')}{h(\mathbf{q}'')} = -1 \tag{5.103a}$$

$$\int'_{\mathbf{q}''}\frac{s(\mathbf{q}'')f(\mathbf{q}'')}{h(\mathbf{q}'')} = \int'_{\mathbf{q}''}\frac{r(\mathbf{q}'')\mathfrak{w}(\mathbf{q}'')}{h(\mathbf{q}'')} = 0\,. \tag{5.103b}$$

Hence, if Eqs. (5.103) are satisfied, the inverse, $\mathcal{O}^{-1}$ [given in (5.101)], cannot be constructed. Additionally, it can be seen directly from the form of $\mathcal{O}^{-1}$ that $h(\mathbf{q}) = 0$ precludes an inverse as well. Because of its dependence on $\mathbf{q}$, this condition gives the continuous part of the spectrum,

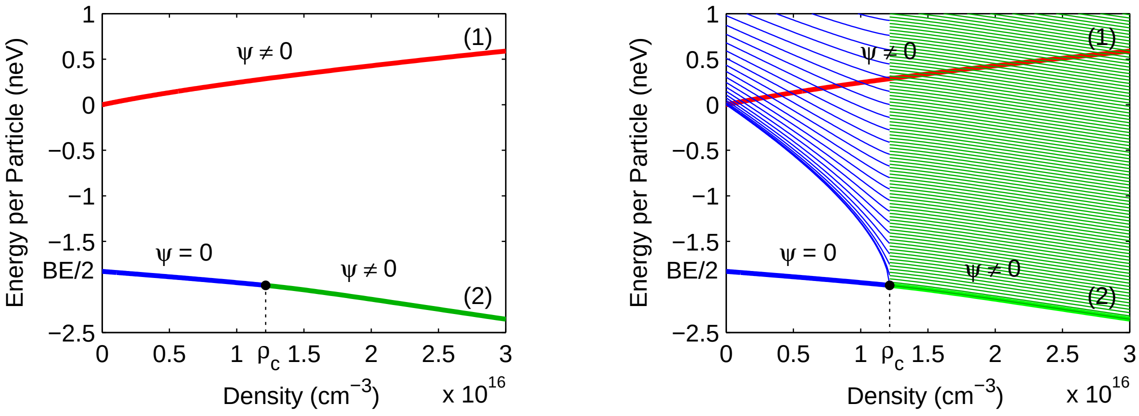
$$\begin{aligned}\Omega &= 2\,\omega(\mathbf{q})\\ &= 2\sqrt{(q^2+\mu)^2-\xi^2}\,.\end{aligned} \tag{5.104}$$

As pointed out in Section 4.3.2, Ω, is interpreted as the energy of two free quasi-bosons and therefore must belong to a continuum. More quantitatively, there is no $\mathbf{q}$ dependence in Eqs. (5.103), hence it must be concluded that the procedure involving the Fredholm alternative only gives the discrete part of the excitations.

We note that unlike the discrete elements, the continuum can be obtained from arguments based on the construction of the inverse. As the form of $h(\mathbf{q})$ is the same regardless of whether $\psi = 0$ or $\psi \neq 0$, Eq. (5.104) can be used to find the continuum for the entire lower state. It can be seen that at zero total momentum, these excitations are parametrized by q^2, with the lowest energy obtained for $\mathbf{q} = 0$. Thus, the continuum boundary is given by the sum of the energy per particle, e, and half of the quasi-bosons' energy, Ω, (5.104):

$$E_{exc} = e + \sqrt{\mu^2-\xi^2}\,. \tag{5.105}$$

As shown in Fig. 5.2(b), this threshold lies above the $\psi = 0$ solution ($\mu \neq \xi$), but intersects with the collapsing state at the critical point, after which it coincides with the $\psi \neq 0$ piece ($\mu = \xi$). Hence the continuum contains the zero mode for the second piece of the collapsing solution. Furthermore, it is now possible to give the decay found in Sec. 5.6 a more concrete physical explanation. Note that the state associated with the complex-valued μ has a corresponding energy per particle that lies inside the continuum of the lower state. Due to energy conservation, the upper solution must evolve into a state that is at the same level. Since there are many excited states within its neighborhood, the decay must represent a transition into collective phonon excitations of the lower state. Because this lower state tends toward collapse, it is assumed that its excitations will follow suit. In this picture, the condensate is lost through decay into another state, as opposed to a physical loss of particles. Of course, as the system collapses, qusiparticles will emerge thus causing a kinematical atom loss of this kind. However, the previous analysis is only valid for dilute systems, as such interactions were not incorporated into the model Hamiltonian of (5.2).



(a) (b)

Figure 5.2: For the case of ^{85}Rb, (a) shows the real part of the energy per particle, $e = u/\rho$ [see Eqs. (5.40), (5.41)] corresponding to the decaying excited state (1). Below this is shown the two-piece collapsing ground state (2) as shown in Fig. 5.1. All results are shown for an applied magnetic field of 162.3G, corresponding to a full s-wave scattering length of 193 Bohr radii. (b) The same curves as in (a), where the hatched regions indicate the continuum of modes belonging to the collapsing lower state. As discussed in the text, the excited "false vacuum" always lies in the continuum of the lower state, thus indicating that the decay represents a transition into collective phonon excitations of the collapsing solution. Note that the density of states for $\psi \neq 0$ is greater than that for $\psi = 0$, as shown by the relative density of the hatched lines above each region.

Chapter 6

Condensate Decay in General

Due to its simplicity, atomic hydrogen was first considered as the ideal candidate for the production of atomic condensates. Consequently, much of the current understanding of BEC physics has its roots in the initial studies of cold hydrogen gas samples. Experimentally, it was observed that these dilute samples were unstable, displaying an increasing atom loss with increasing density. Since relatively high density is required to achieve condensation, it became necessary to explore this decay phenomenon that threatened potentially severe limitations on the attainability of BEC. Although molecule formation had been long recognized as the driving force behind atom loss, the exact kinetic mechanism through which it manifested was at first poorly understood. To fit the experimental observations, a three-body process was eventually identified as being primarily responsible for the loss[1]. Specifically, a three-body recombinant event occurs when an atom causes a molecule to relax into a deeply bound state, releasing its binding energy, resulting in the expulsion of both atom and molecule from the trap (see Fig. 6.1). Although the initial hydrogen gas samples were cold, they were relatively far from quantum degeneracy thereby allowing them to be described classically. As such, the proposed recombinant model was completely consistent with the theoretical framework underpinning the description of these gases.

Although widely accepted, the classical recombinant picture is inconsistent with the notion that a BEC is a single macroscopic quantum object. Because all condensate particles have the same wave function, they can no longer be isolated and treated in an independent kinematic fashion. For example, the proposal of a three-body recombinant event implies that *all particles must simultaneously participate* in the collision, which presents a contradiction. Therefore, isolating the interactions between any two or three constituents becomes a meaningless exercise that should be replaced by a picture treating the behavior of the entire collective.

Given these observations, it becomes tempting to attribute the condensate loss to the coherent mechanism described in the last chapter. To determine whether there is a fit with empirical data, the ^{87}Rb coherent rate is calculated then compared to observation. In the ^{87}Rb experiments, the mean density is $\sim 10^{14}\text{cm}^{-3}$ whereas the scattering length is 5.8nm. By Eq. (5.45), this corresponds to a lifetime of $1/\Gamma \sim 3.6$ms , which is far too quick to be consistent with the observed 16 s. However, it must be remembered that this decay rate was obtained for the specific case of a zero-range attractive background interaction, which may not be applicable to the example at hand. Therefore, we turn back to the more general Hamiltonian of Eq. (5.1) for further analysis.

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[1] H. F. Hess (1983); L. P. H. de Goey (1988).

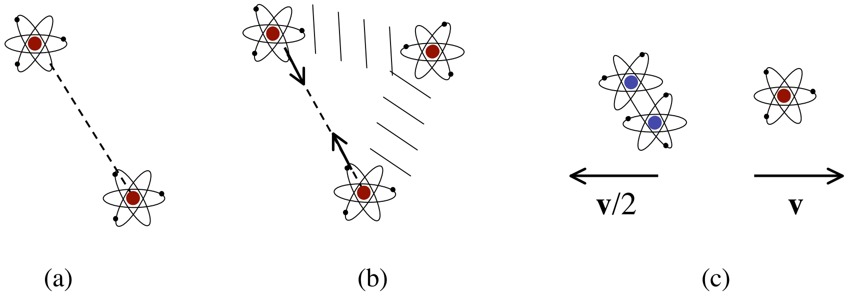

Figure 6.1: A schematic illustrating the three-body recombinant process. (a) An excited molecular state existing in the condensate. (b) A condensate atom in close proximity will perturb the excited pair, causing it to relax into a deeply bound dimer. (c) In this relaxation process, the binding energy is released, being transferred into kinetic energy of the condensate atom and the newly formed dimer. If sufficiently energetic, the products acquire sufficient velocity to overcome the trapping potential.

Section 6.1 reviews the three-body model, providing a quantitative fit to the experimental loss curves. Following this, we examine the general Hamiltonian in Secs. 6.2 and 6.3, arriving at an expansion for the decay rate which contains all the terms $\rho^{3/2}$, ρ^2, $\rho^{5/2}, \ldots$. The dominant lowest order term is seen to compare favorably with the data, where the fit determines the interaction strength. Hence, the decay curve is directly related to parameters in the potential. Finally, Section 6.4 compares the coherent rate with the semi-classical three-body model.

6.1 Three-Body Recombination

Classically, one, two or three-body loss rates are proportional to their corresponding power of the density. For example, a general process containing all three is described by

$$\frac{1}{\rho}\frac{d\rho}{dt} = -L\,\rho^2 - G\,\rho - \frac{1}{\tau_0} \tag{6.1}$$

where L is the three-body rate constant, proportional to a^4 for large, positive scattering lengths, a[1]. Likewise, G is the two-body rate constant describing spin dipole relaxation, a process dependent upon the interaction of atoms with the magnetic trapping fields. Lastly, τ_0 represents a one-body lifetime due to collisions with background gases left in the vacuum chamber after pumping.

Even after the production of BECs in both sodium[2] and rubidium[3], the three-body

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[1] The a^4 dependence has been predicted in many theoretical studies. See, for example, P. O. Fedichev (1996) and P. F. Bedaque (2000). In the experiment by T. Weber (2003), there was sufficient heating of the samples to admit classical recombinant descriptions.

[2] K. B. Davis (1995).

[3] M. H. Anderson (1995).

mindset remained well entrenched in the psyche of atomic physicists who applied it to the losses observed in condensates[1]. In a trapping geometry, it is possible to obtain an equation governing the time evolution of the particle number N, an observable that is directly measurable in such experiments. Assuming a Thomas-Fermi (parabolic) profile, the density has the form[2]

$$\rho(\mathbf{r}) = \frac{1}{2} m\bar{\omega}^2 \, \frac{m}{4\pi\hbar^2 a} \left(r_0^2 - r^2\right), \tag{6.2}$$

where $\bar{\omega} = (\omega_x \, \omega_y \, \omega_z)^{1/3}$ is the mean trap frequency. The condensate radius, r_0, is related to the particle number, N, by

$$r_0 = \left(15\, a\, N \, \frac{\hbar^2}{m^2 \bar{\omega}^2}\right)^{1/5}, \tag{6.3}$$

which is found from the normalization $N = \int d^3 r \rho(r)$. With the density as the weighting function, the average of any quantity, f is

$$\langle f \rangle = \frac{1}{N} \int_{\mathbf{r}} f(\mathbf{r})\, \rho(\mathbf{r})\,. \tag{6.4}$$

Thus, the density-averaged loss rates of two and three body collisions are respectively given by $-G \int \rho(\mathbf{r})^2 = -G\langle\rho\rangle N$ and $-L \int \rho(\mathbf{r})^3 = -L\langle\rho^2\rangle N$. Using the Thomas-Fermi profile of (6.2) the integrals are readily found to be $\langle\rho\rangle = c_2 N^{2/5}$ and $\langle\rho^2\rangle = c_3 N^{4/5}$, with $c_2 = \left[15^{2/5}/(14\pi)\right]\left[m\bar{\omega}/(\hbar\sqrt{a})\right]^{6/5}$ and $c_3 = (7/6)c_2^2$. Hence, the density averaged rate equation is

$$\frac{1}{N}\frac{dN}{dt} = -L\, c_3\, N^{4/5} - G\, c_2\, N^{2/5} - \frac{1}{\tau_0}\,. \tag{6.5}$$

Defining $x \equiv N^{1/5}$ from which $\dot{N} = 5\, x^4\, \dot{x}$, an analytic solution to (6.5) can be obtained by an integration. After some algebra, the result is

$$\begin{aligned} &\ln\left[\frac{\left(4\, L\, c_3\right)^{-1} N^{4/5}}{L c_3\, N^{4/5} + G c_2\, N^{2/5} + 1/\tau_0}\right] + \frac{4}{5\tau_0}\left(t - t_0\right) \\ &+ \frac{2\, G c_2}{\left|\sqrt{G^2\, c_2^2 - 4\, L c_3/\tau_0}\right|} \tan^{-1}\left(\frac{\left|\sqrt{G^2\, c_2^2 - 4 L c_3/\tau_0}\right|}{2\, L c_3\, N^{2/5} + G\, c_2}\right) = 0\,, \end{aligned} \tag{6.6}$$

where

$$t_0 = \frac{5\tau_0}{4} \ln\left(\frac{N_0^{4/5}}{4L^2 c_3^2\, N_0^{4/5} + 4L\, c_3/\tau_0}\right). \tag{6.7}$$

Fitting the time dependent condensate number, $N(t)$, to the experimental loss curves for ^{87}Rb, results in an optimal fit corresponding to all three-body losses with no two-body

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[1] Experimental loss curves can be found in J. Söding (1999).

[2] For more detail in this application of the Thomas-Fermi profile, see Y. Castin and R. Dum, (1996).

contribution $G = 0$[1]. In the case where three-body losses dominate, (6.6) can be solved explicitly for the atom number

$$N(t) = \left[\frac{4Lc_3}{\tau_0} \, \frac{e^{-4(t-t_0)/(5\tau_0)}}{1 - 4L^2 c_3^2 \, e^{-4(t-t_0)/(5\tau_0)}} \right]^{5/4} . \tag{6.8}$$

Depicted in Fig. 6.6, the fit of this equation to the observed losses in ^{87}Rb yields a three-body rate constant of $L = 2.23 \times 10^{-29} \text{cm}^6 \text{s}^{-1}$ and a one-body rate of $\tau_0 = 14.8$s. The closeness of this fit provides compelling evidence for the three-body model.

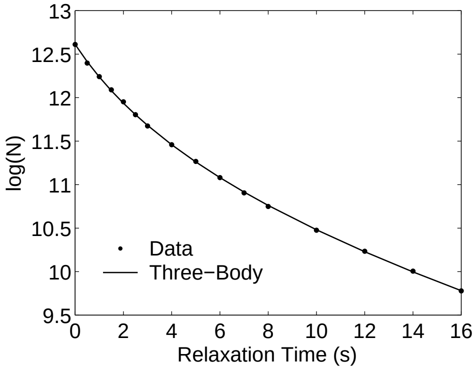

Figure 6.2: Fit of Eq. (6.8) to the loss data of ^{87}Rb. The best fit three-body rate coefficient is found to be $L = 2.23 \times 10^{-29} \text{cm}^6 \text{s}^{-1}$, whereas the one-body time constant is $\tau_0 = 14.8$ s.

6.2 Hamiltonian With a Potential and Molecular Coupling

6.2.1 General Form Factor

Using a general form factor in the separable potential, the method in Sec. (4.2) is used to calculate the pressure corresponding to the Hamiltonian of (5.1)

$$\begin{aligned}
-P = \frac{1}{\mathcal{V}} \langle \hat{H} - \mu \hat{N} \rangle = {} & \int_{\mathbf{k}}' (k^2 - \mu) R(\mathbf{k}) - \frac{1}{2} \mu \psi^2 + \frac{\lambda}{2} \left[\int_{\mathbf{k}}' v(\mathbf{k}) D(\mathbf{k}) \right]^2 + \lambda \frac{1}{2} \psi^2 \int_{\mathbf{k}}' v(\mathbf{k}) D(\mathbf{k}) \\
& + \lambda \int_{\mathbf{k}\,\mathbf{k}'}' v\Big(\frac{\mathbf{k} + \mathbf{k}'}{2} \Big)^2 R(\mathbf{k}) R(\mathbf{k}') + \lambda \psi^2 \int_{\mathbf{k}}' v(\mathbf{k}) R(\mathbf{k}) + \frac{\lambda}{8} \psi^4 \\
& + \Big(\frac{1}{2} \epsilon - \mu \Big) \phi^2 + \alpha \phi \Big[\int_{\mathbf{k}}' v(\mathbf{k}) D(\mathbf{k}) + \frac{1}{2} \psi^2 \Big] ,
\end{aligned} \tag{6.9}$$

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[1] This fit was done in J. Söding (1999). Interestingly, these authors could not find the analytic solution (6.6) for combined two and three body losses.

where $v(0) = 1$. Due to the uniform medium, the fluctuations are diagonal, as in (4.24). The variation on G leads to

$$\frac{\delta P}{\delta G} = 0 \Rightarrow G(\mathbf{k}) = \frac{1}{2}\sqrt{\frac{k^2+\gamma(\mathbf{k})^2+\xi(\mathbf{k})}{k^2+\gamma(\mathbf{k})^2-\xi(\mathbf{k})}}\,. \tag{6.10a}$$

Although having the same form as (5.6a), the quantities γ^2 and ξ are now momentum dependent due to the general form factor:

$$\gamma(\mathbf{k})^2 = -\mu + 2\,\lambda \int_{\mathbf{k}'}' v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)^2 R(\mathbf{k}') + \lambda\, v(\mathbf{k})\,\psi^2 \tag{6.10b}$$

$$\xi(\mathbf{k}) = \Big[\lambda \int_{\mathbf{k}'}' v(\mathbf{k}')D(\mathbf{k}') + \lambda\,\frac{1}{2}\,\psi^2 + \alpha\phi\Big]\, v(\mathbf{k})\,. \tag{6.10c}$$

Extremizing on the mean fields, ψ and ϕ, gives

$$\frac{\delta P}{\delta\psi} = \Big[-\mu + \lambda \int_{\mathbf{k}}' v(\mathbf{k})D(\mathbf{k}) + 2\,\lambda \int_{\mathbf{k}}' v(\mathbf{k})R(\mathbf{k}) + \lambda\,\frac{1}{2}\,\psi^2 + \alpha\phi\Big]\,\psi = 0 \tag{6.11a}$$

$$\frac{\delta P}{\delta\phi} = 0 \Rightarrow \phi = -\frac{\alpha}{\epsilon - 2\mu}\Big[\int_{\mathbf{k}}' v(\mathbf{k})D(\mathbf{k}) + \frac{1}{2}\,\psi^2\Big]\,. \tag{6.11b}$$

Equations (6.10) and (6.11) lead to the equation of state for the uniform medium, once the form factor is specified.

6.2.2 Step Function Form Factor

Given some momentum cutoff, K, we define a step function form factor, as in (2.111). The definition of ξ in (6.10c) then becomes

$$\begin{aligned}\xi(\mathbf{k}) &= \Big[\lambda \int_{\mathbf{k}'}' v(\mathbf{k}')D(\mathbf{k}') + \lambda\,\frac{1}{2}\,\psi^2 + \alpha\phi\Big]\,\theta(K - |\mathbf{k}|) \\ &= \xi\,\theta(K - |\mathbf{k}|)\,.\end{aligned} \tag{6.12}$$

where ξ is the constant $\lambda \int_{\mathbf{k}'} v(\mathbf{k}')D(\mathbf{k}') + (\lambda/2)\psi^2 + \alpha\phi$. Since $\xi(\mathbf{k})$ assumes a step function form as well, G can be written as

$$G(\mathbf{k}) = \begin{cases} \dfrac{1}{2}\sqrt{\dfrac{k^2+\gamma(k)^2+\xi}{k^2+\gamma(k)^2-\xi}} & k \le K \\[2ex] \dfrac{1}{2} & k > K\,. \end{cases} \tag{6.13}$$

When substituted into the definition of the fluctuations (4.24), this form of G gives

$$R(\mathbf{k}) = \frac{1}{2}\left[\frac{k^2+\gamma(k)^2}{\sqrt{[k^2+\gamma(k)^2]^2-\xi^2}}-1\right]\theta(K-|\mathbf{k}|) \tag{6.14a}$$

$$D(\mathbf{k}) = -\frac{\xi}{2}\frac{1}{\sqrt{[k^2+\gamma(k)^2]^2-\xi^2}}\,\theta(K-|\mathbf{k}|)\,. \tag{6.14b}$$

Therefore, it is only required to find $\gamma(\mathbf{k})^2$ for $0 \le |\mathbf{k}| < K$, since all fluctuations vanish outside that range. Within this range, however, $\gamma(\mathbf{k})^2$ depends on $\mathbf{k}$ through a convolution integral:

$$\gamma(\mathbf{k})^2 = -\mu + 2\,\lambda \int'_{\mathbf{k}'} v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)^2 R(\mathbf{k}') + \lambda\,\psi^2\,. \tag{6.15}$$

Since $R(\mathbf{k}')$ is inside the integral, $\mathbf{k}'$ is also limited to the range $0 \le |\mathbf{k}'| < K$. In addition, (6.15) can be simplified by recognizing that the square of the form factor remains a step function:

$$v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)^2 = \theta\Big(K - \frac{1}{2}\sqrt{k^2+k'^2+2\,k\,k' cos\varphi}\Big)\,, \tag{6.16}$$

where φ is the angle between $\mathbf{k}$ and $\mathbf{k}'$. Since both $|\mathbf{k}| = k$ and $|\mathbf{k}'| = k'$ are less than the momentum cutoff, it follows that the square root of the step function's argument must be less than or equal to $2\,K$:

$$\begin{aligned}\sqrt{k^2+k'^2+2\,k\,k' cos\varphi} &\le k + k' \\ &\le 2\,K\,.\end{aligned} \tag{6.17}$$

These inequalities prove that the squared form factor must always be equal to 1 inside the integral of R, thereby allowing the replacement $\int_{\mathbf{k}'} v[(1/2)(\mathbf{k}+\mathbf{k}')]^2 R(\mathbf{k}') = \int_{\mathbf{k}} R(\mathbf{k})$, from which we see that γ is independent of momentum. Concerned only with the range where $|\mathbf{k}| < K$, the step functions are dropped, being replaced with the understanding that there is a momentum cutoff, K, implicit in the limits of all integrals. From these considerations, the variational equations assume the following forms:

$$G(\mathbf{k}) = \frac{1}{2}\sqrt{\frac{k^2+\gamma^2+\xi}{k^2+\gamma^2-\xi}} \Rightarrow \begin{cases} R(\mathbf{k}) = \dfrac{1}{2}\Big[\dfrac{k^2+\gamma^2}{\sqrt{(k^2+\gamma^2)^2-\xi^2}}-1\Big] \\ D(\mathbf{k}) = -\dfrac{\xi}{2}\dfrac{1}{\sqrt{(k^2+\gamma^2)^2-\xi^2}} \end{cases} \tag{6.18}$$

$$\gamma^2 = -\mu + 2\,\lambda \int'_{\mathbf{k}} R(\mathbf{k}) + \lambda\,\psi^2 \tag{6.19}$$

$$\xi = \lambda \int'_{\mathbf{k}} D(\mathbf{k}) + \lambda\,\frac{1}{2}\,\psi^2 + \alpha\phi \tag{6.20}$$

$$\left(\gamma^2 + \xi - \lambda\psi^2\right)\psi = 0 \tag{6.21}$$

$$\phi = -\frac{\alpha}{\epsilon - 2\mu}\left[\int_{\mathbf{k}}' D(\mathbf{k}) + \frac{1}{2}\,\psi^2\right] \tag{6.22}$$

Due to their dependence on the interaction strength, λ, these equations are generalizations of the zero-range case (5.6). In the next section, we explore the possibility that this increased flexibility could be used to account for a coherent decay that is consistent with the observed lifetime in the ordinary BECs[1].

6.3 Quantum Instability

In Sec. (5.6), a complex chemical potential arose because of the requirement of a positive pressure. Since $\gamma^2 = -\mu$ in the zero-range limit, a positive pressure demands a negative γ^2 to lowest order in density. This led to much too fast of a decay to be an accurate model of ordinary condensate behavior. Because the imaginary part of G depends on the size of γ^2, it is reasonable to suspect that making γ^2 less negative will decrease the decay rate. According to Eq. (6.20), γ^2 is arbitrary since it depends on the unknown strength, λ. In addition, by making λ sufficiently large such that $\gamma^2 > 0$, G can become imaginary if $|\xi| > |\gamma^2|$. A focal point in solving the above set of equations lies in determining γ^2 in terms of ξ. Substitution of the molecular field (6.22) into (6.20) gives

$$\xi = \left(\lambda - \frac{\alpha^2}{\epsilon - 2\mu}\right)\left[\int_{\mathbf{k}}' D(\mathbf{k}) + \frac{1}{2}\,\psi^2\right]. \tag{6.23}$$

Due to the fact that there is no a priori way to determine λ, it must be decided at the outset the size of the ratio $|\xi|/|\gamma^2|$, for which there are three regimes of interest: (i) $|\xi| < |\gamma^2|$, (ii) $|\xi| \sim |\gamma^2|$ and (iii) $|\xi| > |\gamma^2|$. Because of these possibilities, two expansions are made. Depending on the regime, we first expand for the appropriate ratio of $|\xi|$ to $|\gamma^2|$, which is then followed by an expansion for low density. In all three regimes, it is assumed that both ξ and γ^2 are less than the momentum cutoff, K.

6.3.1 Case (i): $|\xi| < |\gamma^2|$

Expanding (6.23) requires the expansions of $\int_{\mathbf{k}} R(\mathbf{k})$, $\int_{\mathbf{k}} D(\mathbf{k})$, ψ^2 and μ. To order ξ^2/γ^4, the fluctuation terms are

$$\int_{\mathbf{k}}' R(\mathbf{k}) \simeq \frac{1}{32\pi}\frac{\xi^2}{\gamma} - \frac{\xi^2}{8\pi^2}\frac{1}{K} \tag{6.24a}$$

$$\int_{\mathbf{k}}' D(\mathbf{k}) \simeq -\frac{K}{4\pi^2}\,\xi + \frac{1}{8\pi}\,\xi\gamma\left(1 - \frac{1}{16}\frac{\xi^2}{\gamma^4}\right) - \frac{\xi\gamma^2}{4\pi^2}\frac{1}{K}\,, \tag{6.24b}$$

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[1] "Ordinary condensates" refer to cases like ^{23}Na or ^{87}Rb, where condensates are produced without the need to tune the scattering length.

where we have also expanded for $\gamma \ll K$. Further details may be found in Appendix C.

Because the case of nonvanishing ψ is of interest here, the solution to (6.21) is taken to be

$$\frac{1}{2}\,\psi^2 = \frac{\gamma^2+\xi}{2\,\lambda} \tag{6.25}$$

Along with expansions (6.24), equation (6.19) can be used in explicitly obtaining μ in terms of γ and ξ:

$$\begin{aligned} \mu &= -\gamma^2 + 2\,\lambda \int_{\mathbf{k}}' R(\mathbf{k}) + \lambda\,\psi^2 \\ &= \xi + \frac{\lambda}{16\pi}\,\frac{\xi^2}{\gamma} + \ldots \end{aligned} \tag{6.26}$$

Substitution of these results into (6.23) gives the desired relationship between γ^2 and ξ:

$$\begin{aligned} \xi = &\left[\lambda - \frac{\alpha^2}{\epsilon} - \frac{2\alpha^2}{\epsilon^2}\left(\xi + \frac{\lambda}{16\pi}\,\frac{\xi^2}{\gamma} - \frac{\lambda}{4\pi^2}\,\frac{1}{K}\,\xi^2\right) + \ldots\right] \\ &\times \left[-\frac{\xi}{4\pi^2}\,K + \frac{1}{8\pi}\,\xi\gamma\left(1 - \frac{1}{16}\,\frac{\xi^2}{\gamma^4}\right) - \frac{\xi\gamma^2}{4\pi^2}\,\frac{1}{K} + \frac{\xi+\gamma^2}{2\,\lambda} + \ldots\right], \end{aligned} \tag{6.27}$$

where the denominator $\epsilon - 2\mu$ in (6.23) has been approximated by $(1/\epsilon)(1+2\mu/\epsilon)$.

Finally, we expand γ^2 in powers of $\sqrt{\xi}$:

$$\gamma = \gamma_1\sqrt{\xi} + \gamma_2\xi + \gamma_3\xi^{3/2} + \ldots \tag{6.28a}$$

$$\gamma^2 = \gamma_1^2\,\xi + 2\,\gamma_1\gamma_2\,\xi^{3/2} + (2\gamma_1\gamma_3 + \gamma_2^2)\,\xi^2 + \ldots\,, \tag{6.28b}$$

The first two coefficients, γ_1 and γ_2, are determined by using (6.28) in (6.27) then keeping terms only up to order $\xi^{3/2}$,

$$\xi = \left(\lambda - \frac{\alpha^2}{\epsilon}\right)\left\{\left(\frac{\gamma_1^2+1}{2\,\lambda} - \frac{K}{4\pi^2}\right)\xi + \left[\frac{\gamma_1}{8\pi}\left(1 - \frac{1}{16\,\gamma_1^4}\right) + \frac{\gamma_1\,\gamma_2}{\lambda}\right]\xi^{3/2}\right\} \tag{6.29}$$

Defining the new strength

$$\lambda' = \frac{\lambda}{8\pi a}\,, \tag{6.30}$$

the coefficients are found by equating like powers of ξ in (6.28):

$$\gamma_1^2 = 2\,\lambda' - 1\,, \tag{6.31a}$$

$$\gamma_2 = -a\,\lambda'\left[1 - \frac{1}{16\,(2\lambda'-1)^2}\right]. \tag{6.31b}$$

Like before, the scattering length is related to the strength and the range by $(8\pi a)^{-1} = \lambda^{-1} + K/(4\,\pi^2)$ [see (2.110)].

Obtaining the low-density chemical potential requires three more steps. First, the density is expanded in powers of $\sqrt{\xi}$. Second, this expansion is inverted to give ξ as an expansion in $\sqrt{\rho}$, which is finally inserted into the expression for μ.

Starting from its definition, the density is obtained from ψ^2 and $\int D$ as

$$\begin{aligned}
\rho &= \frac{1}{2}\,\psi^2 + \int_{\mathbf{k}}' R(\mathbf{k}) + \phi^2 \\
&\simeq \frac{1}{2\,\lambda}\left(\xi + \gamma_1^2\xi + 2\,\gamma_1\gamma_2\,\xi^{3/2}\right) + \frac{1}{32\,\pi}\,\frac{1}{\gamma_1}\,\xi^{3/2} \\
&= \frac{\xi}{8\pi a} + f\,\xi^{3/2}\,. \qquad (6.32)
\end{aligned}$$

In the last line, use has been made of (6.30), (6.31), as well as the definition

$$f = \frac{1}{32\pi}\,\frac{1}{\sqrt{2\lambda' - 1}} - \frac{\sqrt{2\lambda' - 1}}{8\pi}\left[1 - \frac{1}{16(2\lambda' - 1)^2}\right]. \qquad (6.33)$$

Obtaining ξ in terms of ρ requires the inversion of (6.32). To avoid dealing with square roots, define $\xi \equiv \eta^2$ and $\rho \equiv \sigma^2$, then expand η in σ. Only terms up to order σ^2 are kept in the expansion of η^2 and η^3:

$$\eta = \eta_1\,\sigma + \eta_2\,\sigma^2 + \dots \qquad (6.34a)$$

$$\eta^2 = \eta_1^2\,\sigma^2 + 2\,\eta_1\eta_2\,\sigma^3 + \dots \qquad (6.34b)$$

$$\eta^3 = \eta_1^3\,\sigma^3 + \dots\,, \qquad (6.34c)$$

where η_1, η_2 and η_3 are to be determined. Inserting the expansions of η into (6.32) gives

$$\sigma^2 = \frac{1}{8\pi a}\left(\eta_1^2\,\sigma^2 + 2\,\eta_1\eta_2\,\sigma^3\right) + f\,\eta_1^3\,\sigma^2\,, \qquad (6.35)$$

from which is found

$$\eta_1 = \sqrt{8\pi a} \qquad (6.36a)$$

$$\eta_1\eta_2 = -4\pi a\,f\,(8\pi a)^{3/2}\,. \qquad (6.36b)$$

Substitution of theses coefficients into (6.34b) completes the inversion

$$\xi = 8\pi a\rho - (8\pi a)^{5/2}\,f\,\rho^{3/2} + \dots \qquad (6.37)$$

Finally, the chemical potential is obtained from (6.26), (6.28a), (6.31a), (6.33) and (6.37):

$$\mu = \xi + \frac{\lambda}{16\pi}\frac{1}{\gamma_1}\xi^{3/2} \tag{6.38}$$

$$= 8\pi a\,\rho + \frac{1}{8\pi}\left(2\,\lambda' - 1\right)^{-3/2}\left(5\lambda'^2 - 5\lambda' + \frac{19}{16}\right)\left(8\pi a\right)^{5/2}\rho^{3/2} + \dots\,. \tag{6.39}$$

If $2\lambda' < 1$, then there is an imaginary part to μ which gives a decay constant of

$$\Gamma = \frac{\hbar}{2m}\frac{1}{4\pi}\left(2\lambda' - 1\right)^{-3/2}\left(5\lambda'^2 - 5\lambda' + \frac{19}{16}\right)\left(8\pi a\right)^{5/2}\rho^{3/2} + \dots\,. \tag{6.40}$$

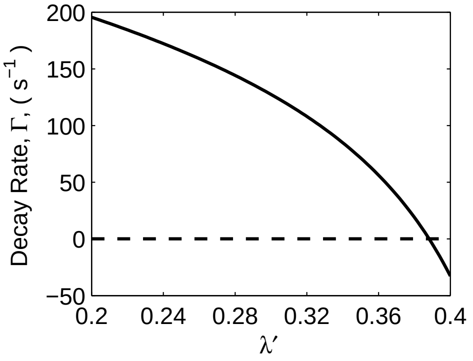

Figure 6.3: For the case of ^{87}Rb at a mean density of 10^{16} cm^{-3}, the solid line shows the rate in Eq. (6.40) plotted as a function of the strength λ' (6.30). In this case, the coherent rate is consistent with the observed rate (dashed line) around the point of intersection at $\lambda' \sim 0.39$. However, by Eq. (6.28b), this is inconsistent with the initial assumption that $|\xi|/|\gamma^2| < 1$

Figure 6.3 shows a plot of this rate as a function of λ' indicating that, to be consistent with observed losses, the value of λ' must be ~ 0.39. This corresponds to $\gamma_1^2 \sim -0.22$ which, when substituted into the leading order term of (6.28b), reveals that $|\xi|/|\gamma^2| \sim 4.5$, a result inconsistent with the original expansion assumption, $|\xi|/|\gamma^2| < 1$.

By the solution of γ_1 (6.31a), it follows that only an attractive interaction, $\lambda \leq 0$, can simultaneously satisfy both the original assumption and the condition for decay $2\lambda' - 1 < 0$. Unfortunately, this leads to rates that are too large to be consistent with experimental observations. Evidently, the more attractive the potential, the faster the decay. Clearly, the other cases must be considered where there is a bound molecular state, yet the potential is sufficiently repulsive to admit a decay rate consistent with measurement.

6.3.2 Case (ii): $|\xi| \sim |\gamma^2|$

For this case, it is convenient to expand ξ in powers of γ:

$$\xi = \xi_0\gamma^2 + \xi_1\gamma^3 + \dots \tag{6.41}$$

By assumption, the first term is the dominant contribution, whereas the second is a small correction. To order γ^3 (C.17) and (C.24) give the fluctuations,

$$\int_{\mathbf{k}}' D(\mathbf{k}) \simeq -\frac{K}{4\pi^2}\,\xi_0\,\gamma^2 + \left(d_1 - \frac{K}{4\pi^2}\,\xi_1\right)\gamma^3 \tag{6.42a}$$

$$\int_{\mathbf{k}}' R(\mathbf{k}) \simeq r_1\,\gamma^3\,, \tag{6.42b}$$

where the dependence of d_1 and r_1 on ξ_0 and ξ_1 can be respectively found in (C.18a) and (C.25). The coefficients ξ_0 and ξ_1 are determined from (6.23), which to order γ^3 can be written as

$$\begin{aligned}\epsilon\,\xi_0\,\gamma^2 + \epsilon\,\xi_1\,\gamma^3 = -\frac{K}{4\pi^2}\,\xi_0\left(\lambda\epsilon - \alpha^2\right)\gamma^2 + \left(d_1 - \frac{K}{4\pi^2}\,\xi_1\right)\left(\lambda\epsilon - \alpha^2\right)\gamma^3 \\ + \left(\lambda\epsilon - \alpha^2\right)\frac{1}{2\lambda}\left(1 + \xi_0\right)\gamma^2 + \left(\lambda\epsilon - \alpha^2\right)\frac{1}{2\lambda}\,\xi_1\,\gamma^3\,.\end{aligned} \tag{6.43}$$

Equating like powers of γ, the solutions are

$$\xi_0 = \frac{1}{2\,\lambda' - 1} \tag{6.44a}$$

$$\xi_1 = \frac{2\,\lambda\,d_1}{2\,\lambda' - 1}\,, \tag{6.44b}$$

where λ' is defined in (6.30) and d_1 in (C.18a).

Following the same basic method as in Case (i), the density up to order γ^3 is

$$\begin{aligned}\rho &\simeq \frac{\xi + \gamma^2}{2\lambda} + r_1\,\gamma^3 \\ &= \frac{1}{2\lambda}\left(\xi_0 + 1\right)\gamma^2 + \left(\frac{\xi_1}{2\lambda} + r_1\right)\gamma^3\,.\end{aligned} \tag{6.45}$$

Since it is small at low density, γ can be expanded in powers of $\sigma = \sqrt{\rho}$. To order σ^3 we have

$$\gamma = \gamma_0\,\sigma + \gamma_1\,\sigma^2 + \gamma_2\,\sigma^3 \tag{6.46a}$$

$$\gamma^2 = \gamma_0^2\,\sigma^2 + 2\gamma_0\,\gamma_1\,\sigma^3 \tag{6.46b}$$

$$\gamma^3 = \gamma_0^3\,\sigma^3 \tag{6.46c}$$

Inserting these expansions into the density yields

$$\sigma^2 = \frac{\xi_0 + 1}{2\lambda}\left(\gamma_0^2\,\sigma^2 + 2\,\gamma_0\,\gamma_1\,\sigma^3\right) + \left(\frac{\xi_1}{2\lambda} + r_1\right)\gamma_0^3\,\sigma^3\,, \tag{6.47}$$

from which the coefficients γ_0 and γ_1 are found to be

$$\gamma_0 = \sqrt{2\lambda - 8\pi a} \tag{6.48a}$$

$$2\gamma_0\gamma_1 = -\big(2\lambda - 8\pi a\big)^{5/2}\big(r_1 + \xi_0 d_1\big) \tag{6.48b}$$

Hence, to order $\rho^{3/2}$, the expansions of γ^2 and γ^3 are

$$\gamma^2 = \big(2\lambda - 8\pi a\big)\,\rho - \big(2\lambda - 8\pi a\big)^{5/2}\big(r_1 + \xi_0 d_1\big)\,\rho^{3/2} \tag{6.49a}$$

$$\gamma^3 = \big(2\lambda - 8\pi a\big)^{3/2}\rho^{3/2}\,. \tag{6.49b}$$

Using these results, the chemical potential in (6.19) is

$$\begin{aligned}\mu &= \xi + 2\lambda \int_{\mathbf{k}}' R(\mathbf{k}) \\ &= \xi_0\gamma^2 + \big(2\lambda r_1 + \xi_1\big)\,\gamma^3 \\ &= 8\pi a\,\rho + \big(2\lambda - 8\pi a\big)^{5/2}\big(r_1 + \xi_0 d_1\big)\,\rho^{3/2} \\ &= 8\pi a\,\rho + \frac{\sqrt{2}}{12\pi^2}\bigg[4 - 5\,\delta_0 + \left(\frac{11}{2} - 9\ln 2\right)\delta_0^2 + \left(3\ln 2 - \frac{1}{2}\right)\delta_0^3 \\ &\qquad + \frac{3}{128}\big(82 - 9\delta_0 - 11\delta_0^2\big)\,\delta_0^2\ln\delta_0\bigg]\,\lambda^{5/2}\rho^{3/2}\,.\end{aligned} \tag{6.50}$$

In the above, the last line follows from the simplification of $r_1 + \xi_0\, d_1$, given by (C.32). Also, from (C.13a) and (6.44a), δ_0 is identified as

$$\delta_0 = 1 - \frac{8\pi a}{\lambda}\,. \tag{6.51}$$

From this definition, the logarithm in (6.50) obtains a nonzero imaginary part only for $\lambda \lesssim 8\pi a$. By the expression for the full scattering length, $(8\pi a)^{-1} = (\lambda - \frac{\alpha^2}{\epsilon})^{-1} + b^{-1}$, this condition on λ is made possible by the inclusion of coupling to the molecular state ($\alpha \neq 0$). Under this assumption, the rate is given by

$$\Gamma = \frac{\hbar}{m}\,\frac{\sqrt{2}}{512\pi^2}\,\big(82 - 9\delta_0 - 11\delta_0^2\big)\,\delta_0^2\,\lambda^{5/2}\,\rho^{3/2}\,. \tag{6.52}$$

By Fig. 6.4, the fit of this rate is consistent with the initial assumption that $\xi \sim \gamma^2$. From the definition of λ' (6.30), this means that the strength is close to the scattering length $\lambda \lesssim 8\pi a$[1]. Given that λ is proportional to the scattering length, the rate roughly acquires an $a^{5/2}$ dependence, reminiscent of the result of the previous chapter. Hence, this is the required regime for coherent decay to apply in ordinary “stable” Bose condensed systems.

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[1] Interestingly, the Gross-Pitaevskii equation requires equality between these two quantities.

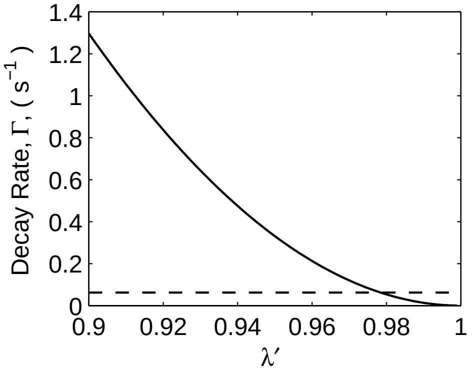

Figure 6.4: For the case of ^{87}Rb at a mean density of 10^{16} cm^{-3}, the solid line shows the rate in Eq. (6.52) plotted as a function of the strength λ' (6.30). In this case, the coherent rate is consistent with the observed rate (dashed line) around the point of intersection at $\lambda' \sim 0.98$. As a check, substitution of (6.44a) into Eq. (6.41) confirms that this fit is consistent with the initial assumption that $|\xi| \sim |\gamma^2|$

6.3.3 Case (iii): $|\xi| > |\gamma^2|$

According to (C.42) and (C.49), defining $\xi = i\eta$, then expanding the fluctuations in γ^2/η results in

$$\int_{\mathbf{k}}' D(\mathbf{k}) = -\frac{K}{4\pi^2}\, i\eta - I\, i\eta^{3/2} - \frac{1}{4\pi^2}\,\frac{1}{K}\,\frac{\gamma^2}{\eta}\, i\eta^2 + O\big(\eta^3\big) \tag{6.53a}$$

$$\int_{\mathbf{k}}' R(\mathbf{k}) = J\,\eta^{3/2} + \frac{1}{4\pi^2}\,\frac{1}{K}\,\frac{\gamma^4}{\eta^2}\,\eta^2 + O\big(\eta^3\big)\,, \tag{6.53b}$$

where I and J are themselves expansions in γ^2/η, given by (C.41d) and (C.50d), respectively. The chemical potential is

$$\begin{aligned}\mu &= -\gamma^2 + 2\lambda \int_{\mathbf{k}}' R(\mathbf{k}) + \lambda\,\psi^2 \\ &= i\eta + 2\lambda J\,\eta^{3/2} + \frac{\lambda}{2\pi^2}\,\frac{1}{K}\,\frac{\gamma^4}{\eta^2}\,\eta^2 + O\big(\eta^2\big)\,, \end{aligned} \tag{6.54}$$

which can be used in the equation (6.23) that determines γ^2 in terms of ξ[1]:

---

[1] Here, we have expanded $\alpha^2/\big(\epsilon - 2\mu\big)$ as was done in (6.27).

$$
\begin{aligned}
\xi &= \left[\lambda - \frac{\alpha^2}{\epsilon}\left(1 + \frac{2\mu}{\epsilon}\right)\right]\left[\int_{\mathbf{k}}' D(\mathbf{k}) + \frac{1}{2}\,\psi^2\right] \\
&= \left[\lambda - \frac{\alpha^2}{\epsilon} - \frac{2\alpha^2}{\epsilon^2}\big(i\eta + 2\lambda J\eta^{3/2}\big)\right]\left[-\frac{K}{4\pi^2}\,i\eta - I i\,\eta^{3/2} - \frac{1}{4\pi^2}\,\frac{1}{K}\,\frac{\gamma^2}{\eta} i\eta^2 + \frac{i\eta + \gamma^2}{2\lambda}\right].
\end{aligned}
\tag{6.55}
$$

In accordance with the assumption $|\xi| > |\gamma^2|$, γ^2 is expanded in powers of $\sqrt{\eta}$,

$$
\gamma = \gamma_1\sqrt{\xi} + \gamma_2\,\xi + \gamma_3\,\xi^{3/2} \tag{6.56a}
$$

$$
\gamma^2 = \gamma_1^2\, i\eta + 2\gamma_1\gamma_2\, i\sqrt{i}\,\eta^{3/2} - \big(\gamma_2^2 + 2\gamma_1\gamma_3\big)\,\eta^2\,. \tag{6.56b}
$$

With these expansions (6.55) can be solved to order η^2,

$$
\begin{aligned}
i\eta = \left(\lambda - \frac{\alpha^2}{\epsilon}\right)\Bigg\{ &- \frac{K}{4\pi^2}\, i\eta \\
&- \Big(I_1 - i\gamma_1^2 I_2 - 2i\sqrt{i}\gamma_1\gamma_2 I_2\sqrt{\eta} - \gamma_1^4 I_3 - 4\sqrt{i}\gamma_1^3\gamma_2 I_3\sqrt{\eta}\Big)\, i\eta^{3/2} \\
&+ \frac{1}{2\lambda}\Big[\big(1 + \gamma_1^2\big)\, i\eta + 2\gamma_1\gamma_2\, i\sqrt{i}\,\eta^{3/2} - \big(\gamma_2^2 + 2\gamma_1\gamma_3\big)\,\eta^2\Big] \\
&+ \left[\frac{1}{4\pi^2}\,\frac{\gamma_1^2}{K} + \left(\lambda - \frac{\alpha^2}{\epsilon}\right)^{-1}\left(-\frac{2\alpha^2}{\epsilon^2}\,\frac{K}{4\pi^2} + \frac{\alpha^2}{\epsilon^2}\,\frac{1}{\lambda}\big(1 + \gamma_1^2\big)\right)\right]\eta^2\Bigg\}\,,
\end{aligned}
\tag{6.57}
$$

where we have used the expansion of I in (C.41d). Equating like powers of η, the coefficients γ_1 and γ_2 are found to be

$$
\gamma_1^2 = 2\lambda' - 1 \tag{6.58a}
$$

$$
\gamma_1\,\gamma_2\,\sqrt{i} = \lambda I_1 - i\lambda\,\gamma_1^2\, I_2 - \lambda\,\gamma_1^4\, I_3\,. \tag{6.58b}
$$

Having expanded γ^2 in $\sqrt{\eta}$, the density equation is now used to obtain an expansion of $\sqrt{\eta}$ in $\sqrt{\rho}$. To order $\eta^{3/2}$ we have

$$
\begin{aligned}
\rho &= \frac{1}{2}\psi^2 + \int_{\mathbf{k}}' R(\mathbf{k}) + \phi^2 \\
&\simeq \frac{i\eta + \gamma^2}{2\lambda} + J\,\eta^{3/2} \\
&= \frac{1}{8\pi a}\, i\eta + \left[J_1 + iI_1 + \gamma_1^2\big(I_2 + iJ_2\big) + \gamma_1^4\left(\frac{3}{2}J_3 - iI_3\right)\right]\eta^{3/2}\,.
\end{aligned}
\tag{6.59}
$$

As in the previous two cases, (6.59) is inverted by expanding $\sqrt{\eta}$ in $\sigma = \sqrt{\rho}$:

$$\sqrt{\eta} = \eta_1\,\sigma + \eta_2\,\sigma^2 \tag{6.60a}$$

$$\eta = \eta_1^2\,\sigma^2 + 2\eta_1\eta_2\,\sigma^3 \tag{6.60b}$$

$$\eta^{3/2} = \eta_1^3\,\sigma^3\,. \tag{6.60c}$$

Substitution of (6.60) into (6.59) gives

$$\sigma^2 = \frac{1}{8\pi a}\,i\left(\eta_1^2\,\sigma^2 + 2\,\eta_1\eta_2\,\sigma^3\right) + \left[J_1 + iI_1 + \gamma_1^2\left(I_2 + iJ_2\right) + \gamma_1^4\left(\frac{3}{2}\,J_3 - iI_3\right)\right]\eta_1^3\,\sigma^3\,, \tag{6.61}$$

from which the coefficients are red off as

$$\eta_1 = \sqrt{-i\,8\pi a} \tag{6.62a}$$

$$2\,\eta_1\eta_2 = i\sqrt{i}\left[J_1 + i\,I_1 + \gamma_1^2\big(I_2 + i\,J_2\big) + \gamma_1^4\left(\frac{3}{2}\,J_3 - i\,I_3\right)\right]\big(8\pi a\big)^{5/2}\,. \tag{6.62b}$$

Using Eqs. (6.60) and (6.62), the chemical potential in (6.54) is

$$\begin{aligned}\mu &= i\eta + 2\lambda\,J\big(-i8\pi a\big)^{3/2}\,\rho^{3/2}\\ &= 8\pi a\,\rho - \sqrt{i}\left[J_1 + iI_1 + \gamma_1^2\big(I_2 + iJ_2\big) + \gamma_1^4\left(\frac{3}{2}\,J_3 - i\,I_3\right)\right]\big(8\pi a\big)^{5/2}\,\rho^{3/2}\\ &\quad + \sqrt{i}\,2\lambda\left(J_1 + i\gamma_1^2\,J_2 + \frac{3}{2}\gamma_1^4\,J_3\right)\big(8\pi a\big)^{3/2}\,\rho^{3/2}\,,\end{aligned} \tag{6.63}$$

thus corresponding to a decay rate of

$$\begin{aligned}\Gamma =& \frac{\hbar}{m}\,\frac{1}{\sqrt{2}}\left\{2\lambda'\left(J_1 + \gamma_1^2\,J_2 + \frac{3}{2}\,\gamma_1^4 J_3\right)\right.\\ &\left. - \left[J_1 + I_1 + \gamma_1^2\left(I_2 + J_2\right) + \gamma_1^4\left(\frac{3}{2}\,J_3 - I_3\right)\right]\right\}\big(8\pi a\big)^{5/2}\,\rho^{3/2}\,.\end{aligned} \tag{6.64}$$

As in the previous two cases, to lowest order we have $\gamma^2 \sim \gamma_1^2\,\xi$. Since $\gamma_1^2 = 2\lambda' - 1$, this series expansion converges the quickest for $\lambda' \sim 1/2$. By figure (6.5), the decay rate given by (6.64) only approaches the observed lifetime for $\lambda' \to 1$. As this limit is approached, however, the initial approximation $|\xi| > |\gamma^2|$, breaks down, thus indicating that Case (ii) is the best approximation.

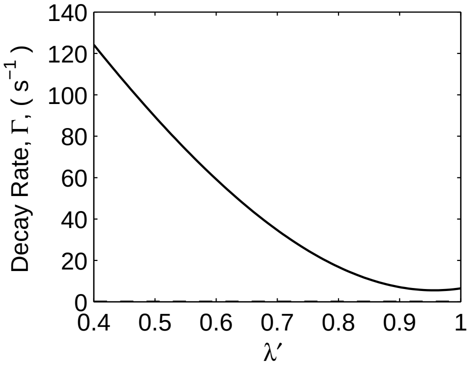

Figure 6.5: For the case of ^{87}Rb at a mean density of 10^{16} cm^{-3}, the solid line shows the rate in Eq. (6.64) plotted as a function of the strength λ' (6.30). In this case, the coherent rate cannot be fit to the observed rate (dashed line), but as λ' approaches 1, the initial approximation, $|\xi| > |\gamma^2|$, becomes less valid.

6.4 Quantum Instability vs. Three-Body Loss

Despite being inconsistent with the quantum mechanical nature of the BEC, the three-body model provides a description that is completely consistent with the observed losses as demonstrated by Fig. 6.1. Although we have shown that a complex chemical potential can arise in a realistic Hamiltonian, the predicted density dependence must be consistent with experimental loss curves. Specifically, it will be tested whether the lowest order term in the coherent decay rate ($\sim \rho^{3/2}$) can be fit as well as the classical three-body rate ($\sim \rho^2$).

Extension of the uniform medium result to the experiments' trapping geometries requires the application of the local density approximation, where it is assumed that each point inside the trap admits a locally uniform value for μ. Proceeding in the same manner as the treatment of the three-body collisional loss of Sec. 6.1, the coherent rate is described by $-L_c \int \rho(\mathbf{r})^{5/2} = -L_c \langle \rho^{3/2} \rangle N$, with N being the total number of atoms in the trap while L_c is the coherent rate coefficient given by Eq. (6.52) of Case (ii):

$$L_c = \frac{\hbar}{m} \frac{\sqrt{2}}{512\pi^2} \left(82 - 9\delta_0 - 11\delta_0^2\right) \delta_0^2 \, \lambda^{5/2} \, . \tag{6.65}$$

With the Thomas-Fermi profile (6.2), the integral is calculated to be $\langle \rho^{3/2} \rangle = c_{5/2} N^{3/5}$, where $c_{5/2} = (75\pi/4096)(7c_2)^{3/2}$ and $c_2 = (15^{2/5}/(14\pi))(m\bar{\omega}/(\hbar\sqrt{a}))^{6/5}$. Inside the chamber, background atoms will impinge on the BEC resulting in quasiparticle excitations which manifest as the loss of individual particles from the collective. Taking τ_0 as the lifetime from this background effect, the averaged coherent rate equation is given by

$$\frac{1}{N}\frac{dN}{dt} = -L_c \, c_{5/2} \, N^{3/5} - \frac{1}{\tau_0} \, . \tag{6.66}$$

Because all experiments are performed at finite temperatures, quasiparticles will be present leading to kinematic losses. But as the temperature of the system is lowered, there are fewer excitations, thus rendering the collective decoherence the dominant mechanism. As a test of this theory, a case is sought where the system is brought sufficiently close to quantum degeneracy. For the example of ^{87}Rb, the theoretically predicted three-body rates ($\sim 10^{-30}$ cm^6 s^{-1})[1] are an order of magnitude too small to be consistent with observation. As a possible explanation of this discrepancy, we choose an appropriate value of δ to fit the time evolution of N [Eq. (6.66)] to the experimental loss data for ^{87}Rb [Fig. 6.6]. Demonstrated in the inset, this data provides no appreciable distinction between the loss as a coherent phenomenon and the best fit semi-classical three-body model.

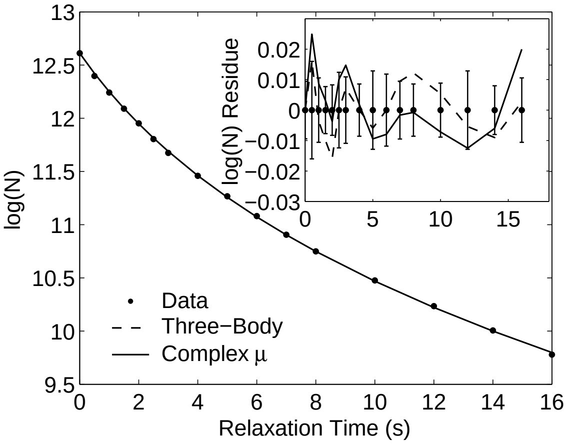

Figure 6.6: Fit of the decay rate given in Eq. (6.66) to the experimental loss data of ^{87}Rb with an inset showing a close up view comparing the difference between the coherent decay and the semi-classical three-body recombinant model described in Sec. 6.1. In a least squares sense, the best fit is obtained for a decay rate coefficient of $L_c = 2.7732 \times 10^{-22}\text{cm}^{9/2}\text{s}^{-1}$ which, by Eq. (6.65) corresponds to an interaction strength $\lambda = (0.954)8\pi a$. Also, the background lifetime is found to be $\tau_0 = 38.8$ s, implying it is not the dominant effect.

Due to a lack of detailed loss data, the value of λ in other atomic species must be found by a coarse one-point lifetime observation. A summary of some different cases is displayed in Table 6.1. The ^{87}Rb strength was found from the loss curve in Fig. 6.6 whereas ^{23}Na, ^{133}Cs and ^{4}He were determined by matching a single observed lifetime measurement[2] to the exponential rate $-L_c(\overline{\rho})^{3/2}$. In the latter cases, an average trap density was used in finding the $1/e$ lifetime. Depicted in the table are experiments in which the loss was primarily due to the internal physics of the BEC itself, but not its interaction with the trapping potential. The only exception is the case for the ^{4}He where the causes of the loss were unclear. Not shown are the cases of ^{7}Li[3] and ^{41}K[4] which involve additional physics thus prohibiting a clean comparison from being made.

At this point it is appropriate to discuss the conditions under which the coherent decay will be readily observed. Because we have no knowledge of the interaction strength, λ, it is

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[1] A. J. Moerdijk (1996) and P. O. Fedichev (1996).

[2] These respective lifetimes were obtained according to observations in K. B. Davis (1995); T. Weber (2003); and A. Robert (2001).

[3] The ^{7}Li BEC has a negative scattering length, rendering it unstable against collapse. See C. C. Bradley (1995).

[4] A condensate of ^{41}K has been achieved only as an admixture with another species: G. Modugno (2001).

difficult to determine whether this effect will dominate the three-body processes. However, if the thermal energy, k_BT, is less than the quasiparticle excitation energy, $\sim 8\pi a\rho$, then losses must occur in this coherent fashion. Moreover, the three-body effect and the coherent mechanism may, after all, not be distinct effects. From the expansion of the chemical potential, $\mu = 8\pi a\rho + \mu_1\,\rho^{3/2} + \mu_2\,\rho^2 + \ldots$, it is evident that the second order complex term can be interpreted as a three-body process. It may in fact be the case that this term dominates the series at some finite temperature.

Isotope	a (nm)	B (G)	$\overline{\rho}$ (10^{14} cm^{-3})	τ (s)	$\frac{\lambda}{8\pi a}$
^{87}Rb	5.8	—	1	16	0.954
^{23}Na	4.5	—	1	1	0.940
^{133}Cs	15.9	23	0.1	15	0.956
^{4}He	20	—	0.1	~ 3	0.988

Table 6.1: Table showing the numerical values of the interaction strength, λ, as determined from a fit of Eq. (6.65) to the observed lifetime, τ. For the ^{133}Cs condensate produced using a Feshbach resonance, we show the magnetic field value, B, corresponding to the scattering length, a, at which the lifetime was observed.

Chapter 7

Macroscopic Quantum Tunneling

In uniform systems, it was shown in Section 5.7 that the collective excitations largely occurred in a continuous spectrum. However, when confined inside a trap, the excitations assume quantized vibrational modes. One interesting situation arises when the quantized modes occur in condensates of species with a negative scattering length. In such cases, the system will have a tendency toward collapse as can be seen from the low-density pressure:

$$\begin{aligned} P &= \mu\rho - u \\ &= 8\pi a\rho^2 - 4\pi a\rho^2 \\ &= 4\pi a\rho^2 \,, \end{aligned} \tag{7.1}$$

where the expressions for the energy density, u, and the chemical potential, μ, are obtained from (5.42) and the argument directly after. But, as the particles become more confined, the Heisenberg uncertainty principle imparts a kinetic energy which can act to counterbalance the collapse, provided the interparticle attraction is not too strong. Being proportional to the product of the scattering length with the square of the density, the interaction strength is determined by the number of condensed atoms. Hence, beyond some critical particle number, the Heisenberg pressure will no longer balance the attraction in the gas. Clearly, there exists a potential energy barrier whose height is determined by the number of condensate atoms as well as their scattering length. For samples close to the critical number, it becomes possible for the condensate to coherently tunnel through the barrier thereby initiating collapse. After obtaining an analysis for attractive atomic condensates, the results are then applied to the collapsing, $\psi = 0$ molecular solution of Section 5.5.

7.1 Trapped Atomic Condensates with $a < 0$

When confined to a harmonic trap, the density distribution can be accurately approximated by a Gaussian which, for the case of spherically symmetric traps, can be characterized by a single parameter, the width of the cloud. According the local density approximation (LDA), every point in the trap can be described by the locally uniform results, where an integration is required to obtain the quantity in total.

By expressing all uniform results in terms of the coordinate dependent density, an expression can be derived for the total energy as a function of the cloud width. Introducing a conjugate momentum, a quantization is performed resulting in a single-particle quantum description of the condensate as a whole, where the width is the coordinate of a an effective mass of a radial "breather mode" of the condensate, moving in an effective potential determined by both the external trap and the interparticle interactions.

7.1.1 Statics

The total energy is given as a functional of the atomic condensate wavefunction, ϕ, where a kinetic energy and a trapping potential are added to the interaction term $u = 4\pi a \psi^2$:

$$E[\psi] = \int_{\mathbf{k}} \left[\frac{1}{\sqrt{2}} \psi^* \left(-\nabla^2 + \Omega\, r^2 \right) \frac{1}{\sqrt{2}} \psi + 4\pi a \left| \frac{1}{\sqrt{2}} \psi \right|^4 \right] , \tag{7.2}$$

where Ω is related to the trap frequency, ω_0, and the unperturbed width of the cloud, d_0, by

$$\Omega = \left(\frac{m\omega_0}{\hbar} \right)^2 = \frac{1}{d_0^4} . \tag{7.3}$$

As a model, the ^{7}Li parameters are used, as given by

$$a = -1.45\,\mathrm{nm} \tag{7.4a}$$

$$d_0 \approx 3.16\,\mu\mathrm{m} \tag{7.4b}$$

$$\omega_0 \approx 908\,\mathrm{s}^{-1} , \tag{7.4c}$$

where $\omega_0 = (\omega_x \omega_y \omega_z)^{1/3}$ is the mean trapping frequency of the experiments[1].

At this point we could extremize Eq. (7.2) on ψ, subject to the constraint of a fixed particle number, N, given by

$$N = \int_{\mathbf{r}} \left[\int_{\mathbf{k}}' R(\mathbf{k}) + \frac{1}{2} \psi^2 \right] \simeq \int_{\mathbf{r}} \frac{1}{2} \psi^2 . \tag{7.5}$$

The resulting nonlinear Schrödinger equation gives a condensate profile remarkably similar to a Gaussian. Therefore, to illustrate the salient features of the theory while avoiding any unnecessary computation, we use a Gaussian trial function,

$$\frac{1}{\sqrt{2}}\, \psi(r) = \psi_0\, e^{-r^2/2\ell^2} , \tag{7.6}$$

which, when substituted into Eq. (7.2) gives a total energy dependent only on the half-width of the cloud, ℓ,

$$E(\ell) = \frac{3}{2}\, \psi_0^2\, \pi^{3/2} \left(\ell + \Omega \ell^5 + \frac{4\pi}{3\sqrt{2}}\, a\, \psi_0^2\, \ell^3 \right) . \tag{7.7}$$

---

[1] These parameters were obtained from C. C. Bradley (1997).

With the Gaussian form, an integration of (7.5) obtains the number in terms of ψ_0 and the half width,

$$N = \psi_0^2\, \pi^{3/2}\, \ell^3\,. \tag{7.8}$$

After solving for ψ_0, the energy can be expressed in N and ℓ:

$$E(\ell) = \frac{3}{2}\, N \left(\ell^{-2} + \Omega \ell^2 + \frac{4}{3\sqrt{2\pi}}\, aN\ell^{-3} \right)\,. \tag{7.9}$$

Given Ω and a, there exists a range of particle numbers for which $E(\ell)$ has a local minimum. This minimum is an equilibrium point around which the condensate can oscillate, where the mode is associated with a collective mass impinging upon the effective potential barrier. As shown in Fig. 7.1(a), there exists some critical particle number, N_c, beyond which the condensate simply collapses. As suggested, this number, along with its associated critical half width, ℓ_c, may be found from the point at which the barrier disappears. Mathematically, this happens for $dE/d\ell = d^2E/d\ell^2 = 0$, which when solved gives[1]

$$\ell_c = \left(\frac{1}{5\Omega} \right)^{1/4} \tag{7.10}$$

$$\begin{aligned} N_c &= -\frac{2\sqrt{2\pi}}{5^{5/4}}\, \frac{d_0}{a} \\ &\simeq -0.671\, \frac{d_0}{a}\,. \end{aligned} \tag{7.11}$$

7.1.2 Collective Dynamics

To calculate the collective dynamics, equation (7.9) is regarded as a potential energy through which the breather modes move. As in the time dependent Gaussian trial functional, the collective motion is found by adding a conjugate variable, Σ, to the exponent of the trial function in (7.6), giving[2]

$$\psi(r) = \psi_0\, e^{-r^2(1/2\ell^2 - i\Sigma)}\,. \tag{7.12}$$

In addition, the action is defined by

$$\begin{aligned} S &= \int L(t)\, dt \\ &= \int dt \int_{\mathbf{r}} \psi^*(r) \left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \psi(r)\,, \end{aligned} \tag{7.13}$$

where $\hat{H} = -\nabla^2 + \Omega\, r^2 + 4\pi a |\psi|^2$. Substitution of the trial function of Eq. (7.12) into the action yields

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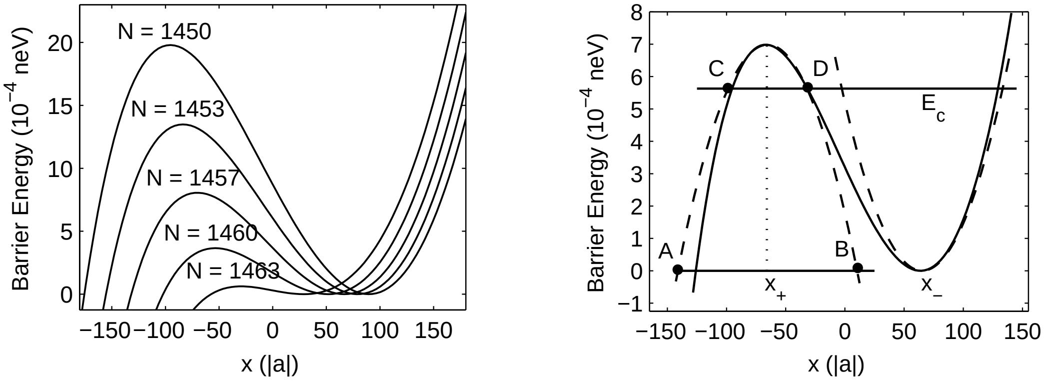
[1] To compare this with numerical results see, for example, A. Eleftheriou (2000).

[2] For notational simplicity, the $1/\sqrt{2}$ factor is dropped in the definition of the mean field.



(a)

(b)

Figure 7.1: For the parameters of ^{7}Li, [see Eqs. (7.4)], (a) depicts the sensitivity of the effective potential (7.9) with respect to the number of condensate atoms, N. When the number is increased, the collective mass acquires more inertia which effectively lowers the barrier height while concomitantly decreasing its width. Beyond some critical particle number, $N_c \sim 1463$, there will be complete collapse due to the disappearance of the well. For $1 - N/N_c = 5 \times 10^{-3}$, part (b) shows a comparison between the full potential (solid line) and the quadratic approximations of (7.19) and (7.21), where the energy zero is chosen to coincide with the local minimum. The lowest level excitation, $E_c = \hbar\omega$, is shown by the top horizontal line, intersecting the barrier at points C and D. In principle, it would be more consistent to evaluate the tunneling time between these two points, but the zero energy points A and B are chosen for simplicity. Consequently, the penetration time will be somewhat overestimated.

$$S = \int dt \left[3\hbar N \Sigma \ell \dot{\ell} - 3\frac{\hbar^2}{m} N \ell^2 \Sigma^2 - \frac{\hbar^2}{2m} V(\ell) + \text{total time derivatives} \right] . \tag{7.14}$$

Here, the static excitation energy of (7.7) is now the quasiparticle excitation potential, or $V(\ell) = E(\ell)$[1]. From the action, the quantity $3\hbar N \Sigma \ell$ is recognized as the canonically conjugate momentum to ℓ. Therefore, the classical Hamiltonian associated with this action is

$$\begin{aligned} H = p\dot{\ell} - L &= 3\frac{\hbar^2}{m} N \ell^2 \Sigma^2 + V(\ell) \\ &= \frac{p^2}{3mN} + V(\ell) \,, \end{aligned} \tag{7.15}$$

---

[1] Using $\ell^2 \dot{\Sigma} = \partial_t(\ell^2 \Sigma) - 2\ell\dot{\ell}\Sigma$, the time derivative in the action (7.13) is given by $-(3/2)\hbar N \ell^2 \dot{\Sigma}$ + total time derivatives. The second term is $\int \psi(r)^* \hat{H} \psi(r) = (\hbar^2/2m)[6N\ell^2\Sigma^2 + V(\ell)]$. We remind the reader that E is on the scale of $\hbar^2/2m$.

from which the collective mass is read off as

$$m_c = \frac{3}{2} mN \,. \tag{7.16}$$

Having obtained the collective mass, any of the standard approximation techniques may be used at this point to obtain the tunneling time. For macroscopic tunneling to occur, the size of the cloud must be close to the critical half-width obtained in (7.10). Defining $x = \ell - \ell_c$, we expand the potential to cubic order around the critical width:

$$\begin{aligned} V(x) = \frac{N}{\ell_c^2} \Bigg[\frac{9}{5} \left(1 - \frac{4}{9}\frac{N}{N_c}\right) - \frac{12}{5}\frac{1}{\ell_c} \left(1 - \frac{N}{N_c}\right) x + \frac{24}{5}\frac{1}{\ell_c^2} \left(1 - \frac{N}{N_c}\right) x^2 \\ -6\frac{1}{\ell_c^3} \left(1 - \frac{4}{3}\frac{N}{N_c}\right) x^3 + \ldots \Bigg] . \end{aligned} \tag{7.17}$$

Differentiating this expansion, then setting the result to zero, both the peak of the potential barrier, x_+, as well as the location of the well, x_-, are found to lowest order in the parameter $1 - N/N_c$[1]:

$$x_\pm = \mp \ell_c \sqrt{\frac{2}{5} \left(1 - \frac{N}{N_c}\right)} \,. \tag{7.18}$$

These points are the locations of the local maximum and minimum of the potential. To find the approximate parameters of the effective confining potential, (7.17) is expanded to quadratic order around $x_\pm$. As shown by Fig. 7.1(b), the well is given by the expansion around x_-:

$$\begin{aligned} V_-(x) &= \frac{1}{2} \frac{d^2 V}{dx^2}\bigg|_{x=x_-} (x - x_-)^2 \\ &= 6\sqrt{10}\, \frac{N}{d_0^4} \sqrt{1 - \frac{N}{N_c}} (x - x_+)^2 \,. \end{aligned} \tag{7.19}$$

Equating the coefficient with $m_c\omega^2/2$, we obtain the ground state harmonic frequency to lowest order in $1 - N/N_c$,

$$\omega = (160)^{1/4} \omega_0 \left(1 - \frac{N}{N_c}\right)^{1/4} , \tag{7.20}$$

which is in agreement with the result obtained by Ueda and Leggett[2].

In quantum decay processes, the tunneling rate can be closely approximated by an exponential form, $\Gamma = A e^{-(\hbar/2m) S_0}$, where the prefactor, A is proportional to the "attack" frequency, ω, given in (7.20). Since this prefactor is outweighed by the exponential, the quantity of most interest is S_0. To evaluate this exponent we first use the instanton approach then compare the result with that obtained in the WKB approximation. In simplifying the

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[1] To lowest order in $1 - N/N_c$, we have $N/N_c = 1 - (1 - N/N_c) \approx 1$.

[2] M. Ueda and A. J. Leggett (1998).

subsequent analysis, the potential in Eq. (7.17) is expanded around x_+ to quadratic order. Taking the height to be the difference between the local maximum and the local minimum, $V(x_+) - V(x_-)$, results in

$$\begin{aligned} V_+ &= V(x_+) - V(x_-) + \frac{1}{2}\frac{d^2V}{dx^2}\bigg|_{x=x_+}(x-x_+)^2 \\ &= \frac{16\sqrt{2}}{5}\frac{N}{d_0^2}\left(1-\frac{N}{N_c}\right)^{3/2} - 6\sqrt{10}\,\frac{N}{d_0^4}\sqrt{1-\frac{N}{N_c}}\,(x-x_+)^2\ . \end{aligned} \tag{7.21}$$

In the instanton formalism, the rate exponent is found to be the extremum of an imaginary time action,

$$S = \int dt\left[V_+(x) + \frac{m\,m_c}{\hbar^2}\,\dot{x}^2\right], \tag{7.22}$$

where the integral is evaluated between the two turning points, A and B, shown in Fig. 7.1(b). Extremizing this functional, the bounce trajectory is found from

$$\frac{\delta S}{\delta x} = 0 \quad\Rightarrow\quad \dot{x} = \hbar\sqrt{\frac{1}{m\,m_c}V_+(x)}\,. \tag{7.23}$$

Substitution of the quadratic form of the potential in Eq. (7.21) results in

$$\dot{x} = \frac{4(2^{3/4})}{\sqrt{15}}\sqrt{\frac{\hbar\omega_0}{m}}\left(1-\frac{N}{N_c}\right)^{3/4}\cos(\omega t)\,. \tag{7.24}$$

Using Eqs. (7.23) and (7.24) in (7.22), the extremized action is found to be

$$\frac{\hbar}{2m}S_0 = \frac{1}{\hbar}\int_0^{\pi/\omega} dt\, m_c\dot{x}^2 \simeq 2N\left(1-\frac{N}{N_c}\right)^{5/4}\ . \tag{7.25}$$

Between the same two turning points, A and B, in Fig. 7.1(b), the WKB approximation provides an alternate expression for the exponent,

$$\frac{\hbar}{2m}S_0 = \int_A^B dx\sqrt{V_+(x)} \simeq 1.63\sqrt{N}\left(1-\frac{N}{N_c}\right)^{5/4}\ . \tag{7.26}$$

Comparing this with the instanton result, there is an unchanged dependence on the parameter $1 - N/N_c$, whereas the dependence on N is linear in the former case, as opposed to the square root. Assuming a prefactor[1] of $A = \omega(15\hbar S_0/(4\pi m))^{1/2}$, equation (7.25) is used to calculate a tunneling rate of $\Gamma_T = 1.88s^{-1}$, for $1 - N/N_c = 5\times10^{-3}$. As the number of condensate atoms, N, is decreased, the barrier grows according to Fig. 7.1(a), and the tunneling becomes less significant.

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[1] The prefactor was taken from Ueda and Leggett. *ibid.*

7.2 Trapped Molecular Condensates

Because molecules have inherently more degrees of freedom than their constituent atoms, the production of molecular Bose-Einstein condensates could open up new directions into the study of these degenerate gases. However, molecular condensate formation has remained an elusive experimental challenge due to the added rovibrational energy level structure. To overcome this difficulty, a number of experiments have been proposed whereby molecules can be produced by changing an external field parameter, thereby altering the potentials seen by the atoms. Included in these schemes is the melting of a Mott insulator[1] and magnetic field sweeps across a Feshbach resonance. In the latter case, molecular condensates have been produced from fermionic species by traversing the BCS-BEC crossover regime[2]. Although the application of the same method to an atomic BEC has only achieved ultracold molecules[3], the exploitation of a Feshbach resonance remains an encouraging avenue for molecular BEC production.

As discussed in Sec. 5.4, the zero-temperature statics of an atom-molecule system coupled through a Feshbach resonance naturally gives rise to a collapsing molecular ground state exhibiting highly unusual properties, resulting from an admixture of condensed molecules with correlated atom pairs. Due to the coupling between pairs and molecules, this solution has unusual properties that cannot be ascribed to a condensate created directly from molecules alone[4].

7.2.1 Effective Molecule-Molecule Scattering Length

Just as in the case of pure atomic condensates, the molecular condensate exhibits a macroscopic tunneling effect as well. Characterizing this effect requires an understanding of the intermolecular interactions, arising from an effective molecule-molecule scattering length. Since this scattering length is tunable, the tunneling rate is adjustable. However, finding the effective scattering length requires a further examination of the uniform static results in Secs. 5.4 and 5.5.

For large weakly bound molecules close to resonance, the interactions can be determined by the two-body forces between each pair of atoms in the scattering reaction. With a diagrammatic method, the corresponding intermolecular scattering length, a_{mm}, has been shown to be proportional to the atomic scattering length[5] as $a_{mm} = 4a$. However, it is unclear whether this result is applicable to the molecular condensate which is the true ground state of the coupled system. In this case, a_{mm} is found from an expansion of the energy density to order ϕ^4.

Since there is no atomic field, the density is simply $\rho = \int R(\mathbf{k}) + \phi^2$. Taking $\mu = -\gamma^2$, the expansions for both the pressure [Eq. (5.33)] and the pair density [Eq. (5.30b)], gives the energy density as

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[1] D. Jaksch (2002).

[2] C. A. Regal (2004).

[3] K. Xu (2003).

[4] A proposal to create an all-molecular condensate by the conversion of its coupled atom-molecule counterpart can be found in S. J. J. M. F. Kokkelmans (2001).

[5] M. W. J. Romans (2004).

$$\begin{aligned} u &= -P - \gamma^2 \rho \\ &= \frac{1}{512\pi}\frac{\xi^4}{\gamma^3} - \gamma^2\left[\int_{\mathbf{k}}' R(\mathbf{k}) + \phi^2\right] \\ &= \frac{1}{512\pi}\frac{\xi^4}{\gamma^3} - \frac{\xi^2\gamma}{32\pi}\left(1+\frac{3}{32}\frac{\xi^2}{\gamma^4}\right) - \gamma^2\phi^2 \,. \end{aligned} \tag{7.27}$$

This expansion involves γ^2, ξ^2 and ϕ^2, but we seek to eliminate the first two in favor of the last. Facilitating this manipulation is the fact that only the low-density ($\xi \to 0$) results are important. To find γ to order ξ^2, we use Eq. (5.31),

$$\frac{1}{8\pi a_{bg}} - \frac{\gamma}{8\pi} + \frac{\alpha^2}{\epsilon + 2\gamma^2} + \frac{\xi^2}{128\pi}\frac{1}{\gamma^3} = 0\,, \tag{7.28}$$

the lowest order ($\xi = 0$) solution of which gives the binding energy, $2\gamma_0^2$:

$$\left(\gamma_0 - \frac{1}{a_{bg}}\right) = \frac{8\pi\alpha^2}{\epsilon + 2\gamma_0^2}\,. \tag{7.29}$$

Since any higher order terms will depend on a similar configuration of parameters, it is convenient at this point to define the quantity

$$z = \frac{2\pi\alpha^2}{\gamma_0}\frac{1}{(\gamma_0 - 1/a_{bg})^2}\,, \tag{7.30}$$

from which α^2 and ϵ can be expressed as

$$2\pi\alpha^2 = \gamma_0\left(\gamma_0 - \frac{1}{a_{bg}}\right)^2 z \tag{7.31a}$$

$$(\epsilon + 2\gamma_0^2) = 4\gamma_0\left(\gamma_0 - \frac{1}{a_{bg}}\right) z\,. \tag{7.31b}$$

The low-density expansion of γ is

$$\gamma = \gamma_0 + \gamma_0'\xi^2 + \dots\,, \tag{7.32}$$

where the coefficients are found from (7.28):

$$\left.\frac{d\gamma}{d\xi^2}\right|_{\xi=0} \equiv \gamma_0' = \frac{1}{\gamma_0^3}\frac{1}{1+z}\,. \tag{7.33}$$

Having explicitly obtained γ up to order ξ^2, it is now possible to express the molecular field, ϕ, in terms of ξ. Recalling the solution for ϕ given in Eq. (5.8b), we have

$$\begin{aligned}\phi &= -\frac{\alpha\xi}{\epsilon + 2\gamma^2} \\ &= -\frac{\alpha\xi}{\epsilon + 2\gamma_0^2}\left(1 - \frac{4\gamma_0\gamma_0'}{\epsilon + 2\gamma_0^2}\xi^2 + \dots\right) .\end{aligned} \tag{7.34}$$

Squaring this expression then inverting it gives ξ^2 in terms of ϕ^2,

$$\xi^2 = 32\pi\gamma_0 z\,\phi^2 + \frac{2048\pi^2}{\gamma_0 - 1/a_{bg}}\,\frac{1}{\gamma_0}\,\frac{z}{1+z}\,\phi^4 + \dots . \tag{7.35}$$

Substitution of (7.32), (7.33) and (7.35) into (7.27) gives the energy density to order ϕ^4,

$$u = u_0\phi^2 + 4\pi a_{mm}\phi^4 \,, \tag{7.36}$$

where

$$u_0 = -\gamma_0^2(1+z) \,. \tag{7.37}$$

The coefficient in front of the ϕ^4 term is identified as the effective molecule-molecule scattering length, given by

$$a_{mm} = -\frac{z}{\gamma_0}\left[\frac{16}{1+z}\left(1 + \frac{\gamma_0}{\gamma_0 - 1/a_{bg}}\right) + z\left(\frac{1}{4} + \frac{8}{1+z}\right)\right] \tag{7.38}$$

It is instructive to examine the forms of a_{mm} in both the limit of tight binding ($\gamma_0 \to \infty$) and in the large molecule limit ($\gamma_0 \to 0$). In each case, we have

$$a_{mm} \to -\frac{64\pi\alpha^2}{\gamma_0^4}\,; \quad \gamma_0 \to \infty \tag{7.39a}$$

$$a_{mm} \to -\frac{\pi^2\alpha^4 a_{bg}^4}{\gamma_0^3}\,; \quad \gamma_0 \to 0 \,. \tag{7.39b}$$

7.2.2 Statics

Analogous to the atomic condensate case, a Gaussian is taken for the position dependence of the molecular field inside a trap:

$$\phi(r) = \phi_0 e^{-r^2/2\ell^2} \,. \tag{7.40}$$

In this case, however, the total atom number is

$$N = \int_{\mathbf{r}}\left[\int_{\mathbf{k}}' R(\mathbf{k}) + \phi^2\right] , \tag{7.41}$$

where the atom pairing term is comparable in magnitude to the condensate term. Using the expansion of $R(\mathbf{k})$ to order ϕ^2 we have

$$\begin{aligned} N &= -\frac{u_0}{\gamma_0^2}\int_{\mathbf{r}} \phi^2 \\ &= -\frac{u_0}{\gamma_0^2}\,\phi_0^2\,\pi^{3/2}\,\ell^3\,, \end{aligned} \tag{7.42}$$

from which the depletion ratio, ζ, defined as the fraction of condensate molecules, is given as

$$\zeta = -\frac{\gamma_0^2}{u_0}. \tag{7.43}$$

In ordinary atomic condensates[1], this factor is unity because the lowest order pair correlation density involves a term depending on the cube of the mean atomic field, not the square. Since N will always be multiplied by ζ, it is convenient to define a renormalized particle number as

$$N' = \zeta N. \tag{7.44}$$

Using Eq. (7.42), ϕ_0 is eliminated in favor of N', giving a total energy

$$\begin{aligned} E[\ell] &= \int_{\mathbf{k}} \left[\phi^*\left(-\frac{1}{2}\nabla^2 + 2\,\Omega\,r^2\right)\phi + u_0\,|\phi|^2 + 4\pi a_{mm}\,|\phi|^4\right] \\ &= u_0 N' + \frac{3}{4}N'\left(\ell^{-2} + 4\Omega\ell^2 + \frac{8}{3\sqrt{2\pi}}a_{mm}N'\ell^{-3}\right)\,. \end{aligned} \tag{7.45}$$

From the identification of the binding energy as $-2\gamma_0^2$, it follows that the first term in the total energy is simply the energy of N atoms paired into molecules. Comparing this with (7.9), we see that by setting $\Omega \to 4\Omega$ and $a \to 2\,a_{mm}$ in Eqs. (7.10) and (7.11), the critical number of particles, N_c', is found to be

$$\begin{aligned} N_c' &= -\frac{\sqrt{\pi}}{5^{5/4}}\frac{d_0}{a_{mm}} \\ &\simeq -0.237\frac{d_0}{a_{mm}}\,, \end{aligned} \tag{7.46}$$

whereas the critical half-width, ℓ_c, is given by

$$\ell_c = \left(\frac{1}{20\Omega}\right)^{1/4}\,. \tag{7.47}$$

As shown by Figure 7.2, the critical particle number becomes unbounded as the system asymptotically approaches the noninteracting molecular regime.

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[1] Compare with Eq. (7.8).

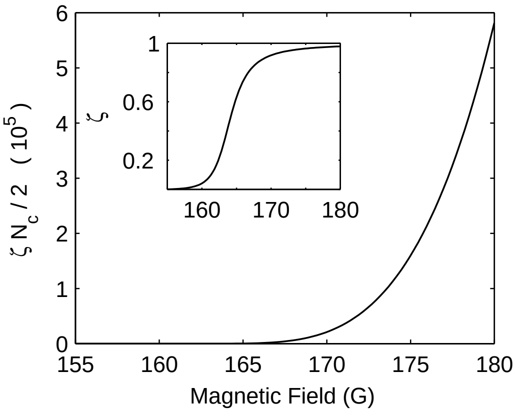

Figure 7.2: A plot showing the renormalized critical particle number in Eq. (7.46), as a function of the magnetic field. As a_{mm} approaches zero with increasing magnetic field, the system tends toward stability, having an unbounded particle number. Over the same field range, the inset shows the behavior of the depletion ratio, ζ. Taken together, these results suggest that increasing the molecular condensate fraction ($\zeta \to 1$) stabilizes the system against collapse.

7.2.3 Collective Dynamics

With the replacement of N by the renormalized particle number in (7.44), all results from Sec. 7.1.2 simply carry over. By defining the dynamic trial functional as

$$\phi(r) = \phi_0 e^{-r^2(1/2\ell^2 - i\Sigma)} \,, \tag{7.48}$$

the effective mass is

$$m_{eff} = \frac{3}{4} m_m N' \,, \tag{7.49}$$

where m_m is the molecular mass ($m_m = 2m$). Also, the effective potential, along with its corresponding approximations are[1]

$$\begin{aligned} V(x) = \frac{N'}{\ell_c^2} \Bigg[& u_0 \ell_c^2 + \frac{9}{10}\left(1 - \frac{4}{9}\frac{N}{N_c}\right) - \frac{6}{5}\frac{1}{\ell_c}\left(1 - \frac{N}{N_c}\right) x + \frac{12}{5}\frac{1}{\ell_c^2}\left(1 - \frac{N}{N_c}\right) x^2 \\ & - 3\frac{1}{\ell_c^3}\left(1 - \frac{4}{3}\frac{N}{N_c}\right) x^3 + \ldots \Bigg] \end{aligned} \tag{7.50}$$

$$V_-(x) = 3\sqrt{10}\,\frac{N'}{d_0^4}\sqrt{1 - \frac{N}{N_c}}(x - x_+)^2 \tag{7.51}$$

$$V_+ = \frac{8\sqrt{2}}{5}\frac{N'}{d_0^2}\left(1 - \frac{N}{N_c}\right)^{3/2} - 3\sqrt{10}\,\frac{N'}{d_0^4}\sqrt{1 - \frac{N}{N_c}}\,(x - x_+)^2 \,. \tag{7.52}$$

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[1] In the molecular case, ℓ_c is given by (7.47), not (7.10).

These results are summarized in Fig. 7.3

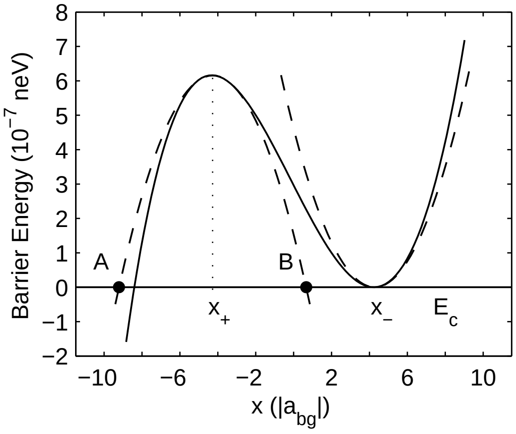

Figure 7.3: The full potential of Eq. (7.50) (solid line) is compared to the quadratic expansions of Eqs. (7.51) and (7.52) (dashed curves) for the ^{85}Rb parameters of Table 2.1. We take a trap half width of $d_0 \approx 320 a_{bg}$ with a critical number of molecules, $N_c = 1308$, and $1 - N/N_c = 10^{-3}$. These values give a combined molecule and pair average density of 10^{12} cm^{-3} with a depletion factor of $\zeta = 0.75$. As shown by the solid horizontal line, the collective ground state excitation energy, E_c, is very near zero. All tunneling paths are evaluated between A and B, the points where $V_+ = E_c \approx 0$.

Finally, the tunneling exponents corresponding to Eqs. (7.25) and (7.26) remain unchanged in form, but are now dependent upon N' instead of N:

$$\frac{\hbar}{2m} S_0 \simeq \begin{cases} 2N' \left(1 - \frac{N}{N_c}\right)^{5/4} ; & \text{Instanton} \\ 1.63\sqrt{N'} \left(1 - \frac{N}{N_c}\right)^{5/4} ; & \text{WKB} \end{cases} \tag{7.53}$$

Taking a prefactor of $A = \omega(15\hbar S_0/(4\pi m))^{1/2}$, we use the instanton result of Eq. (7.53) to compare the tunneling rate, Γ_T, to the two-body relaxation loss rate, Γ_{relax} of the molecules. Since there is no current data on the molecule-molecule relaxation, we take a number from the inelastic two-body losses seen in cold ^{85}Rb clouds: $K_2 \approx 10^{-14}$ cm^3 / s^1. Using the numerical values from Fig. (7.3) gives $\Gamma_T \approx 5$ s^{-1} whereas $\Gamma_{relax} \approx .01$ s^{-1}. Thus, the tunneling rate is seen to dominate the decay in this example. As shown in Fig. (7.2), the critical number of particles may be tuned arbitrarily close to the number in the original sample, offering a degree of flexibility not present in attractive systems without a resonance.

There remain significant practical complications in the actual production of the molecular condensate. Reaching the BEC regime requires high molecular densities with an elastic to inelastic collision ratio of greater than unity. Further, relaxation losses oppose the cooling process by ejecting more particles from the center of the trap, in direct opposition to the evaporative cooling process in which energetic atoms at the edge are expelled in greater

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[1] J. L. Roberts (2000).

number. When ejected, these molecules will heat the surrounding particles thereby inhibiting the cooling even further. Although these limitations are restrictive, encouraging results have been attained in the production of cold degenerate molecules. Furthermore, many of these loss issues may be avoided by using a Mott transition for molecular condensate formation. After overcoming these experimental challenges, many new aspects remain to be explored in molecular condensates arising from a Feshbach resonance.

One interesting application can be seen from the plot of the depletion ratio, shown in the inset of Fig. 7.2. Toward resonance, there is a dominance of correlated pairs whereas further away, the molecular condensate comprises most of the density. Between these limits exists a BCS-BEC crossover region analogous to that in fermionic systems. However, a closer inspection of Fig. 5.1 reveals an important distinction from the fermion case. At some magnetic field, the uniform system will reach a critical density at which a phase transition takes place, thus giving rise to a discontinuity at the corresponding point in the bosonic crossover. Further study of this effect and its implications could shed new light onto the BCS-BEC transition.

Chapter 8

Further Considerations

This chapter concludes by discussing some other problems of current interest within the BEC community. First, Section 8.1 applies the variational Gaussian formalism to the Bose-Hubbard model. In this process, it is shown how the addition of an auxiliary field simplifies the problem. Using a double resonance model, Section 8.2 discusses the interacting Fermi gas, analyzed using the Bogoliubov transformations. By specifically including a molecular component, some interesting issues arise as to the nature of the BCS-BEC crossover. In all cases, the material presented here is not carried out to completion, as it is intended only to provide an initial impetus into new directions.

8.1 Bose-Hubbard Model

One important problem in solid state physics concerns the theoretical distinction between conductors and insulators. To address this issue, the Hubbard model was put forth. Based on a tight binding scheme, this model describes an insulator as a lattice where the electrons are tightly bound around their constituent atoms. Unlike the tight binding approximation, however, the Hubbard model allows for the inclusion of the Coulomb repulsion between electrons. If the repulsion exceeds the on site attraction, then the electrons may "hop" between adjacent sites, thereby establishing a mobility that is characteristic of conductors. Hence, there is a competition between the mutual repulsion and the on site attraction, where equality marks the point of a quantum phase transition.

The same basic model applies to zero temperature, atomic bosons confined in an optical lattice. Unlike the solid state case, the lattice here can be tailored by the interference of multiple counter propagating laser beams. Hence, the relative strength of interparticle repulsions compared to on site attraction may be tuned by adjusting the power of the externally applied optical field. This degree of control allows a direct manipulation of the analogous quantum phase transition between the Mott insulator phase and the Bose-Einstein condensate[1].

We discuss the case of the one dimensional lattice, as the two and three dimensional cases follow from appropriate generalizations. The second-quantized Hamiltonian is

$$\hat{H} - \mu\hat{N} = -J\sum_{\langle i,j\rangle}\big(\hat{a}_i^\dagger\hat{a}_j + \hat{a}_j^\dagger\hat{a}_i\big) + \frac{1}{2}U\sum_i \hat{n}_i\big(\hat{n}_i - 1\big) + \sum_i \epsilon_i\hat{n}_i - \mu\sum_i \hat{n}_i\,, \tag{8.1}$$

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[1] See the experiment in M. Greiner (2002). For theoretical studies see D. Jaksch (1998) and D. van Oosten (2001).

where $\hat{a}_i^\dagger$ and $\hat{a}_i$ are the respective creation and annihilation operators for bosons on site i, whence it follows that $\hat{n}_i$ counts the number on each site. Having defined J[1] as the "hopping strength," the first term of Eq. (8.1) represents the energy lost or gained when an atom jumps to an adjacent site[2]. The second term is the interparticle repulsion, with U the strength of the interaction. Also, ϵ_i denotes a general energy offset which is introduced to accommodate any other external field[3] aside from the optical lattice. Finally, the last term reflects the constraint of N total particles, where the Lagrange multiplier, μ, is identified as the chemical potential in the usual way.

Before analyzing this Hamiltonian with the Gaussian formalism of Chapter 4, it is first convenient to express (8.1) in the compact form

$$\hat{H} - \mu\hat{N} = \sum_{ij} \hat{a}_i^\dagger K_{ij} \hat{a}_j + \sum_{ijk\ell} \hat{a}_i^\dagger \hat{a}_j^\dagger \, V_{ij;k\ell} \, \hat{a}_\ell \hat{a}_k \,, \tag{8.2}$$

which is made possible through the identification of the "kinetic" and "interaction" matrices:

$$K_{ij} = -J\big(\delta_{ij-1} + \delta_{ij+1}\big) + \big(\epsilon_i - \mu\big)\,\delta_{ij} \tag{8.3a}$$

$$V_{ij;k\ell} = \frac{1}{2} U \delta_{ij}\,\delta_{k\ell}\,\delta_{jk}\,. \tag{8.3b}$$

Following the procedure of Eqs. (4.3), the creation and annihilation operators are decomposed into coordinates and momenta:

$$\hat{a}_j^\dagger = \frac{1}{\sqrt{2}}\big(\hat{\phi}_j - i\hat{\pi}_j\big) \tag{8.4a}$$

$$\hat{a}_j = \frac{1}{\sqrt{2}}\big(\hat{\phi}_j + i\hat{\pi}_j\big)\,. \tag{8.4b}$$

The action of $\hat{\phi}_j$ and $\hat{\pi}_j$ is the same as in Eqs. (4.7).

As before, the many-body wave function has the variational Gaussian ansatz,

$$\Psi(\phi) = N e^{-\delta\phi_i \frac{1}{4} G_{ij}^{-1} \delta\phi_j}\,, \tag{8.5}$$

where G_{ij}^{-1} is the width and $\delta\phi$ is the field, ϕ' minus its mean value ϕ. In this expression, G and ϕ are the variational parameters determined by extremizing the expectation value of the Hamiltonian. Finding the expectation value in terms of the variational parameters is most easily accomplished by recasting the Hamiltonian in terms of the creation and destruction operators $(\hat{c}_j^\dagger, \hat{c}_j)$ of the many-body state (8.5). The first step in this strategy is to construct $\hat{c}_j^\dagger$ and $\hat{c}_j$ using the actions of $\hat{\phi}_j$ and $\hat{\pi}_j$ as a guide:

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[1] Although J can be calculated from the intensity of the standing wave, it is just treated as some parameter here. For further details, refer to M. Greiner, *loc. cit.* or D. Jaksch, *loc. cit.*

[2] The sum is over all nearest neighbor pairs, as indicated by the notation $\langle ij \rangle$.

[3] These may include the harmonic trapping potential.

$$\hat{c}_j^\dagger = \frac{1}{2\sqrt{2}}\big(\hat{\phi}_j - \phi_j - 2\,G_{jk} i\hat{\pi}_k\big) \tag{8.6a}$$

$$\hat{c}_j^\dagger = \frac{1}{2\sqrt{2}}\big(\hat{\phi}_j - \phi_j + 2\,G_{jk} i\hat{\pi}_k\big)\,. \tag{8.6b}$$

Here and throughout, the Einstein summation convention is used, where it is implicitly understood that repeated indices are summed. From these constructions, it is readily verified that

$$\hat{c}_j|\Psi\rangle = 0 \tag{8.7a}$$

$$\hat{c}_j^\dagger|\Psi\rangle = \frac{1}{\sqrt{2}}\,\delta\phi_j|\Psi\rangle \tag{8.7b}$$

Finally, the commutation relations are

$$\big[\hat{c}_j^\dagger, \hat{c}_i\big] = -\frac{1}{2}\,G_{ij} \tag{8.8a}$$

$$\big[\hat{c}_j^\dagger, \hat{c}_i^\dagger\big] = \big[\hat{c}_j, \hat{c}_i\big] = 0\,, \tag{8.8b}$$

which follow from (8.6) and the usual commutator $[i\hat{\pi}_k, \hat{\phi}_i] = \delta_{ik}$

The action of the boson annihilation operator on the many-body ansatz (8.5) gives

$$\begin{aligned}\hat{a}_j|\Psi\rangle &= \frac{1}{\sqrt{2}}\left(\delta\phi_j + \phi_j + \frac{\delta}{\delta\phi_j}\right)|\Psi\rangle \\ &= \frac{1}{\sqrt{2}}\left(\delta\phi_j + \phi_j - \frac{1}{2}G^{-1}_{jk}\,\delta\phi_k\right)|\Psi\rangle\,.\end{aligned} \tag{8.9}$$

By this result, it is easy to express $\hat{a}_j^\dagger$ and $\hat{a}_j$ in terms of $\hat{c}_j^\dagger$ and $\hat{c}_j$:

$$\hat{a}_j^\dagger = \alpha^+_{jk}\hat{c}_k^\dagger + \alpha^-_{jk}\hat{c}_k + \frac{1}{\sqrt{2}}\phi_j \tag{8.10a}$$

$$\hat{a}_j = \alpha^-_{jk}\hat{c}_k^\dagger + \alpha^+_{jk}\hat{c}_k + \frac{1}{\sqrt{2}}\phi_j \tag{8.10b}$$

where we have defined

$$\alpha^+_{jk} = \delta_{jk} + \frac{1}{2}G^{-1}_{jk} \tag{8.11a}$$

$$\alpha^-_{jk} = \delta_{jk} - \frac{1}{2}G^{-1}_{jk}\,. \tag{8.11b}$$

It is now possible to use Eqs. (8.7), (8.8), (8.10) and (8.11) to calculate the expectation value. The kinetic term is

$$\begin{aligned}\langle\Psi|\hat{a}_i^\dagger\hat{a}_j|\Psi\rangle &= \langle\Psi|\alpha_{ij}^-\,\hat{c}_k\,\alpha_{j\ell}^-\,\hat{c}_\ell^\dagger + \frac{1}{2}\,\phi_i\phi_j|\Psi\rangle \\ &= \alpha_{ij}^-\,\frac{1}{2}\,G_{k\ell}\alpha_{\ell j}^- + \frac{1}{2}\,\phi_i\phi_j\,.\end{aligned} \tag{8.12}$$

A straightforward calculation reveals that

$$\begin{aligned}\alpha_{ik}^-\,\frac{1}{2}G_{k\ell}\,\alpha_{\ell j}^- &= \frac{1}{2}\left(\frac{1}{4}G_{ij}^{-1} + G_{ij} - \delta_{ij}\right) \\ &\equiv R_{ij}\end{aligned} \tag{8.13a}$$

$$\begin{aligned}\alpha_{ik}^+\,\frac{1}{2}G_{k\ell}\,\alpha_{\ell j}^- &= -\frac{1}{2}\left(\frac{1}{4}G_{ij}^{-1} - G_{ij}\right) \\ &\equiv -D_{ij}\end{aligned} \tag{8.13b}$$

Substitution of (8.13a) into (8.14) gives

$$\langle\Psi|\hat{a}_i^\dagger\hat{a}_j|\Psi\rangle = R_{ij} + \frac{1}{2}\phi_i\phi_j\,. \tag{8.14}$$

Similarly, the interaction term is found to be

$$\begin{aligned}\langle\Psi|\hat{a}_i^\dagger\hat{a}_k^\dagger\hat{a}_j\hat{a}_\ell|\Psi\rangle =& D_{ik}D_{j\ell} - \frac{1}{2}\phi_j\phi_\ell D_{ik} + R_{ij}R_{k\ell} + R_{i\ell}R_{jk} \\ &+ \frac{1}{2}\phi_j\phi_k R_{i\ell} + \frac{1}{2}\phi_\ell\phi_k R_{ij} + \frac{1}{2}\phi_i\phi_j R_{\ell k} + \frac{1}{2}\phi_i\phi_\ell R_{kj} \\ &- \frac{1}{2}\phi_i\phi_k D_{j\ell} + \frac{1}{4}\phi_i\phi_j\phi_k\phi_\ell\,.\end{aligned} \tag{8.15}$$

With these results the expectation value of the Hamiltonian is

$$\langle\hat{H} - \mu\hat{N}\rangle = \sum_{ij}\left[K_{ij}\left(R_{ij} + \frac{1}{2}\phi_i\phi_j\right) + V_{ij}\left(D_{ij}^2 - \phi_i^2 D_{ij} + 2R_{ij}^2 + 2\phi_i^2 R_{ij} + \frac{1}{4}\phi_i^2\phi_j^2\right)\right], \tag{8.16}$$

where

$$V_{ij} = \frac{1}{2}U\delta_{ij}\,. \tag{8.17}$$

Unfortunately, the corresponding variational equations do not admit an analytic solution due to the quadratic terms in R and D. That is, taking the variation on G_{mn} results in

$$\begin{aligned}\sum_{ij}\Bigg\{ \big[K_{ij} + 2V_{ij}\big(2R_{ij} + \phi_i^2\big)\big]\frac{1}{2}\Big(-\frac{1}{4}G^{-1}_{im}G^{-1}_{nj} + \delta_{im}\delta_{jn}\Big) \\ + V_{ij}\big(2D_{ij} - \phi_i^2\big)\frac{1}{2}\Big(\frac{1}{4}G^{-1}_{im}G^{-1}_{nj} + \delta_{im}\delta_{jn}\Big)\Bigg\} = 0\,,\end{aligned} \tag{8.18}$$

which is a quartic matrix equation. Due to this complexity, it is worthwhile to consider the modified model discussed in Sec. 2.6.4, where the interactions are replaced by coupling to a Feshbach state. Introducing the following replacement

$$\sum_{ijk\ell} \hat{a}_i^\dagger \hat{a}_j^\dagger \, V_{ij;k\ell}\, \hat{a}_\ell \hat{a}_k \to (\varepsilon - 2\mu)\chi^2 + \frac{g}{2}\,\chi \sum_{ij} \delta_{ij}\, \hat{a}_i \hat{a}_j + \text{ H. c. } , \tag{8.19}$$

leads to

$$\langle \hat{H} - \mu \hat{N} \rangle = \sum_{ij} \Big[K_{ij}\Big(R_{ij} + \frac{1}{2}\phi_i\phi_j \Big) + g\chi\delta_{ij}\Big(-D_{ij} + \frac{1}{2}\phi_i\phi_j \Big) \Big] + (\varepsilon - 2\mu)\chi^2\,. \tag{8.20}$$

Here, ε is the energy of the molecular state relative to the continuum, whereas g is the coupling between the molecules and the scattering continuum (see Fig. 2.7). From the two-body scattering, the strength of the potential is related to these parameters by

$$U = -\frac{\varepsilon}{g^2}\,. \tag{8.21}$$

The variation on the mean molecular field, χ, obtains $\chi = (\varepsilon - 2\mu)^{-1} g \sum_i (-D_{ii} + \phi_i^2/2)$. Because g and ε are themselves variables, it is simpler to define $g\chi \equiv \xi$, then treating it as an adjustable parameter. The simplification (8.20) is evident in the equation for G,

$$\begin{aligned}\frac{\delta \langle \hat{H} - \mu \hat{N} \rangle}{\delta G_{mn}} = \sum_{ij} \Big[K_{ij}\frac{1}{2}\Big(-\frac{1}{4}G^{-1}_{im}G^{-1}_{nj} + \delta_{im}\delta jn \Big) \\ + \xi\delta_{ij}\frac{1}{2}\Big(\frac{1}{4}G^{-1}_{im}G^{-1}_{nj} + \delta_{im}\delta_{jn} \Big) \Big] = 0\,.\end{aligned} \tag{8.22}$$

Because ξ is arbitrary, this equation can be satisfied only if the quantity inside the sum vanishes. Defining the matrices,

$$A_{ij} = K_{ij} - \xi\delta_{ij} \tag{8.23a}$$

$$B_{ij} = K_{ij} + \xi\delta_{ij}\,, \tag{8.23b}$$

allows the variational equation for G can be cast in the matrix form

$$-\frac{1}{4}\, G^{-1}\, A\, G^{-1} + B = 0\,, \tag{8.24}$$

which, as shown by the analysis leading up to Eq. (5.55), has a symmetric solution given by

$$G = \frac{1}{2}\frac{1}{\sqrt{B}}\sqrt{\sqrt{B}\,A\,\sqrt{B}}\,\frac{1}{\sqrt{B}}\,. \tag{8.25}$$

Lastly, an extremization on the mean field, ϕ_i, gives

$$K_{ij}\phi_j + \xi\phi_i = 0 \tag{8.26}$$

One solution to the above equation is clearly $\phi_i = 0\,\forall i$, which corresponds to the Mott insulator phase, where there is no condensate for the particles are bound to their local lattice sites. The other solution corresponds to the atomic condensate, with the quantum phase transition occurring at $\phi = 0$. In either case, the complete solution can be obtained from (8.25), (8.26) and the total particle number constraint:

$$N = \sum_i \left(R_{ii} + \frac{1}{2}\phi_i^2 \right). \tag{8.27}$$

8.2 Interacting Fermi Gas

Because of its application to superconductivity as well as other condensed matter systems, the case of the interacting fermi gas is a topic of current interest. Due to the Pauli exclusion principle, there can be no s-wave scattering between fermions in the same state. Hence, we consider an equal mixture of fermions in two distinct spin states, which will be labeled by the subscripts ↑ and ↓. In the zero-range limit of an attractive potential, it is simplest to model the interaction by a molecular coupling term, as was done for the bosons in Eq. (5.2). The grand canonical Hamiltonian is

$$\begin{aligned}\hat{K} = \hat{H} - \mu\hat{N} = &\sum_{\mathbf{k}\sigma}\left(k^2-\mu\right)\hat{\psi}^\dagger_{\mathbf{k}\sigma}\hat{\psi}_{\mathbf{k}\sigma} + 2\left(\varepsilon - 2\mu\right)\sum_{\mathbf{k}}\hat{\chi}^\dagger_{\mathbf{k}}\hat{\chi}_{\mathbf{k}} \\ &+ \frac{g}{\sqrt{2}}\sum_{\mathbf{k}'',\mathbf{k},\mathbf{k}'}\hat{\chi}^\dagger_{\mathbf{k}''}F_{\mathbf{k}'',\mathbf{k}\mathbf{k}'}\left(\hat{\psi}_{\mathbf{k}\uparrow}\hat{\psi}_{-\mathbf{k}'\downarrow} - \hat{\psi}_{-\mathbf{k}\downarrow}\hat{\psi}_{\mathbf{k}'\uparrow}\right) + \text{H. c.}\,,\end{aligned} \tag{8.28}$$

where $F_{\mathbf{k}'',\mathbf{k}\mathbf{k}'} = \delta_{\mathbf{k}'',(\mathbf{k}-\mathbf{k}')/2}$ is the usual δ-function form factor, $\hat{\chi}$ is the molecular field operator producing the interaction, and σ is the spin index. Taking the mean for the molecular field operator gives

$$\hat{K} = \sum_{\mathbf{k}\sigma}\left(k^2-\mu\right)\hat{\psi}^\dagger_{\mathbf{k}\sigma}\hat{\psi}_{\mathbf{k}\sigma} + 2\left(\frac{1}{2}\varepsilon - \mu\right)\mathcal{V}\chi^2 + \xi\sum_{\mathbf{k}}\hat{\psi}_{\mathbf{k}\uparrow}\hat{\psi}_{-\mathbf{k}\downarrow} + \text{H. c.}\,, \tag{8.29}$$

where $\mathcal{V}$ is the volume and $\xi \equiv g\chi$. Using the standard Bogoliubov transformation, the new operators, $\hat{\alpha}_{\mathbf{k}}$ and $\hat{\beta}_{\mathbf{k}}$ are defined through[1]

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[1] This is the approach used in Chapter 10 of A. L. Fetter and J. D. Walecka (2003). Alternatively, a variational approach could have been used, with a trial functional given by $|\phi\rangle = \prod_{\mathbf{k}}\big(u(\mathbf{k}) + v(\mathbf{k})\hat{\psi}^\dagger_{\mathbf{k}\uparrow}\hat{\psi}^\dagger_{-\mathbf{k}\downarrow}\big)|0\rangle$, which is a generalization of (3.67a).

$$\hat{\psi}_{\mathbf{k}\uparrow} = u(\mathbf{k})\hat{\alpha}_{\mathbf{k}} + v(\mathbf{k})\hat{\beta}^{\dagger}_{-\mathbf{k}} \tag{8.30a}$$

$$\hat{\psi}_{\mathbf{k}\downarrow} = u(\mathbf{k})\hat{\beta}_{-\mathbf{k}} - v(\mathbf{k})\hat{\alpha}^{\dagger}_{\mathbf{k}} \,. \tag{8.30b}$$

A canonical transformation is achieved only if the new operators satisfy

$$\begin{gathered}\left\{\hat{\alpha}_{\mathbf{k}}, \hat{\alpha}^{\dagger}_{\mathbf{k}'}\right\} = \left\{\hat{\beta}_{\mathbf{k}}, \hat{\beta}^{\dagger}_{\mathbf{k}'}\right\} = \delta_{\mathbf{k}\mathbf{k}'} \\ \text{All other anticommutators} = 0\,. \end{gathered} \tag{8.31}$$

Imposing the initial anticommutation relations, $\{\hat{\psi}_{\mathbf{k}\sigma}, \hat{\psi}^{\dagger}_{\mathbf{k}'\sigma'}\} = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}$, it follows that

$$u(\mathbf{k})^2 + v(\mathbf{k})^2 = 1\,. \tag{8.32}$$

The various terms in the Hamiltonian (8.29) can be expressed in $\hat{\alpha}$ and $\hat{\beta}$. Starting with the kinetic terms, we have

$$\hat{\psi}^{\dagger}_{\mathbf{k}\uparrow}\hat{\psi}_{\mathbf{k}'\uparrow} = N\left(\hat{\psi}^{\dagger}_{\mathbf{k}\uparrow}\hat{\psi}_{\mathbf{k}'\uparrow}\right) + \langle\hat{\psi}^{\dagger}_{\mathbf{k}\uparrow}\hat{\psi}_{\mathbf{k}'\uparrow}\rangle\,, \tag{8.33}$$

where the normal ordered product is given by

$$\begin{aligned} N\left(\hat{\psi}^{\dagger}_{\mathbf{k}\uparrow}\hat{\psi}_{\mathbf{k}'\uparrow}\right) &= N\left\{\left[u(\mathbf{k})\hat{\alpha}^{\dagger}_{\mathbf{k}} + v(\mathbf{k})\hat{\beta}_{-\mathbf{k}}\right]\left[u(\mathbf{k}')\hat{\alpha}_{\mathbf{k}'} + v(\mathbf{k}')\hat{\beta}^{\dagger}_{-\mathbf{k}'}\right]\right\} \\ &= u(\mathbf{k})u(\mathbf{k}')\hat{\alpha}^{\dagger}_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}'} - v(\mathbf{k})v(\mathbf{k}')\hat{\beta}^{\dagger}_{-\mathbf{k}'}\hat{\beta}_{-\mathbf{k}} + u(\mathbf{k})v(\mathbf{k}')\hat{\alpha}^{\dagger}_{\mathbf{k}}\hat{\beta}^{\dagger}_{-\mathbf{k}'} + v(\mathbf{k})u(\mathbf{k}')\hat{\beta}_{-\mathbf{k}}\hat{\alpha}_{\mathbf{k}'}\,. \end{aligned} \tag{8.34}$$

Defining the vacuum such that $\hat{\beta}^{\dagger}|0\rangle = \hat{\alpha}^{\dagger}|0\rangle = 0$, the mean value is

$$\begin{aligned} \langle\hat{\psi}^{\dagger}_{\mathbf{k}\uparrow}\hat{\psi}_{\mathbf{k}'\uparrow}\rangle &= \langle\left[u(\mathbf{k})\hat{\alpha}^{\dagger}_{\mathbf{k}} + v(\mathbf{k})\hat{\beta}_{-\mathbf{k}}\right]\left[u(\mathbf{k}')\hat{\alpha}_{\mathbf{k}'} + v(\mathbf{k}')\hat{\beta}^{\dagger}_{-\mathbf{k}'}\right]\rangle \\ &= v(\mathbf{k})^2\delta_{\mathbf{k}\mathbf{k}'}\,. \end{aligned} \tag{8.35}$$

Similar results are obtained for the remaining terms

$$\hat{\psi}^{\dagger}_{\mathbf{k}\downarrow}\hat{\psi}_{\mathbf{k}'\downarrow} = N\left(\hat{\psi}^{\dagger}_{\mathbf{k}\downarrow}\hat{\psi}_{\mathbf{k}'\downarrow}\right) + v(\mathbf{k})^2\delta_{\mathbf{k}\mathbf{k}'} \tag{8.36a}$$

$$\hat{\psi}_{\mathbf{k}\uparrow}\hat{\psi}_{-\mathbf{k}'\downarrow} = N\left(\hat{\psi}_{\mathbf{k}\uparrow}\hat{\psi}_{-\mathbf{k}'\downarrow}\right) - u(\mathbf{k})v(\mathbf{k})\delta_{\mathbf{k}\mathbf{k}'}\,. \tag{8.36b}$$

$$N\left(\hat{\psi}^{\dagger}_{\mathbf{k}\downarrow}\hat{\psi}_{\mathbf{k}'\downarrow}\right) = u(\mathbf{k})u(\mathbf{k}')\hat{\beta}^{\dagger}_{\mathbf{k}}\hat{\beta}_{\mathbf{k}'} - v(\mathbf{k})v(\mathbf{k}')\hat{\alpha}^{\dagger}_{-\mathbf{k}'}\hat{\alpha}_{-\mathbf{k}} - u(\mathbf{k})v(\mathbf{k}')\hat{\beta}^{\dagger}_{\mathbf{k}}\hat{\alpha}^{\dagger}_{-\mathbf{k}'} - v(\mathbf{k})u(\mathbf{k}')\hat{\alpha}_{-\mathbf{k}}\hat{\beta}_{\mathbf{k}'} \tag{8.37a}$$

$$N\left(\hat{\psi}_{\mathbf{k}\uparrow}\hat{\psi}_{-\mathbf{k}'\downarrow}\right) = u(\mathbf{k})u(\mathbf{k}')\hat{\alpha}_{\mathbf{k}}\hat{\beta}_{-\mathbf{k}'} - v(\mathbf{k})v(\mathbf{k}')\hat{\beta}^{\dagger}_{-\mathbf{k}}\hat{\alpha}^{\dagger}_{\mathbf{k}'} + u(\mathbf{k})v(\mathbf{k}')\hat{\alpha}^{\dagger}_{\mathbf{k}'}\hat{\alpha}_{\mathbf{k}} + u(\mathbf{k}')v(\mathbf{k})\hat{\beta}^{\dagger}_{-\mathbf{k}}\hat{\beta}_{-\mathbf{k}'}\,. \tag{8.37b}$$

Using (8.34)-(8.37), the Hamiltonian can be expressed as

$$\hat{K} = U + \hat{H}_1 + \hat{H}_2\,, \tag{8.38}$$

where

$$U = 2\sum_{\mathbf{k}}(k^2-\mu)v(\mathbf{k})^2 + 2\left(\frac{1}{2}\varepsilon - \mu\right)V\left(\frac{\xi}{g}\right)^2 - 2\xi\sum_{\mathbf{k}}u(\mathbf{k})v(\mathbf{k}) \tag{8.39}$$

$$\hat{H}_1 = \sum_{\mathbf{k}}\left(\hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + \hat{\beta}^\dagger_{-\mathbf{k}}\hat{\beta}_{-\mathbf{k}}\right)\left\{\left[u(\mathbf{k})^2 - v(\mathbf{k})^2\right](k^2-\mu) + 2\xi u(\mathbf{k})v(\mathbf{k})\right\} \tag{8.40}$$

$$\hat{H}_2 = \sum_{\mathbf{k}}\left(\hat{\alpha}^\dagger_{\mathbf{k}}\hat{\beta}^\dagger_{-\mathbf{k}} + \hat{\beta}_{-\mathbf{k}}\hat{\alpha}_{\mathbf{k}}\right)\left\{2u(\mathbf{k})v(\mathbf{k})(k^2-\mu) - \xi\left[u(\mathbf{k})^2 - v(\mathbf{k})^2\right]\right\}\,. \tag{8.41}$$

Evidently, the Hamiltonian may be diagonalized by setting $\hat{H}_2$ to zero which can be done by requiring $2(k^2-\mu)u(\mathbf{k})v(\mathbf{k}) = \xi[u(\mathbf{k})^2 - v(\mathbf{k})^2]$, thus resulting in a total energy composed of the ground state, U, plus the sum of quasiparticle excitations, $\hat{H}_1$. Solving the diagonalization equation is facilitated by defining $u(\mathbf{k}) \equiv \cos\theta_{\mathbf{k}}$ and $v(\mathbf{k}) \equiv \sin\theta_{\mathbf{k}}$, from which we have

$$\begin{aligned}\hat{H}_2 = 0 \Rightarrow (k^2-\mu)\sin 2\theta_{\mathbf{k}} &= \xi\cos 2\theta_{\mathbf{k}} \\ \tan 2\theta_{\mathbf{k}} &= \frac{\xi}{k^2-\mu}\,.\end{aligned} \tag{8.42}$$

From this result, it is straightforward to solve for $\sin 2\theta_{\mathbf{k}}$ and $\cos 2\theta_{\mathbf{k}}$,

$$\sin 2\theta_{\mathbf{k}} = 2u(\mathbf{k})v(\mathbf{k}) = \frac{\xi}{\sqrt{(k^2-\mu)^2+\xi^2}} \tag{8.43a}$$

$$\cos 2\theta_{\mathbf{k}} = u(\mathbf{k})^2 - v(\mathbf{k})^2 = \frac{k^2-\mu}{\sqrt{(k^2-\mu)^2+\xi^2}}\,. \tag{8.43b}$$

Finally, using the constraint, $u(\mathbf{k})^2 + v(\mathbf{k})^2 = 1$, we have

$$u(\mathbf{k})v(\mathbf{k}) = \frac{1}{2}\frac{\xi}{\sqrt{(k^2-\mu)^2+\xi^2}} \tag{8.44a}$$

$$u(\mathbf{k})^2 = \frac{1}{2}\left[1 + \frac{k^2-\mu}{\sqrt{k^2-\mu)^2+\xi^2}}\right] \tag{8.44b}$$

$$v(\mathbf{k})^2 = \frac{1}{2}\left[1 - \frac{k^2-\mu}{\sqrt{k^2-\mu)^2+\xi^2}}\right]\,. \tag{8.44c}$$

8.2.1 Tha Gap Equation

After diagonalization, the Hamiltonian consists of a ground state part, U, and a sum over the excitations, $\hat{H}_1$, where

$$\hat{H}_1 = \sum_{\mathbf{k}} \sqrt{(k^2-\mu)^2+\xi^2}\left(\hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + \hat{\beta}^\dagger_{-\mathbf{k}}\hat{\beta}_{-\mathbf{k}}\right) . \tag{8.45}$$

Each quasiparticle contributes an energy of $\sqrt{(k^2-\mu)^2+\xi^2}$, implying the existence of a gap in energy between the ground state and the excitation spectrum[1]. The equation for the gap function is obtained by extremizing the ground state energy with respect to ξ:[2]

$$\frac{\delta U}{\delta \xi} = 0 \Rightarrow \begin{cases} \xi = 0 & \text{Normal Solution} \\ 1 = -\dfrac{1}{4\pi^2}\dfrac{\lambda}{1-\mu\lambda^2}\displaystyle\int_0^K \dfrac{k^2\,dk}{\sqrt{(k^2-\mu)^2+\xi^2}} & \text{Superconducting Solution} \end{cases} \tag{8.46}$$

Here, we have used $g = \sqrt{-2/\lambda}$ and $\varepsilon = 2/\lambda^2$, in accordance with Sec. 2.6.4.

The superconducting solution may be put into a more convenient form for numerical computations by using the following integration by parts formulae:

$$\int \frac{k^n\,dk}{\sqrt{(k^2-\mu)^2+\xi^2}} = 2\mu\frac{n-2}{n-1}\int\frac{k^{n-2}\,dk}{\sqrt{(k^2-\mu)^2+\xi^2}} - \frac{n-3}{n-1}(\mu^2+\xi^2)\int\frac{k^{n-4}\,dk}{\sqrt{(k^2-\mu)^2+\xi^2}} + \frac{k^{n-3}}{n-1}\sqrt{(k^2-\mu)^2+\xi^2} \tag{8.47a}$$

$$\int \frac{k^2(k^2-\mu)}{\left[(k^2-\mu)^2+\xi^2\right]^{3/2}}\,dk = -k\,\frac{1}{2}\left[(k^2-\mu)^2+\xi^2\right]^{-1/2} + \frac{1}{2}\int\frac{dk}{\sqrt{(k^2-\mu)^2+\xi^2}} . \tag{8.47b}$$

By defining

$$x \equiv \sqrt{\mu^2+\xi^2} \tag{8.48a}$$

$$r \equiv \sqrt{\frac{x+\mu}{2x}} , \tag{8.48b}$$

the superconductor gap equation in (8.46) can be expressed in terms of elliptic integrals[3]:

$$\frac{1}{a} + \frac{2}{\pi}\sqrt{x}\left[F(r) - 2E(r)\right] = 0 . \tag{8.49}$$

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[1] When compared to the bosonic case [see (5.27)] there is a sign difference in the expression for the quasiparticle excitation spectrum. As a result, the zero-range fermionic case does not exhibit the coherent decay, as found in Sec. 5.6.

[2] The gap function was first obtained by J. Bardeen, L. N. Cooper and J. R. Schrieffer (1957).

[3] I. S. Gradshteyn and I. M. Ryzhik (2000), Sec. 3.165, p. 290.

8.2.2 The Complete Superconductor Solution

According to (8.39), the ground state energy density is

$$u = \frac{1}{2\pi^2} \int_0^K k^4 \left[1 - \frac{k^2 - \mu}{\sqrt{(k^2-\mu)^2 + \xi^2}} \right] dk - \frac{\xi^2}{\lambda} - \frac{\xi^2}{2\pi^2} \int_0^K \frac{k^2\, dk}{\sqrt{(k^2-\mu)^2 + \xi^2}} \,. \tag{8.50}$$

In addition to the gap equation (8.49) and the number density,

$$\begin{aligned} \rho &= 2 \int'_{\mathbf{k}} v(\mathbf{k})^2 \\ &= \frac{1}{2\pi^2} \int_0^K \left[k^2 - \frac{k^4 - \mu k^2}{\sqrt{(k^2-\mu)^2 + \xi^2}} \right] dk \,, \end{aligned} \tag{8.51}$$

Eq. (8.50) specifies the complete solution to the problem. Using the integration by parts (8.47a) and the definitions (8.48), Eqs. (8.50) and (8.51) can be more compactly expressed as

$$u = \frac{1}{5\pi^2}(2x^2 - \mu)\sqrt{x}E(r) - \frac{x-\mu}{10\pi^2}(2x+\mu)\sqrt{x}F(r) - \frac{x^2-\mu}{8\pi a} \tag{8.52}$$

$$\rho = \frac{1}{3\pi^2}\mu\sqrt{x}E(r) + \frac{x-\mu}{6\pi^2}\sqrt{x}F(r) \,. \tag{8.53}$$

8.3 Interacting Fermi Gas with Two Feshbach States

A model is considered where, in addition to simulating the interparticle interactions, a second bound state consisting of real molecules is introduced. In this case, superfluidity is understood to emerge due to a condensation of the boson-like pairs[1]. The grand canonical Hamiltonian is

$$\begin{aligned} \hat{K} = & \sum_{\mathbf{k}\sigma} \left(k^2 - \mu\right) \hat{\psi}^\dagger_{\mathbf{k}\sigma} \hat{\psi}_{\mathbf{k}\sigma} + 2\left(\varepsilon - 2\mu\right) \sum_{\mathbf{k}} \hat{\chi}^\dagger_{\mathbf{k}} \hat{\chi}_{\mathbf{k}} + 2\left(\epsilon - 2\mu\right) \sum_{\mathbf{k}} \hat{\phi}^\dagger_{\mathbf{k}} \hat{\phi}_{\mathbf{k}} \\ & + \frac{g}{\sqrt{2}} \sum_{\mathbf{k}'',\mathbf{k},\mathbf{k}'} \hat{\chi}^\dagger_{\mathbf{k}''} F_{\mathbf{k}'',\mathbf{k}\mathbf{k}'} \left(\hat{\psi}_{\mathbf{k}\uparrow} \hat{\psi}_{-\mathbf{k}'\downarrow} - \hat{\psi}_{-\mathbf{k}\downarrow} \hat{\psi}_{\mathbf{k}'\uparrow} \right) + \text{H. c.} \\ & + \frac{\alpha}{\sqrt{2}} \sum_{\mathbf{k}'',\mathbf{k},\mathbf{k}'} \hat{\phi}^\dagger_{\mathbf{k}''} F_{\mathbf{k}'',\mathbf{k}\mathbf{k}'} \left(\hat{\psi}_{\mathbf{k}\uparrow} \hat{\psi}_{-\mathbf{k}'\downarrow} - \hat{\psi}_{-\mathbf{k}\downarrow} \hat{\psi}_{\mathbf{k}'\uparrow} \right) + \text{H. c.} \,, \end{aligned} \tag{8.54}$$

where the molecular fields (ϕ, χ) with their associated detunings (ϵ, ε) and couplings (α, g), are all defined in accordance with the conventions of Sec. 2.6. Since this analysis proceeds

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[1] E. Timmermans (2001).

in much the same way as that of Sec. 8.2, only the end results are quoted here. Thus, the complete solution to the double resonance case is[1]

$$u = \frac{1}{5\pi^2}(2x^2-\mu)\sqrt{x}E(r) - \frac{x-\mu}{10\pi^2}(2x+\mu)\sqrt{x}F(r) - (x^2-\mu)\left[\frac{\epsilon\alpha^2}{(\epsilon-2\mu)^2} - \frac{2\alpha^2}{\epsilon-2\mu} - \frac{1}{8\pi a}\right] \tag{8.55}$$

$$\rho = \frac{1}{3\pi^2}\,\mu\sqrt{x}E(r) + \frac{x-\mu}{6\pi^2}\sqrt{x}F(r) + 2\frac{\alpha^2(x^2-\mu^2)}{(\epsilon-2\mu)^2}\,. \tag{8.56}$$

Given x, μ is found from the gap equation

$$\frac{1}{a} + \frac{8\pi\alpha^2}{\epsilon-2\mu} + \frac{2}{\pi}\sqrt{x}\left[F(r)-2E(r)\right] = 0\,, \tag{8.57}$$

where x and r are given by (8.48).

8.4 BCS-BEC Crossover

In work undertaken by Leggett (1979), attention has been drawn to the distinction between BCS pairs and the molecular BEC. In particular, the question to be addressed is whether there is a phase transition that separates the regime of correlated Cooper pairs from that of the molecular BEC. Although it was found that such a "transition" occurs continuously, a criterion for the crossover is the change of sign of the chemical potential, μ. For positive values of μ, the system is BCS-like, whereas $\mu < 0$ implies a condensate. Unlike Leggett, we have explicitly included a molecular component, suggesting an alternate way to identify the transition, by using a direct comparison of the molecular BEC density to the BCS pair density.

From the expression

$$\rho = \int_{\mathbf{k}}' v(\mathbf{k})^2 + 2\frac{\xi^2}{(\epsilon-2\mu)^2}\,, \tag{8.58}$$

it is evident that $\xi \to 0$ corresponds to the low-density limit. However, care must be exercised when taking this limit, since it is really the ratio

$$z \equiv \frac{\xi}{\mu}\,, \tag{8.59}$$

that must be considered small, thus leading to a logarithmic expansion of the gap equation. Defining $k' = \sqrt{1-r^2}$, we have[2]

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[1] For specifics as to how the zero-range limit is taken, see the double resonance boson case in Chapter 5.

[2] The expansion of $F(k')$ and $E(k')$ can be found in 8.113.3 and 8.114.3 of Gradshteyn and Ryzhik, p. 852.

$$\begin{aligned} p(z)^{-1} \equiv \sqrt{\frac{x}{\mu}}\big[F(k') - 2E(k')\big] &= \sqrt{\frac{x}{\mu}}\left[\ln 4 - \ln k' + \frac{1}{4}\big(-3\ln 4 + 3\ln k' + 1\big)k'^2 + \ldots\right] \\ &= \ln\frac{8}{z} - \frac{1}{16}z^2\ln z + \frac{3}{8}\left(1 + \frac{1}{2}\ln 2\right)z^2 + \frac{159}{1024}\,z^4\,\ln z - \ldots\,. \end{aligned} \tag{8.60}$$

Taking $p(z) \simeq -1/\ln(z/8)$, the gap equation can be solved for z, giving

$$z \simeq 8\exp\left\{\frac{\pi}{2\sqrt{\mu}}\frac{1}{a(\epsilon - 2\mu)}\right\}, \tag{8.61}$$

where $1/a(\epsilon - 2\mu) = 1/a + 4\pi\alpha^2/(\epsilon - 2\mu)$. Using the expansions of the elliptic integrals, F and E, the leading order pair density can be obtained in terms of the chemical potential as

$$\rho_p = \int_{\mathbf{k}}' v(\mathbf{k})^2 \simeq \frac{1}{3\pi^2}\mu^{3/2}\,, \tag{8.62}$$

whereas the molecular condensate density is

$$\begin{aligned} \rho_m &= 2\,\frac{\alpha^2\xi^2}{(\epsilon - 2\mu)^2} \\ &\simeq \frac{128\alpha^2\mu^2}{(\epsilon - 2\mu)^2}\,\exp\left\{\frac{\pi}{\sqrt{\mu}}\,\frac{1}{a(\epsilon - 2\mu)}\right\}. \end{aligned} \tag{8.63}$$

A comparison of these two populations indicates that even for $\mu > 0$, there may be a dominance of the molecular BEC, depending on the value of the scattering length which is tuned through the external magnetic field. Hence, some question arises as to whether the sign change of μ is an adequate indicator of the crossover transition.

Appendix A

RPA Expansion for a Model Hamiltonian with a Two-Body Potential

In this section the grand canonical Hamiltonian of Eq. (4.22) is expanded to second order in the variations given by Eqs. (4.48).

A.1 Expansion of R, D and ψ^2

Assuming a separable form for the potential [see Eqs. (2.107) and (4.35)], the Hamiltonian of Eq. (4.22) in the momentum space representation is

$$\begin{aligned}
K = {}& \int_{\mathbf{k}}' (k^2 - \mu) \left[R(\mathbf{k}, \mathbf{k}, t) + \psi^*(\mathbf{k}, t)\psi(\mathbf{k}, t) \right] \\
&+ \frac{\lambda}{2} \int_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''}' \delta(\mathbf{k} - \mathbf{k}' - \mathbf{k}'' + \mathbf{k}''') v\Big(\frac{\mathbf{k} + \mathbf{k}'}{2}\Big) v\Big(\frac{\mathbf{k}'' + \mathbf{k}'''}{2}\Big) \Big[D^*(\mathbf{k}, \mathbf{k}', t) D(\mathbf{k}'', \mathbf{k}''', t) \\
&\qquad - D^*(\mathbf{k}, \mathbf{k}', t)\psi(\mathbf{k}'', t)\psi(\mathbf{k}''', t) + 2R(\mathbf{k}', \mathbf{k}'', t)R(\mathbf{k}, \mathbf{k}''', t) \\
&\qquad + 4\psi^*(\mathbf{k}', t)\psi(\mathbf{k}'', t)R(\mathbf{k}, \mathbf{k}''', t) - D(\mathbf{k}'', \mathbf{k}''', t)\psi^*(\mathbf{k}, t)\psi^*(\mathbf{k}', t) \\
&\qquad + \psi(\mathbf{k}''', t)\psi(\mathbf{k}'', t)\psi^*(\mathbf{k}, t)\psi^*(\mathbf{k}', t) \Big]
\end{aligned} \tag{A.1}$$

where

$$\begin{aligned}
R(\mathbf{k}, \mathbf{k}', t) = {}& \frac{1}{2} \left[\frac{1}{4} G^{-1}(\mathbf{k}, \mathbf{k}', t) + G(\mathbf{k}, \mathbf{k}', t) - \delta(\mathbf{k} - \mathbf{k}') \right] \\
&+ 2 \int_{\mathbf{k}'',\mathbf{k}'''}' \Sigma(\mathbf{k}, \mathbf{k}'', t) G(\mathbf{k}'', \mathbf{k}''', t) \Sigma(\mathbf{k}''', \mathbf{k}', t)
\end{aligned} \tag{A.2a}$$

$$\begin{aligned}D(\mathbf{k},\mathbf{k}',t) =&\frac{1}{2}\left[\frac{1}{4}G^{-1}(\mathbf{k},\mathbf{k}',t) - G(\mathbf{k},\mathbf{k}',t)\right] + 2\int_{\mathbf{k}'',\mathbf{k}'''}^{\prime}\Sigma(\mathbf{k},\mathbf{k}'',t)G(\mathbf{k}'',\mathbf{k}''',t)\Sigma(\mathbf{k}''',\mathbf{k}',t)\\ &- i\int_{\mathbf{k}''}^{\prime}\left[\Sigma(\mathbf{k},\mathbf{k}'',t)G(\mathbf{k}'',\mathbf{k}',t) + G(\mathbf{k},\mathbf{k}'',t)\Sigma(\mathbf{k}'',\mathbf{k}',t)\right]\end{aligned} \tag{A.2b}$$

$$\psi(\mathbf{k},t) = \frac{1}{\sqrt{2}}\Big[\phi(\mathbf{k},t) + i\pi(\mathbf{k},t)\Big]\,. \tag{A.2c}$$

The small, time-dependent, nonuniform deviations in G, Σ, ϕ and π are given in Eqs. (4.48), (4.50) and (4.51), but are reproduced here for convenience.

$$G(\mathbf{k},\mathbf{k}',t) = G(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}') + \delta G(\mathbf{k},\mathbf{k}',t) \tag{A.3a}$$

$$\Sigma(\mathbf{k},\mathbf{k}') = \delta\Sigma(\mathbf{k},\mathbf{k}',t) \tag{A.3b}$$

$$\phi(\mathbf{k},t) = \phi\delta(\mathbf{k}) + \delta\phi(\mathbf{k},t) \tag{A.3c}$$

$$\pi(\mathbf{k},t) = \delta\pi(\mathbf{k},t) \tag{A.3d}$$

$$\begin{aligned}G^{-1}(\mathbf{k},\mathbf{k}',t) =& G(\mathbf{k})^{-1}\delta(\mathbf{k}-\mathbf{k}') - G(\mathbf{k})^{-1}\delta G(\mathbf{k},\mathbf{k}',t)G(\mathbf{k}')^{-1}\\ &+ G(\mathbf{k})^{-1}\int_{\mathbf{k}''}^{\prime}\delta G^{*}(\mathbf{k},\mathbf{k}'',t)G(\mathbf{k}'')^{-1}\delta G(\mathbf{k}'',\mathbf{k}',t)G(\mathbf{k}')^{-1}\,.\end{aligned} \tag{A.3e}$$

Expanding K to second order first requires an expansion of R, D, and ψ, in terms of the variations in Eqs. (A.3). Using the general forms of Eqs. (A.2) obtains

$$R(\mathbf{k},\mathbf{k}',t) = R^{(0)}(\mathbf{k},\mathbf{k}',t) + R^{(1)}(\mathbf{k},\mathbf{k}',t) + R^{(2)}(\mathbf{k},\mathbf{k}',t)\,, \tag{A.4}$$

where

$$\begin{aligned}R^{(0)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\left[\frac{1}{4}G(\mathbf{k})^{-1} + G(\mathbf{k}) - 1\right]\delta(\mathbf{k}-\mathbf{k}')\\ &= R(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}')\end{aligned} \tag{A.5a}$$

$$R^{(1)}(\mathbf{k},\mathbf{k}',t) = \frac{1}{2}\left[-\frac{1}{4}G(\mathbf{k})^{-1}G(\mathbf{k}')^{-1} + 1\right]\delta G(\mathbf{k},\mathbf{k}',t) \tag{A.5b}$$

$$\begin{aligned}R^{(2)}(\mathbf{k},\mathbf{k}',t) =& \frac{1}{8}G(\mathbf{k})^{-1}\int_{\mathbf{k}''}^{\prime}\delta G^{*}(\mathbf{k},\mathbf{k}'',t)\,G(\mathbf{k}'')^{-1}\,\delta G(\mathbf{k}'',\mathbf{k}',t)G(\mathbf{k}')^{-1}\\ &+ 2\int_{\mathbf{k}''}\delta\Sigma^{*}(\mathbf{k},\mathbf{k}'',t)\,G(\mathbf{k}'')\,\delta\Sigma(\mathbf{k}'',\mathbf{k}',t)\,.\end{aligned} \tag{A.5c}$$

Similarly, the first few orders of the other fluctuations are:

$$\begin{aligned} D^{(0)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\left[\frac{1}{4}G(\mathbf{k})^{-1} - G(\mathbf{k})\right]\delta(\mathbf{k}-\mathbf{k}') \\ &= D(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}') \end{aligned} \tag{A.6a}$$

$$D^{(1)}(\mathbf{k},\mathbf{k}',t) = -\frac{1}{2}\left[\frac{1}{4}G(\mathbf{k})^{-1}G(\mathbf{k}')^{-1} + 1\right]\delta G(\mathbf{k},\mathbf{k}',t) - i\left[G(\mathbf{k}) + G(\mathbf{k}')\right]\delta\Sigma(\mathbf{k},\mathbf{k}',t) \tag{A.6b}$$

$$\begin{aligned} D^{(2)}(\mathbf{k},\mathbf{k}',t) = {} & \frac{1}{8}G(\mathbf{k})^{-1}\int'_{\mathbf{k}''}\delta G^*(\mathbf{k},\mathbf{k}'',t)\,G(\mathbf{k}'')^{-1}\,\delta G(\mathbf{k}'',\mathbf{k}',t)G(\mathbf{k}')^{-1} \\ & + 2\int_{\mathbf{k}''}\delta\Sigma^*(\mathbf{k},\mathbf{k}'',t)\,G(\mathbf{k}'')\,\delta\Sigma(\mathbf{k}'',\mathbf{k}',t) \\ & - i\int'_{\mathbf{k}''}\left[\delta\Sigma^*(\mathbf{k},\mathbf{k}'',t)\delta G(\mathbf{k}'',\mathbf{k}',t) + \delta G^*(\mathbf{k},\mathbf{k}'',t)\delta\Sigma(\mathbf{k}'',\mathbf{k}',t)\right] . \end{aligned} \tag{A.6c}$$

An expansion of products of the atomic field gives,

$$\psi^*\psi^{(0)}(\mathbf{k},\mathbf{k}',t) = \frac{1}{2}\phi^2\,\delta(\mathbf{k})\delta(\mathbf{k}') \tag{A.7a}$$

$$\begin{aligned} \psi^*\psi^{(1)}(\mathbf{k},\mathbf{k}',t) = {} & \frac{1}{2}\phi\,\delta(\mathbf{k}')\left[\delta\phi(\mathbf{k},t) - i\delta\pi(\mathbf{k},t)\right] \\ & + \frac{1}{2}\phi\,\delta(\mathbf{k})\left[\delta\phi(\mathbf{k}',t) + i\delta\pi(\mathbf{k}',t)\right] \end{aligned} \tag{A.7b}$$

$$\begin{aligned} \psi^*\psi^{(2)}(\mathbf{k},\mathbf{k}',t) = {} & \frac{1}{2}\left[\delta\phi^*(\mathbf{k},t)\delta\phi(\mathbf{k}',t) + i\delta\phi^*(\mathbf{k},t)\delta\pi(\mathbf{k}',t)\right. \\ & \left. -i\delta\phi(\mathbf{k}',t)\delta\pi^*(\mathbf{k},t) + \delta\pi^*(\mathbf{k},t)\delta\pi(\mathbf{k}',t)\right] , \end{aligned} \tag{A.7c}$$

$$\psi\psi^{(0)}(\mathbf{k},\mathbf{k}',t) = \frac{1}{2}\phi^2\,\delta(\mathbf{k})\delta(\mathbf{k}') \tag{A.8a}$$

$$\begin{aligned} \psi\psi^{(1)}(\mathbf{k},\mathbf{k}',t) = {} & \frac{1}{2}\phi\,\delta(\mathbf{k}')\left[\delta\phi(\mathbf{k},t) + i\delta\pi(\mathbf{k},t)\right] \\ & + \frac{1}{2}\phi\,\delta(\mathbf{k})\left[\delta\phi(\mathbf{k}',t) + i\delta\pi(\mathbf{k}',t)\right] \end{aligned} \tag{A.8b}$$

$$\begin{aligned} \psi\psi^{(2)}(\mathbf{k},\mathbf{k}',t) = {} & \frac{1}{2}\left[\delta\phi^*(\mathbf{k},t)\delta\phi(\mathbf{k}',t) + i\delta\phi^*(\mathbf{k},t)\delta\pi(\mathbf{k}',t)\right. \\ & \left. +i\delta\phi(\mathbf{k}',t)\delta\pi^*(\mathbf{k},t) - \delta\pi^*(\mathbf{k},t)\delta\pi(\mathbf{k}',t)\right] , \end{aligned} \tag{A.8c}$$

Using these expansions, we calculate the second order contributions from each of the terms in K.

A.2 Second Order Kinetic Contribution

The kinetic energy part is contained in the first integral of Eq. (A.1). From Eqs. (A.5), the second order part of $\displaystyle\int'_{\mathbf{k}}(k^2-\mu)R(\mathbf{k},\mathbf{k},t)$ is

$$\begin{aligned}\int'_{\mathbf{k}}(k^2-\mu)R^{(2)}(\mathbf{k},\mathbf{k},t) &= \int'_{\mathbf{k},\mathbf{k}'}(k^2-\mu)\Big[\frac{1}{8}\delta G^*(\mathbf{k}',\mathbf{k},t)\,G(\mathbf{k})^{-2}\,G(\mathbf{k}')^{-1}\delta G(\mathbf{k},\mathbf{k}',t)\\ &\qquad + \delta\Sigma^*(\mathbf{k}',\mathbf{k},t)\,2G(\mathbf{k}')\,\delta\Sigma(\mathbf{k},\mathbf{k}',t)\Big]\\ = \int'_{\mathbf{q},\mathbf{P}}\Big[\Big(\mathbf{q}+\frac{1}{2}\mathbf{P}\Big)^2-\mu\Big]&\Big[\frac{1}{8}\delta G^*(\mathbf{q},-\mathbf{P},t)G\Big(\mathbf{q}+\frac{1}{2}\mathbf{P}\Big)^{-2}G\Big(\mathbf{q}-\frac{1}{2}\mathbf{P}\Big)^{-1}\delta G(\mathbf{q},\mathbf{P},t)\\ &\qquad +\delta\Sigma^*(\mathbf{q},-\mathbf{P},t)\,2G\Big(\mathbf{q}-\frac{1}{2}\mathbf{P}\Big)\,\delta\Sigma(\mathbf{q},\mathbf{P},t)\Big]\\ = \int'_{\mathbf{q},\mathbf{P}}\Big[&\delta G^*(\mathbf{q},\mathbf{P},t)(k^2-\mu)R_{G^2}(\mathbf{q},\mathbf{P})\delta G(\mathbf{q},\mathbf{P},t)\\ &\qquad + \delta\Sigma^*(\mathbf{q},\mathbf{P},t)(k^2-\mu)R_{\Sigma^2}(\mathbf{q},\mathbf{P})\delta\Sigma(\mathbf{q},\mathbf{P},t)\Big]\,,\end{aligned}\tag{A.9}$$

where we identify

$$\mathbf{P}=\mathbf{k}-\mathbf{k}' \qquad\qquad \mathbf{P}'=\mathbf{k}''-\mathbf{k}''' \tag{A.10a}$$

$$\mathbf{q}=\frac{1}{2}(\mathbf{k}+\mathbf{k}') \qquad\qquad \mathbf{q}'=\frac{1}{2}(\mathbf{k}''+\mathbf{k}''')\,. \tag{A.10b}$$

As given by Eq. (4.52), we have used the transformation $\delta G^*(\mathbf{k}',\mathbf{k},t)\to\delta G^*(\mathbf{q},\mathbf{P},t)$, where the symmetry under the inversion $\mathbf{P}\to-\mathbf{P}$ is implicit in the following definitions

$$(k^2-\mu)R_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P})=\frac{1}{16}\Big[(\mathbf{q}_+^2-\mu)G_+^{-2}G_-^{-1}+(\mathbf{q}_-^2-\mu)G_-^{-2}G_+^{-1}\Big]\delta(\mathbf{q}-\mathbf{q}') \tag{A.11a}$$

$$(k^2-\mu)R_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})=\Big[(\mathbf{q}_+^2-\mu)G_-+(\mathbf{q}_-^2-\mu)G_+\Big]\delta(\mathbf{q}-\mathbf{q}')\,. \tag{A.11b}$$

For notational simplicity, we use the ± subscript to denote a coordinate shift of $\pm\mathbf{P}/2$ in the argument of any function f such that

$$f_\pm=f\Big(\mathbf{q}\pm\frac{1}{2}\mathbf{P}\Big)\,,\qquad f'_\pm=f\Big(\mathbf{q}'\pm\frac{1}{2}\mathbf{P}'\Big)\,. \tag{A.12}$$

Using Eq. (A.7), the second order contribution from $\int'_{\mathbf{k}} (k^2-\mu)\psi^*(\mathbf{k},t)\psi(\mathbf{k},t)$ is

$$\begin{aligned}\int'_{\mathbf{k}} (k^2-\mu)\psi^*\psi^{(2)}(\mathbf{k},\mathbf{k},t) &= \int'_{\mathbf{k}} (k^2-\mu)\frac{1}{2}\left[|\delta\phi(\mathbf{k},t)|^2 + |\delta\pi(\mathbf{k},t)|^2\right] \\ &= \int'_{\mathbf{P}} \big[\delta\phi^*(\mathbf{P},t)(k^2-\mu)\psi^*\psi_{\phi^2}(\mathbf{P})\delta\phi(\mathbf{P},t) \\ &\qquad + \delta\pi^*(\mathbf{P},t)(k^2-\mu)\psi^*\psi_{\pi^2}(\mathbf{P})\delta\pi(\mathbf{P},t)\big]\ ,\end{aligned} \tag{A.13}$$

where

$$(k^2-\mu)\psi^*\psi_{\phi^2}(\mathbf{P}) = \frac{1}{2}(\mathbf{P}^2-\mu) \tag{A.14a}$$

$$(k^2-\mu)\psi^*\psi_{\pi^2}(\mathbf{P}) = \frac{1}{2}(\mathbf{P}^2-\mu)\,. \tag{A.14b}$$

In contrast, the second order potential is somewhat more complicated as it involves products of the quantities expanded in Eqs. (A.4)-(A.8).

A.3 Second Order Potential Contribution

It is convenient to separate the two types of products in the potential. Discussing each individually, the first is characterized by a self product whereas the other involves a cross product.

A.3.1 Products of Quantities with Themselves

We list the second order contribution for each of the self-product terms, D^*D, RR and $|\psi|^4$, respectively.

D*D:

$$\begin{aligned}\int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} &\delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)v\Big(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\Big)\Big[D^{*(0)}(\mathbf{k},\mathbf{k}',t)D^{(2)}(\mathbf{k}'',\mathbf{k}''',t) \\ &+D^{*(1)}(\mathbf{k},\mathbf{k}',t)D^{(1)}(\mathbf{k}'',\mathbf{k}''',t)+D^{*(2)}(\mathbf{k},\mathbf{k}',t)D^{(0)}(\mathbf{k}'',\mathbf{k}''',t)\Big]\end{aligned} \tag{A.15}$$

Using the zero, first and second order terms in Eqs. (A.6), this becomes

$$\begin{aligned}= \int'_{\mathbf{k},\mathbf{k}''} v(\mathbf{k})v(\mathbf{k}'')D(\mathbf{k}'') \int'_{\mathbf{k}'} \Big[&\delta G^*(\mathbf{k}',\mathbf{k},t)\frac{1}{8}G(\mathbf{k})^{-2}G(\mathbf{k}')^{-1}\delta G(\mathbf{k},\mathbf{k}',t) \\ &+ \delta\Sigma^*(\mathbf{k}',\mathbf{k},t)\,2G(\mathbf{k}')\,\delta\Sigma(\mathbf{k},\mathbf{k}',t)\Big]\end{aligned}$$

$$+ \int'_{\mathbf{k},\mathbf{k}''} v(\mathbf{k}) v(\mathbf{k}'') D(\mathbf{k}) \int'_{\mathbf{k}'} \Big[\delta G^*(\mathbf{k}',\mathbf{k}'',t) \frac{1}{8} G(\mathbf{k}'')^{-2} G(\mathbf{k}')^{-1} \delta G(\mathbf{k}'',\mathbf{k}',t)$$

$$+ \delta\Sigma^*(\mathbf{k}',\mathbf{k}'',t)\, 2G(\mathbf{k}')\, \delta\Sigma(\mathbf{k}'',\mathbf{k}',t) \Big]$$

$$+ \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''') v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big) v\Big(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\Big) \delta G^*(\mathbf{k},\mathbf{k}',t) \frac{1}{4} \left[\frac{1}{4} G(\mathbf{k})^{-1} G(\mathbf{k}')^{-1} + 1 \right]$$

$$\times \left[\frac{1}{4} G(\mathbf{k}'')^{-1} G(\mathbf{k}''')^{-1} + 1 \right] \delta G(\mathbf{k}'',\mathbf{k}''',t)$$

$$+ \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''') v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big) v\Big(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\Big) \delta\Sigma^*(\mathbf{k},\mathbf{k}',t) \left[G(\mathbf{k}) + G(\mathbf{k}') \right]$$

$$\times \left[G(\mathbf{k}'') + G(\mathbf{k}''') \right] \delta\Sigma(\mathbf{k}'',\mathbf{k}''',t)\,, \qquad \text{(A.16)}$$

which can be written more compactly as

$$\int'_{\mathbf{q},\mathbf{q}',\mathbf{P}} \left[\delta G^*(\mathbf{q},\mathbf{P},t) D^2_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) \delta G(\mathbf{q}',\mathbf{P},t) + \delta\Sigma^*(\mathbf{q},\mathbf{P},t) D^2_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) \delta\Sigma(\mathbf{q}',\mathbf{P},t) \right]\,, \qquad \text{(A.17)}$$

where we have used the momenta in Eqs. (A.10) with $\mathbf{P} = \mathbf{P}'$. In the notation of Eq. (A.12), it can be deduced from (A.16) that the matrices $D^2_{G^2}$ and $D^2_{\Sigma^2}$ are given by

$$D^2_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) = \int'_{\mathbf{k}} v(\mathbf{k}) D(\mathbf{k}) \left[\frac{1}{8} v\Big(\mathbf{q} + \frac{1}{2}\mathbf{P}\Big) G_+^{-2} G_-^{-1} + \frac{1}{8} v\Big(\mathbf{q} - \frac{1}{2}\mathbf{P}\Big) G_-^{-2} G_+^{-1} \right] \delta(\mathbf{q}-\mathbf{q}')$$

$$+ v(\mathbf{q}) v(\mathbf{q}') \frac{1}{4} \left(\frac{1}{4} G_+^{-1}\, G_-^{-1} + 1 \right) \left(\frac{1}{4} G_+'^{-1}\, G_-'^{-1} + 1 \right) \qquad \text{(A.18a)}$$

$$D^2_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) = \int'_{\mathbf{k}} v(\mathbf{k}) D(\mathbf{k}) \left[2v\Big(\mathbf{q} + \frac{1}{2}\mathbf{P}\Big) G_- + 2v\Big(\mathbf{q} - \frac{1}{2}\mathbf{P}) G_+ \right] \delta(\mathbf{q}-\mathbf{q}')$$

$$+ v(\mathbf{q}) v(\mathbf{q}') (G_+ + G_-)(G'_+ + G'_-) \qquad \text{(A.18b)}$$

2RR:

$$\int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''') v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big) v\Big(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\Big)\, 2 \Big[R^{*(0)}(\mathbf{k}',\mathbf{k}'',t) R^{(2)}(\mathbf{k},\mathbf{k}''',t)$$

$$+ R^{*(1)}(\mathbf{k}',\mathbf{k}'',t) R^{(1)}(\mathbf{k},\mathbf{k}''',t) + R^{*(2)}(\mathbf{k}',\mathbf{k}'',t) R^{(0)}(\mathbf{k},\mathbf{k}''',t) \Big] \qquad \text{(A.19)}$$

Using the zero, first and second order terms of Eq. (A.5), this becomes

$$
\begin{aligned}
&= \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'''} v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big) v\Big(\frac{-\mathbf{k}-\mathbf{k}'}{2}\Big)\, 2R(\mathbf{k}') \Big[\delta G^*(\mathbf{k},\mathbf{k}''',t)\,\frac{1}{8}\,G(\mathbf{k})^{-2}\,G(\mathbf{k}''')^{-1}\,\delta G(\mathbf{k}''',\mathbf{k},t) \\
&\qquad\qquad + \delta\Sigma^*(\mathbf{k},\mathbf{k}''',t)\,2G(\mathbf{k}''')\,\delta\Sigma(\mathbf{k}''',\mathbf{k},t)\Big] \\
&+ \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'''} v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big) v\Big(\frac{-\mathbf{k}-\mathbf{k}'}{2}\Big)\, 2R(\mathbf{k}) \Big[\delta G^*(\mathbf{k}',\mathbf{k}''',t)\,\frac{1}{8}\,G(\mathbf{k}')^{-2}\,G(\mathbf{k}''')^{-1}\,\delta G(\mathbf{k}''',\mathbf{k}',t) \\
&\qquad\qquad + \delta\Sigma^*(\mathbf{k}',\mathbf{k}''',t)\,2G(\mathbf{k}''')\,\delta\Sigma(\mathbf{k}''',\mathbf{k}',t)\Big] \\
&+ \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''') v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big) v\Big(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\Big) \delta G^*(\mathbf{k},\mathbf{k}''',t)\frac{1}{2}\Big[-\frac{1}{4}G(\mathbf{k}')^{-1}G(\mathbf{k}'')^{-1}+1\Big] \\
&\qquad\qquad \times\Big[-\frac{1}{4}G(\mathbf{k})^{-1}G(\mathbf{k}''')^{-1}+1\Big]\,\delta G(\mathbf{k}',\mathbf{k}'',t)\,. \qquad (A.20)
\end{aligned}
$$

In analogy to (A.17) this can be written concisely as

$$
\int'_{\mathbf{q},\mathbf{q}',\mathbf{P}} \big[\delta G^*(\mathbf{q},\mathbf{P},t) R^2_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) \delta G(\mathbf{q}',\mathbf{P},t) + \delta\Sigma^*(\mathbf{q},\mathbf{P},t) R^2_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) \delta\Sigma(\mathbf{q}',\mathbf{P},t)\big]\ , \qquad (A.21)
$$

where

$$
\begin{aligned}
R^2_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) =\ & 2\int'_{\mathbf{k}} R(\mathbf{k}) \Big[v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big)\,\frac{1}{8}\,G_+^{-2}\,G_-^{-1} \\
&\qquad v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big)\,\frac{1}{8}\,G_-^{-2}\,G_+^{-1}\Big]\,\delta(\mathbf{q}-\mathbf{q}') \\
&+ v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{q}'+\frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{q}'+\frac{1}{4}\mathbf{P}\Big)\,\frac{1}{2}\,\Big(-\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\Big)\,\Big(-\frac{1}{4}G_+'^{-1}\,G_-'^{-1}+1\Big)
\end{aligned}
\qquad (A.22a)
$$

$$
\begin{aligned}
R^2_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) =\ & 2\int'_{\mathbf{k}} R(\mathbf{k}) \Big[v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big)\,2\,G_- \\
&\qquad + v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big)\,2\,G_+\Big]\ . \qquad (A.22b)
\end{aligned}
$$

To express the arguments of R as $\mathbf{q}$, $\mathbf{q}'$ and $\mathbf{P}$, it is necessary to change variables such that

$$\mathbf{P} = \mathbf{k} + \mathbf{k}''' \qquad \mathbf{P}' = \mathbf{k}'' + \mathbf{k}' \tag{A.23a}$$

$$\mathbf{q} = \frac{1}{2}(\mathbf{k} - \mathbf{k}''') \qquad \mathbf{q}' = \frac{1}{2}(\mathbf{k}' - \mathbf{k}'')\,. \tag{A.23b}$$

$\psi\psi\psi^*\psi^*$**:**

$$\begin{aligned}
&\int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k} - \mathbf{k}' - \mathbf{k}'' + \mathbf{k}''') v\Big(\frac{\mathbf{k} + \mathbf{k}'}{2}\Big) v\Big(\frac{\mathbf{k}'' + \mathbf{k}'''}{2}\Big) \Big[\psi\psi^{(0)}(\mathbf{k}''', \mathbf{k}'', t)\, \psi^*\psi^{*\,(2)}(\mathbf{k}, \mathbf{k}', t) \\
&\qquad + \psi\psi^{(1)}(\mathbf{k}''', \mathbf{k}'', t)\, \psi^*\psi^{*\,(1)}(\mathbf{k}, \mathbf{k}', t) + \psi\psi^{(2)}(\mathbf{k}''', \mathbf{k}'', t)\, \psi^*\psi^{*\,(0)}(\mathbf{k}, \mathbf{k}', t)\Big] \\
&= \int'_{\mathbf{P}} v(0) v(\mathbf{P}) \frac{1}{2}\phi^2 \left[|\delta\phi(\mathbf{P}, t)|^2 - |\delta\pi(\mathbf{P}, t)|^2\right] \\
&+ \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k} - \mathbf{k}' - \mathbf{k}'' + \mathbf{k}''') v\Big(\frac{\mathbf{k} + \mathbf{k}'}{2}\Big) v\Big(\frac{\mathbf{k}'' + \mathbf{k}'''}{2}\Big) \frac{1}{4}\phi^2 \\
&\qquad \times \Big\{\delta(\mathbf{k}''')\delta(\mathbf{k}) \left[\delta\phi^*(\mathbf{k}', t) - i\delta\pi^*(\mathbf{k}', t)\right] \left[\delta\phi(\mathbf{k}'', t) + i\delta\pi(\mathbf{k}'', t)\right] \\
&\qquad\quad + \delta(\mathbf{k}''')\delta(\mathbf{k}') \left[\delta\phi^*(\mathbf{k}, t) - i\delta\pi^*(\mathbf{k}, t)\right] \left[\delta\phi(\mathbf{k}'', t) + i\delta\pi(\mathbf{k}'', t)\right] \\
&\qquad\quad + \delta(\mathbf{k}'')\delta(\mathbf{k}) \left[\delta\phi^*(\mathbf{k}', t) - i\delta\pi^*(\mathbf{k}', t)\right] \left[\delta\phi(\mathbf{k}''', t) + i\delta\pi(\mathbf{k}''', t)\right] \\
&\qquad\quad + \delta(\mathbf{k}'')\delta(\mathbf{k}') \left[\delta\phi^*(\mathbf{k}, t) - i\delta\pi^*(\mathbf{k}, t)\right] \left[\delta\phi(\mathbf{k}''', t) + i\delta\pi(\mathbf{k}''', t)\right]\Big\} \\
&= \int'_{\mathbf{P}} \Big[\delta\phi^*(\mathbf{P}, t)\, |\psi|^4_{\phi^2}(\mathbf{P})\, \delta\phi(\mathbf{P}, t) + \delta\pi^*(\mathbf{P}, t)\, |\psi|^4_{\pi^2}(\mathbf{P})\, \delta\pi(\mathbf{P}, t)\Big]\ ,
\end{aligned} \tag{A.24}$$

where

$$|\psi|^4_{\phi^2}(\mathbf{P}) = \phi^2 \left[\frac{1}{2} v(0) v(\mathbf{P}) + v\Big(\frac{1}{2}\mathbf{P}\Big) v\Big(\frac{1}{2}\mathbf{P}\Big)\right] \tag{A.25a}$$

$$|\psi|^4_{\phi^2}(\mathbf{P}) = \phi^2 \left[v\Big(\frac{1}{2}\mathbf{P}\Big) v\Big(\frac{1}{2}\mathbf{P}\Big) - \frac{1}{2} v(0) v(\mathbf{P})\right]\ . \tag{A.25b}$$

A.3.2 Cross-Products Between Quantities

In a similar vein, the cross terms in the potential are also evaluated using the expansions of (A.4)-(A.8).

$\mathbf{D}^*\psi\psi + \mathbf{D}\psi^*\psi^*$:

$$\int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)v\Big(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\Big)\Big[D^{*\,(0)}(\mathbf{k},\mathbf{k}',t)\,\psi\psi^{(2)}(\mathbf{k}'',\mathbf{k}''',t)$$
$$+ D^{*\,(1)}(\mathbf{k},\mathbf{k}',t)\,\psi\psi^{(1)}(\mathbf{k}'',\mathbf{k}''',t) + D^{*\,(2)}(\mathbf{k},\mathbf{k}',t)\,\psi\psi^{(0)}(\mathbf{k}'',\mathbf{k}''',t) + \text{H.c.}\Big] \quad \text{(A.26)}$$

Using the zero, first and second order terms of Eqs. (A.6) and (A.8) gives

$$= \int'_{\mathbf{k},\mathbf{k}'} v(\mathbf{k})v(\mathbf{k}')D(\mathbf{k})\,\big[|\delta\phi(\mathbf{k}',t)|^2 - |\delta\pi(\mathbf{k}',t)|^2\big]$$
$$+ \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)v\Big(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\Big)\delta G^*(\mathbf{k},\mathbf{k}',t)\Big(-\frac{1}{2}\Big)\,\Big[\frac{1}{4}G(\mathbf{k})^{-1}\,G(\mathbf{k}')^{-1}+1\Big]$$
$$\times\,\phi\,\big[\delta(\mathbf{k}'')\,\delta\phi(\mathbf{k}''',t) + \delta(\mathbf{k}''')\,\delta\phi(\mathbf{k}'',t)\big]$$
$$+ \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)v\Big(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\Big)\delta\Sigma^*(\mathbf{k},\mathbf{k}',t)\,\big[-G(\mathbf{k})-G(\mathbf{k}')\big]$$
$$\times\,\phi\,\big[\delta(\mathbf{k}'')\,\delta\pi(\mathbf{k}''',t) + \delta(\mathbf{k}''')\,\delta\pi(\mathbf{k}'',t)\big]$$
$$+ \int'_{\mathbf{k}} v(0)v(\mathbf{k})\phi^2 \int'_{\mathbf{k}'}\Big[\delta G^*(\mathbf{k},\mathbf{k}',t)\frac{1}{8}G(\mathbf{k})^{-2}\,G(\mathbf{k}')^{-1}\delta G(\mathbf{k}',\mathbf{k},t)$$
$$+ \delta\Sigma^*(\mathbf{k},\mathbf{k}',t)\,2G(\mathbf{k}')\,\delta\Sigma(\mathbf{k}',\mathbf{k},t)\Big]$$
$$= \int'_{\mathbf{q},\mathbf{q}',\mathbf{P}} \big[\delta G^*(\mathbf{q},\mathbf{P},t)D\psi\psi_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P})\delta G(\mathbf{q},\mathbf{P},t) + \delta\Sigma^*(\mathbf{q},\mathbf{P},t)D\psi\psi_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})\delta\Sigma(\mathbf{q},\mathbf{P},t)\big]$$
$$+ \int'_{\mathbf{q},\mathbf{P}} [\delta G^*(\mathbf{q},\mathbf{P},t)D\psi\psi_{G\phi}(\mathbf{q},\mathbf{P})\delta\phi(\mathbf{P},t) + \delta\Sigma^*(\mathbf{q},\mathbf{P},t)D\psi\psi_{\Sigma\pi}(\mathbf{q},\mathbf{P})\delta\pi(\mathbf{P},t)]$$
$$+ \int'_{\mathbf{P}} \big[\delta\phi^*(\mathbf{P},t)D\psi\psi_{\phi^2}(\mathbf{P})\delta\phi(\mathbf{P},t) + \delta\pi^*(\mathbf{P},t)D\psi\psi_{\pi^2}(\mathbf{P})\delta\pi(\mathbf{P},t)\big]\;, \quad \text{(A.27)}$$

where

$$D\psi\psi_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) = v(0)\frac{1}{2}\phi^2\,\Big[v\Big(\mathbf{q}+\frac{1}{2}\mathbf{P}\Big)\frac{1}{8}G_+^{-2}\,G_-^{-1} + v\Big(\mathbf{q}-\frac{1}{2}\mathbf{P}\Big)\frac{1}{8}G_-^{-2}\,G_+^{-1}\Big]\,\delta(\mathbf{q}-\mathbf{q}') \quad \text{(A.28a)}$$

$$D\psi\psi_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) = v(0)\frac{1}{2}\phi^2\,\Big[v\Big(\mathbf{q}+\frac{1}{2}\mathbf{P}\Big)\,2\,G_- + v\Big(\mathbf{q}-\frac{1}{2}\mathbf{P}\Big)\,2\,G_+\Big]\,\delta(\mathbf{q}-\mathbf{q}') \quad \text{(A.28b)}$$

$$D\psi\psi_{G\phi}(\mathbf{q},\mathbf{P}) = -\left[v(\mathbf{q})v\Big(\frac{1}{2}\mathbf{P}\Big) + v(\mathbf{q})v\Big(-\frac{1}{2}\mathbf{P}\Big)\right]\frac{1}{2}\phi\left(\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\right) \tag{A.28c}$$

$$D\psi\psi_{\Sigma\pi}(\mathbf{q},\mathbf{P}) = -\left[v(\mathbf{q})v\Big(\frac{1}{2}\mathbf{P}\Big) + v(\mathbf{q})v\Big(-\frac{1}{2}\mathbf{P}\Big)\right]\phi(G_+ + G_-) \tag{A.28d}$$

$$D\psi\psi_{\phi^2}(\mathbf{P}) = v(\mathbf{P})\int_{\mathbf{k}}' v(\mathbf{k})\,D(\mathbf{k}) \tag{A.28e}$$

$$D\psi\psi_{\pi^2}(\mathbf{P}) = -v(\mathbf{P})\int_{\mathbf{k}}' v(\mathbf{k})\,D(\mathbf{k})\,. \tag{A.28f}$$

$\mathbf{4\psi^*\psi R}$:

$$\int_{\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}'''}' \delta(\mathbf{k}-\mathbf{k}'-\mathbf{k}''+\mathbf{k}''')v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)v\Big(\frac{\mathbf{k}''+\mathbf{k}'''}{2}\Big)\Big[4\psi^*\psi^{(0)}(\mathbf{k}',\mathbf{k}'',t)\,R^{(2)}(\mathbf{k},\mathbf{k}''',t)$$
$$+4\psi^*\psi^{(1)}(\mathbf{k}',\mathbf{k}'',t)\,R^{(1)}(\mathbf{k},\mathbf{k}''',t) + 4\psi^*\psi^{(2)}(\mathbf{k}',\mathbf{k}'',t)\,R^{(0)}(\mathbf{k},\mathbf{k}''',t)\Big]\,. \tag{A.29}$$

Using the zero, first and second order terms of Eqs. (A.5) and (A.7) gives

$$= \int_{\mathbf{k},\mathbf{k}'}' v\Big(\frac{1}{2}\mathbf{k}\Big)v\Big(-\frac{1}{2}\mathbf{k}\Big)\,2\,\phi^2\left[\delta G^*(\mathbf{k},\mathbf{k}',t)\frac{1}{8}G(\mathbf{k})^{-2}\,G(\mathbf{k}')^{-1}\delta G(\mathbf{k}',\mathbf{k},t)\right.$$
$$\left. + \,\delta\Sigma^*(\mathbf{k},\mathbf{k}',t)\,2G(\mathbf{k}')\delta\Sigma(\mathbf{k}',\mathbf{k},t)\right]$$
$$+\int_{\mathbf{k},\mathbf{k}',\mathbf{k}'''}' \delta(\mathbf{k}-\mathbf{k}'+\mathbf{k}''')v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{k}'\Big)v\Big(\frac{1}{2}\mathbf{k}'''\Big)4\,\phi\,\delta\phi^*(\mathbf{k}',t)\frac{1}{2}\left[-\frac{1}{4}G(\mathbf{k})^{-1}\,G(\mathbf{k}''')^{-1}+1\right]\delta G(\mathbf{k},\mathbf{k}''',t)$$
$$+\int_{\mathbf{k},\mathbf{k}'}' v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{k}'\Big)v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{k}'\Big)\,2\,\left\{\delta\phi^*(\mathbf{k}',t)R(\mathbf{k})\delta\phi(\mathbf{k}',t)+\delta\pi^*(\mathbf{k}',t)R(\mathbf{k})\delta\pi(\mathbf{k}',t)\right\}\,. \tag{A.30}$$

Employing the coordinate transformations of Eqs. (A.23) results in the more compact form

$$= \int_{\mathbf{q},\mathbf{q}',\mathbf{P}}' \left[\delta G^*(\mathbf{q},\mathbf{P},t)\,\psi^*\psi R_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P})\,\delta G(\mathbf{q},\mathbf{P},t) + \delta\Sigma^*(\mathbf{q},\mathbf{P},t)\,\psi^*\psi R_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})\,\delta\Sigma(\mathbf{q},\mathbf{P},t)\right]$$
$$+\int_{\mathbf{q},\mathbf{P}}' \delta G^*(\mathbf{q},\mathbf{P},t)\psi^*\psi R_{G\phi}(\mathbf{q},\mathbf{P})\delta\phi(\mathbf{P},t)$$
$$+\int_{\mathbf{P}}' \left[\delta\phi^*(\mathbf{P},t)\,\psi^*\psi R_{\phi^2}(\mathbf{P})\,\delta\phi(\mathbf{P},t) + \delta\pi^*(\mathbf{P},t)\,\psi^*\psi\,R_{\pi^2}(\mathbf{P})\,\delta\pi(\mathbf{P},t)\right] \tag{A.31}$$

where

$$\psi^*\psi R_{G^2}(\mathbf{q},\mathbf{q}'\mathbf{P}) = \frac{1}{8}\phi^2 \Big[v\Big(\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big) G_+^{-2}\,G_-^{-1} + v\Big(\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big) G_-^{-2} G_+^{-1} \Big]\, \delta(\mathbf{q}-\mathbf{q}') \quad \text{(A.32a)}$$

$$\psi^*\psi R_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) = 2\,\phi^2 \Big[v\Big(\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big) G_- + v\Big(\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big) G_+ \Big]\, \delta(\mathbf{q}-\mathbf{q}') \quad \text{(A.32b)}$$

$$\psi^*\psi R_{G\phi}(\mathbf{q},\mathbf{P}) = v\Big(\frac{1}{2}\mathbf{q}+\frac{3}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big)\, 2\,\phi\, \Big(-\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\Big) \quad \text{(A.32c)}$$

$$\psi^*\psi R_{\phi^2}(\mathbf{P}) = \int_{\mathbf{k}}' v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{P}\Big) R(\mathbf{k}) \quad \text{(A.32d)}$$

$$\psi^*\psi\, R_{\pi^2}(\mathbf{P}) = \int_{\mathbf{k}}' v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{P}\Big) R(\mathbf{k})\,. \quad \text{(A.32e)}$$

A.4 Matrix Form of RPA

Expressed in a compact matrix form, the grand canonical Hamiltonian of Eq. (A.1) has the second order expansion

$$K_{RPA} = \frac{1}{2} \begin{bmatrix} \delta G^*(\mathbf{q},\mathbf{P}) & \delta\phi^*(\mathbf{P}) \end{bmatrix} \begin{bmatrix} \mathfrak{A}_{GG}(\mathbf{q},\mathbf{q}',\mathbf{P}) & \mathfrak{A}_{G\phi}(\mathbf{q}',\mathbf{P}) \\ \mathfrak{A}_{\phi G}(\mathbf{q},\mathbf{P}) & \mathfrak{A}_{\phi\phi}(\mathbf{P}) \end{bmatrix} \begin{bmatrix} \delta G(\mathbf{q}',\mathbf{P}) \\ \delta\phi(\mathbf{P}) \end{bmatrix} + \frac{1}{2} \begin{bmatrix} \delta\Sigma^*(\mathbf{q},\mathbf{P}) & \delta\pi^*(\mathbf{P}) \end{bmatrix} \begin{bmatrix} \mathfrak{B}_{\Sigma\Sigma}(\mathbf{q},\mathbf{q}',\mathbf{P}) & \mathfrak{B}_{\Sigma\pi}(\mathbf{q}',\mathbf{P}) \\ \mathfrak{B}_{\pi\Sigma}(\mathbf{q},\mathbf{P}) & \mathfrak{B}_{\pi\pi}(\mathbf{P}) \end{bmatrix} \begin{bmatrix} \delta\Sigma(\mathbf{q}',\mathbf{P}) \\ \delta\pi(\mathbf{P}) \end{bmatrix}, \quad \text{(A.33)}$$

where the matrix elements are found by combining the results given in Eqs. (A.11), (A.14), (A.18), (A.22), (A.25), (A.28) and (A.32).

A.4.1 $\mathfrak{A}$ Matrix Elements

Starting with the terms involving δG^2, we simply read off the corresponding contributions from each of the previous expansions, thus obtaining

$$\mathfrak{A}_{GG}(\mathbf{q},\mathbf{q}',\mathbf{P}) = 2\,(k^2-\mu) R_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) + \lambda \big[D^2_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) + R^2_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) - D\psi\psi_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) + \psi^*\psi R_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) \big] \quad \text{(A.34)}$$

An explicit substitution of each of these quantities results in the rather lengthy expression

$$
\begin{aligned}
&= \frac{1}{8}\left[(\mathbf{q}_+{}^2-\mu)G_+^{-2}\,G_-^{-1}+(\mathbf{q}_-{}^2-\mu)G_-^{-2}\,G_+^{-1}\right]\delta(\mathbf{q}-\mathbf{q}')\\
&\quad+\lambda\int_{\mathbf{k}}^{\prime} v(\mathbf{k})D(\mathbf{k})\left[\frac{1}{8}\,v\Big(\mathbf{q}+\frac{1}{2}\mathbf{P}\Big)G_+^{-2}\,G_-^{-1}+\frac{1}{8}\,v\Big(\mathbf{q}-\frac{1}{2}\mathbf{P}\Big)G_-^{-2}\,G_+^{-1}\right]\delta(\mathbf{q}-\mathbf{q}')\\
&\quad+\lambda\,v(\mathbf{q})v(\mathbf{q}')\frac{1}{4}\left(\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\right)\left(\frac{1}{4}G_+'^{-1}\,G_-'^{-1}+1\right)\\
&\quad+2\,\lambda\int_{\mathbf{k}}^{\prime} R(\mathbf{k})\left[v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big)v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big)\frac{1}{8}G_+^{-2}\,G_-^{-1}\right.\\
&\quad\left.+\,v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big)v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big)\frac{1}{8}G_-^{-2}\,G_+^{-1}\right]\delta(\mathbf{q}-\mathbf{q}')\\
&+\lambda\,v\Big(\frac{1}{2}\mathbf{q}+\frac{1}{2}\mathbf{q}'+\frac{1}{4}\mathbf{P}\Big)v\Big(-\frac{1}{2}\mathbf{q}-\frac{1}{2}\mathbf{q}'+\frac{1}{4}\mathbf{P}\Big)\frac{1}{2}\left(-\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\right)\left(-\frac{1}{4}G_+'^{-1}\,G_-'^{-1}+1\right)\\
&\quad-\lambda\,v(0)\frac{1}{2}\phi^2\left[v\Big(\mathbf{q}+\frac{1}{2}\mathbf{P}\Big)\,\frac{1}{8}\,G_+^{-2}\,G_-^{-1}+v\Big(\mathbf{q}-\frac{1}{2}\mathbf{P}\Big)\,\frac{1}{8}\,G_-^{-2}\,G_+^{-1}\right]\delta(\mathbf{q}-\mathbf{q}')\\
&\quad+\lambda\,\frac{1}{8}\,\phi^2\left[v\Big(\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big)v\Big(-\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big)G_+^{-2}\,G_-^{-1}\right.\\
&\qquad\left.+\,v\Big(\frac{1}{2}\mathbf{q}-\frac{1}{4}\mathbf{P}\Big)v\Big(-\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big)G_-^{-2}\,G_+^{-1}\right]\delta(\mathbf{q}-\mathbf{q}')\,.
\end{aligned}
\tag{A.35}
$$

With the separable potential we define $V(\mathbf{k},\mathbf{k}',\mathbf{k}'',\mathbf{k}''')=v\big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{k}'\big)v\big(\frac{1}{2}\mathbf{k}''+\frac{1}{2}\mathbf{k}'''\big)$ and $v(\mathbf{k})=v(-\mathbf{k})$. Hence, this allows γ^2 and ξ, defined in Eqs. (4.47), to be written as

$$
\gamma(\mathbf{k})^2=-\mu+2\lambda\int_{\mathbf{k}'}^{\prime} v\Big(\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)v\Big(-\frac{\mathbf{k}+\mathbf{k}'}{2}\Big)R(\mathbf{k}')+\lambda\phi^2v(\mathbf{k})v(-\mathbf{k}) \tag{A.36a}
$$

$$
\xi(\mathbf{k})=\lambda\,v(\mathbf{k})\int_{\mathbf{k}'}^{\prime} v(\mathbf{k}')D(\mathbf{k}')-\frac{\lambda}{2}\phi^2v(0)v(\mathbf{k})\,. \tag{A.36b}
$$

From (A.35) it can be seen that $\mathfrak{A}_{GG}$ can be conveniently split into a sum of diagonal and off-diagonal pieces:

$$
\mathfrak{A}_{GG}(\mathbf{q},\mathbf{q}',\mathbf{P})=s_K(\mathbf{q},\mathbf{P})\delta(\mathbf{q}-\mathbf{q}')+S_K(\mathbf{q},\mathbf{q}',\mathbf{P})\,. \tag{A.37}
$$

Using Eqs. (A.36), the respective diagonal and non-diagonal parts can be more compactly written as

$$s_K(\mathbf{q},\mathbf{P}) = \frac{1}{8}\,G_+^{-2}\,G_-^{-1}\left(\mathbf{q}_+{}^2+\gamma_+^2+\xi_+\right)+\frac{1}{8}\,G_-^{-2}\,G_+^{-1}\left(\mathbf{q}_-{}^2+\gamma_-^2+\xi_-\right) \tag{A.38a}$$

$$\begin{aligned}
S_K(\mathbf{q},\mathbf{q}',\mathbf{P}) &= \frac{\lambda}{4}v(\mathbf{q})v(\mathbf{q}')\left(\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\right)\left(\frac{1}{4}G_+'^{-1}\,G_-'^{-1}+1\right)\\
&\quad+\frac{\lambda}{2}\,v\Big(\frac{1}{2}\mathbf{q}+\frac{1}{2}\mathbf{q}'+\frac{1}{4}\mathbf{P}\Big)v\Big(-\frac{1}{2}\mathbf{q}-\frac{1}{2}\mathbf{q}'+\frac{1}{4}\mathbf{P}\Big)\left(-\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\right)\left(-\frac{1}{4}G_+'^{-1}\,G_-'^{-1}+1\right)
\end{aligned} \tag{A.38b}$$

The remaining matrix elements are calculated similarly.

$$\begin{aligned}
\mathfrak{A}_{G\phi}(\mathbf{q},\mathbf{P}) = \mathfrak{A}_{\phi G}(\mathbf{q},\mathbf{P}) &= c_K(\mathbf{q},\mathbf{P})\\
&= -\frac{\lambda}{2}D\,\psi\psi_{\,G\phi}(\mathbf{q},\mathbf{P})+\frac{\lambda}{2}\psi^*\psi\,R_{G\phi}(\mathbf{q},\mathbf{P})\\
&= \lambda\,\frac{1}{4}\,\phi\left[v(\mathbf{q})v\Big(\frac{1}{2}\mathbf{P}\Big)+v(\mathbf{q})v\Big(-\frac{1}{2}\mathbf{P}\Big)\right]\left(\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\right)\\
&\quad+\lambda\,\phi\,v\Big(\frac{1}{2}\mathbf{q}+\frac{3}{4}\mathbf{P}\Big)v\Big(-\frac{1}{2}\mathbf{q}+\frac{1}{4}\mathbf{P}\Big)\left(-\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\right)\,.
\end{aligned} \tag{A.39}$$

$$\begin{aligned}
\mathfrak{A}_{\phi\phi}(\mathbf{P}) = A(\mathbf{P}) &= 2\,(k^2-\mu)\psi^*\psi_{\,\phi^2}(\mathbf{P})+\lambda|\psi|^4_{\phi^2}(\mathbf{P})-\lambda D\,\psi\psi_{\,\phi^2}(\mathbf{P})+\lambda\psi^*\psi\,R_{\phi^2}(\mathbf{P})\\
&= \mathbf{P}^2-\mu+\lambda\,\phi^2\,\left[\frac{1}{2}v(0)v(\mathbf{P})+v\Big(\frac{1}{2}\mathbf{P}\Big)v\Big(\frac{1}{2}\mathbf{P}\Big)\right]-\lambda\,v(\mathbf{P})\int_{\mathbf{k}}'v(\mathbf{k})D(\mathbf{k})\\
&\quad+2\lambda\int_{\mathbf{k}}'v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{P}\Big)v\Big(-\frac{1}{2}\mathbf{k}-\frac{1}{2}\mathbf{P}\Big)R(\mathbf{k})\\
&= \mathbf{P}^2+\gamma(\mathbf{P})^2-\xi(\mathbf{P})\,.
\end{aligned} \tag{A.40}$$

A.4.2 $\mathfrak{B}$ Matrix Elements

$$\begin{aligned}
\mathfrak{B}_{\Sigma\Sigma}(\mathbf{q},\mathbf{q}',\mathbf{P}) &= 2\,(k^2-\mu)R_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})+\lambda\left[D^2_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})+R^2_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})\right.\\
&\qquad\left.-D\,\psi\psi_{\,\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})+\psi^*\psi\,R_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})\right]
\end{aligned} \tag{A.41}$$

$$\begin{aligned}
&= 2\,\left[(\mathbf{q}_+{}^2-\mu)G_-+(\mathbf{q}_-{}^2-\mu)G_+\right]\delta(\mathbf{q}-\mathbf{q}')\\
&\quad+2\,\lambda\int_{\mathbf{k}}'v(\mathbf{k})D(\mathbf{k})\left[v\Big(\mathbf{q}+\frac{1}{2}\mathbf{P}\Big)G_-+v\Big(\mathbf{q}-\frac{1}{2}\mathbf{P}\Big)G_+\right]\delta(\mathbf{q}-\mathbf{q}')
\end{aligned}$$

$$
\begin{aligned}
&+ \lambda\, v(\mathbf{q})v(\mathbf{q}')(G_+ + G_-)(G'_+ + G'_-) \\
&+ 4\,\lambda \int'_{\mathbf{k}} R(\mathbf{k}) \Big[v\Big(\frac{1}{2}\mathbf{k} + \frac{1}{2}\mathbf{q} + \frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k} - \frac{1}{2}\mathbf{q} - \frac{1}{4}\mathbf{P}\Big) G_- \\
&\qquad\qquad + v\Big(\frac{1}{2}\mathbf{k} + \frac{1}{2}\mathbf{q} - \frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k} - \frac{1}{2}\mathbf{q} + \frac{1}{4}\mathbf{P}\Big) G_+ \Big]\, \delta(\mathbf{q} - \mathbf{q}') \\
&- \lambda\, v(0)\phi^2 \Big[v\Big(\mathbf{q} + \frac{1}{2}\mathbf{P}\Big) G_- + v\Big(\mathbf{q} - \frac{1}{2}\mathbf{P}\Big) G_+ \Big]\, \delta(\mathbf{q} - \mathbf{q}') \\
&+ 2\,\lambda\,\phi^2 \Big[v\Big(\frac{1}{2}\mathbf{q} + \frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{q} - \frac{1}{4}\mathbf{P}\Big) G_- \\
&\qquad\qquad + v\Big(\frac{1}{2}\mathbf{q} - \frac{1}{4}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{q} + \frac{1}{4}\mathbf{P}\Big) G_+ \Big]\, \delta(\mathbf{q} - \mathbf{q}')\,. \qquad \text{(A.42)}
\end{aligned}
$$

In analogy with Eq. (A.37), $\mathfrak{B}_{\Sigma\Sigma}$ can be split into diagonal and off-diagonal parts as well:

$$
\mathfrak{B}_{\Sigma\Sigma}(\mathbf{q}, \mathbf{q}', \mathbf{P}) = s_M(\mathbf{q}, \mathbf{P})\, \delta(\mathbf{q} - \mathbf{q}') + S_M(\mathbf{q}, \mathbf{q}', \mathbf{P})\,, \tag{A.43}
$$

where

$$
s_M(\mathbf{q}, \mathbf{P}) = 2\left(\mathbf{q_+}^2 + \gamma_+^2 + \xi_+\right) G_- + 2\left(\mathbf{q_-}^2 + \gamma_-^2 + \xi_-\right) G_+ \tag{A.44a}
$$

$$
S_M(\mathbf{q}, \mathbf{q}', \mathbf{P}) = \lambda(G_+ + G_-)(G'_+ + G'_-)\,. \tag{A.44b}
$$

The remaining elements follow in like fashion.

$$
\begin{aligned}
\mathfrak{B}_{\Sigma\pi}(\mathbf{q}, \mathbf{P}) = \mathfrak{B}_{\pi\Sigma}(\mathbf{q}, \mathbf{P}) = c_M(\mathbf{q}, \mathbf{P}) \\
&= -\frac{\lambda}{2} D\, \psi\psi_{\,\Sigma\pi}(\mathbf{q}, \mathbf{P}) \\
&= \frac{\lambda}{2}\,\phi\, \Big[v(\mathbf{q}) v\Big(\frac{1}{2}\mathbf{P}\Big) + v(\mathbf{q}) v\Big(-\frac{1}{2}\mathbf{P}\Big) \Big] (G_+ + G_-)
\end{aligned} \tag{A.45}
$$

$$
\begin{aligned}
\mathfrak{B}_{\pi\pi}(\mathbf{P}) &= B(\mathbf{P}) \\
&= 2\,(k^2 - \mu)\psi^*\psi_{\,\pi^2}(\mathbf{P}) + \lambda\left[|\psi|^4_{\pi^2}(\mathbf{P}) - D\,\psi\psi_{\,\pi^2}(\mathbf{P}) + \psi^*\psi\, R_{\pi^2}(\mathbf{P}) \right] \\
&= \mathbf{P}^2 - \mu + \lambda\,\phi^2 \Big[v\Big(\frac{1}{2}\mathbf{P}\Big) v\Big(\frac{1}{2}\mathbf{P}\Big) - \frac{1}{2} v(0) v(\mathbf{P}) \Big] + \lambda v(\mathbf{P}) \int'_{\mathbf{k}} v(\mathbf{k}) D(\mathbf{k}) \\
&\qquad + 2\,\lambda \int'_{\mathbf{k}} v\Big(\frac{1}{2}\mathbf{k} + \frac{1}{2}\mathbf{P}\Big) v\Big(-\frac{1}{2}\mathbf{k} - \frac{1}{2}\mathbf{P}\Big) R(\mathbf{k}) \\
&= \mathbf{P}^2 + \gamma(\mathbf{P})^2 + \xi(\mathbf{P})
\end{aligned} \tag{A.46}
$$

Appendix B

RPA Expansion for a Double Resonance Model

In this section we expand the grand canonical Hamiltonian of Eq. (5.4) to second order in the variations given by Eqs. (5.57). This procedure is carried out in much the same way as was accomplished in Appendix A, except that a molecular coupling term takes the place of the potential.

B.1 Expansion of R, D, ψ^2, ϕ^2, χ^2 and ξ

The general time-dependent, nonuniform representation of the Hamiltonian in (5.2) is given by

$$\begin{aligned} K = & \int'_{\mathbf{k}} (k^2 - \mu) \left[R(\mathbf{k},\mathbf{k},t) + \psi^*(\mathbf{k},t)\psi(\mathbf{k},t) \right] \\ & + (\epsilon - 2\mu) \int'_{\mathbf{k}} \phi^*(\mathbf{k},t)\phi(\mathbf{k},t) + (\epsilon - 2\mu) \int'_{\mathbf{k}} \chi^*(\mathbf{k},t)\chi(\mathbf{k},t) \\ & + \frac{1}{2} \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}''} \delta(\mathbf{k}'' - \mathbf{k} + \mathbf{k}') v(\mathbf{q}) \Big\{ \xi^*(\mathbf{k}'',t) \left[D(\mathbf{k},\mathbf{k}',t) + \psi(\mathbf{k},t)\psi(\mathbf{k}',t) \right] \\ & \qquad\qquad + \xi(\mathbf{k}'',t) \left[D^*(\mathbf{k},\mathbf{k}',t) + \psi^*(\mathbf{k},t)\psi^*(\mathbf{k}',t) \right] \Big\} \end{aligned} \tag{B.1}$$

where $v(\mathbf{q})$ is the molecular form factor given in the separable potential of Eq. (2.107). The fluctuations R and D are given by Eqs. (A.2a) and (A.2b), respectively, whereas the mean fields assume the form of (A.2c):

$$\psi(\mathbf{k},t) = \frac{1}{\sqrt{2}} \Big[\psi(\mathbf{k},t) + i\pi(\mathbf{k},t) \Big] , \tag{B.2a}$$

$$\phi(\mathbf{k},t) = \frac{1}{\sqrt{2}} \Big[\phi(\mathbf{k},t) + i\omega(\mathbf{k},t) \Big] , \tag{B.2b}$$

$$\chi(\mathbf{k},t) = \frac{1}{\sqrt{2}} \Big[\chi(\mathbf{k},t) + i\nu(\mathbf{k},t) \Big] , \tag{B.2c}$$

with ψ, ϕ and χ representing the mean atomic field, the mean molecular field and the mean auxiliary field, respectively. The expansions of R and D are identical to those of Eqs. (A.5) and (A.6), while the required mean field product terms are

$$\psi^*\psi^{(0)}(\mathbf{k},\mathbf{k}',t) = \frac{1}{2}\psi^2\,\delta(\mathbf{k})\delta(\mathbf{k}') \tag{B.3a}$$

$$\begin{aligned}\psi^*\psi^{(1)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\psi\,\delta(\mathbf{k}')\left[\delta\psi(\mathbf{k},t) - i\delta\pi(\mathbf{k},t)\right] \\ &\quad + \frac{1}{2}\psi\,\delta(\mathbf{k})\left[\delta\psi(\mathbf{k}',t) + i\delta\pi(\mathbf{k}',t)\right]\end{aligned} \tag{B.3b}$$

$$\begin{aligned}\psi^*\psi^{(2)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\left[\delta\psi^*(\mathbf{k},t)\delta\psi(\mathbf{k}',t) + i\delta\psi^*(\mathbf{k},t)\delta\pi(\mathbf{k}',t)\right. \\ &\quad \left. - i\delta\psi(\mathbf{k}',t)\delta\pi^*(\mathbf{k},t) + \delta\pi^*(\mathbf{k},t)\delta\pi(\mathbf{k}',t)\right] ,\end{aligned} \tag{B.3c}$$

$$\psi\psi^{(0)}(\mathbf{k},\mathbf{k}',t) = \frac{1}{2}\psi^2\,\delta(\mathbf{k})\delta(\mathbf{k}') \tag{B.4a}$$

$$\begin{aligned}\psi\psi^{(1)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\psi\,\delta(\mathbf{k}')\left[\delta\psi(\mathbf{k},t) + i\delta\pi(\mathbf{k},t)\right] \\ &\quad + \frac{1}{2}\psi\,\delta(\mathbf{k})\left[\delta\psi(\mathbf{k}',t) + i\delta\pi(\mathbf{k}',t)\right]\end{aligned} \tag{B.4b}$$

$$\begin{aligned}\psi\psi^{(2)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\left[\delta\psi^*(\mathbf{k},t)\delta\psi(\mathbf{k}',t) + i\delta\psi^*(\mathbf{k},t)\delta\pi(\mathbf{k}',t)\right. \\ &\quad \left. + i\delta\psi(\mathbf{k}',t)\delta\pi^*(\mathbf{k},t) - \delta\pi^*(\mathbf{k},t)\delta\pi(\mathbf{k}',t)\right] ,\end{aligned} \tag{B.4c}$$

$$\phi^*\phi^{(0)}(\mathbf{k},\mathbf{k}',t) = \frac{1}{2}\phi^2\,\delta(\mathbf{k})\delta(\mathbf{k}') \tag{B.5a}$$

$$\begin{aligned}\phi^*\phi^{(1)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\phi\,\delta(\mathbf{k}')\left[\delta\phi(\mathbf{k},t) - i\delta\omega(\mathbf{k},t)\right] \\ &\quad + \frac{1}{2}\phi\,\delta(\mathbf{k})\left[\delta\phi(\mathbf{k}',t) + i\delta\omega(\mathbf{k}',t)\right]\end{aligned} \tag{B.5b}$$

$$\begin{aligned}\phi^*\phi^{(2)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\left[\delta\phi^*(\mathbf{k},t)\delta\phi(\mathbf{k}',t) + i\delta\phi^*(\mathbf{k},t)\delta\omega(\mathbf{k}',t)\right. \\ &\quad \left. - i\delta\phi(\mathbf{k}',t)\delta\omega^*(\mathbf{k},t) + \delta\omega^*(\mathbf{k},t)\delta\omega(\mathbf{k}',t)\right] ,\end{aligned} \tag{B.5c}$$

$$\chi^*\chi^{(0)}(\mathbf{k},\mathbf{k}',t) = \frac{1}{2}\chi^2\,\delta(\mathbf{k})\delta(\mathbf{k}') \tag{B.6a}$$

$$\begin{aligned}\chi^*\chi^{(1)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\chi\,\delta(\mathbf{k}')\left[\delta\chi(\mathbf{k},t) - i\delta\nu(\mathbf{k},t)\right] \\ &\quad + \frac{1}{2}\chi\,\delta(\mathbf{k})\left[\delta\chi(\mathbf{k}',t) + i\delta\nu(\mathbf{k}',t)\right]\end{aligned} \tag{B.6b}$$

$$\begin{aligned}\chi^*\chi^{(2)}(\mathbf{k},\mathbf{k}',t) &= \frac{1}{2}\left[\delta\chi^*(\mathbf{k},t)\delta\chi(\mathbf{k}',t) + i\delta\chi^*(\mathbf{k},t)\delta\nu(\mathbf{k}',t)\right. \\ &\quad \left. - i\delta\chi(\mathbf{k}',t)\delta\nu^*(\mathbf{k},t) + \delta\nu^*(\mathbf{k},t)\delta\nu(\mathbf{k}',t)\right] ,\end{aligned} \tag{B.6c}$$

$$\begin{aligned}\xi^{(0)}(\mathbf{k}'',t) &= \xi\delta(\mathbf{k}'') \\ &= (\lambda\alpha\phi + g\chi)\delta(\mathbf{k}'')\,,\end{aligned} \tag{B.7a}$$

$$\begin{aligned}\xi^{(1)}(\mathbf{k}'',t) &= \delta\xi(\mathbf{k}'',t) \\ &= \left[\lambda\alpha\delta\phi(\mathbf{k}'',t) + g\delta\chi(\mathbf{k}'',t)\right] + i\left[\lambda\alpha\delta\omega(\mathbf{k}'',t) + g\delta\nu(\mathbf{k}'',t)\right]\,.\end{aligned} \tag{B.7b}$$

Along with Eqs. (A.2a) and (A.2b), these expansions are used to calculate the second order contributions from each of the terms in the Hamiltonian given by (B.1).

B.2 Second Order Kinetic Contribution

To second order in the variations, the kinetic energy is given by

$$\begin{aligned}\int_{\mathbf{k}}^{\prime}(k^2-\mu)\Big[R^{(2)}(\mathbf{k},\mathbf{k},t) + \psi^*\psi^{(2)}(\mathbf{k},\mathbf{k},t)\Big] = \int_{\mathbf{q},\mathbf{P}}^{\prime}&\left[\delta G^*(\mathbf{q},\mathbf{P},t)(k^2-\mu)R_{G^2}(\mathbf{q},\mathbf{P})\delta G(\mathbf{q},\mathbf{P},t)\right. \\ &\left.+\delta\Sigma^*(\mathbf{q},\mathbf{P},t)(k^2-\mu)R_{\Sigma^2}(\mathbf{q},\mathbf{P})\delta\Sigma(\mathbf{q},\mathbf{P},t)\right] \\ +\int_{\mathbf{P}}^{\prime}\delta\psi^*(\mathbf{P},t)(k^2-\mu)\psi^*\psi_{\psi^2}(\mathbf{P})\delta\psi(\mathbf{P},t) &+ \delta\pi^*(\mathbf{P},t)(k^2-\mu)\psi^*\psi_{\pi^2}(\mathbf{P})\delta\pi(\mathbf{P},t)\,,\end{aligned} \tag{B.8}$$

where the $(k^2-\mu)R$ and $(k^2-\mu)\psi^*\psi$ terms are given by Eqs. (A.11) and (A.14), respectively. There remains the second order molecular contribution as well as that of the coupling, both of which are far more easily obtained when compared to the corresponding potential terms calculated in Section A.3.

B.3 Second Order Contribution from Molecules

As seen in the Hamiltonian of (B.1), the molecular detunings are part of the total energy. As such, their RPA terms are

$$\begin{aligned}(\epsilon-2\mu)\int_{\mathbf{k}}^{\prime}\phi^*\phi^{(2)}(\mathbf{k},\mathbf{k},t) &+ (\varepsilon-2\mu)\int_{\mathbf{k}}^{\prime}\chi^*\chi^{(2)}(\mathbf{k},\mathbf{k},t) \\ = \int_{\mathbf{P}}^{\prime}&\Big[\delta\phi^*(\mathbf{P},t)\phi^*\phi_{\phi^2}(\mathbf{P})\delta\phi(\mathbf{P},t) + \delta\omega^*(\mathbf{P},t)\phi^*\phi_{\omega^2}(\mathbf{P})\delta\omega(\mathbf{P},t) \\ &+\delta\chi^*(\mathbf{P},t)\chi^*\chi_{\chi^2}(\mathbf{P})\delta\chi(\mathbf{P},t) + \delta\nu^*(\mathbf{P},t)\chi^*\chi_{\nu^2}(\mathbf{P})\delta\nu(\mathbf{P},t)\Big]\,.\end{aligned} \tag{B.9}$$

Reading off the results from Eqs. (B.5c), (B.6c), we identify

$$\phi^*\phi_{\phi^2}(\mathbf{P}) = \phi^*\phi_{\omega^2}(\mathbf{P}) = \frac{1}{2}\epsilon - \mu\,, \tag{B.10a}$$

$$\chi^*\chi_{\chi^2}(\mathbf{P}) = \chi^*\chi_{\nu^2}(\mathbf{P}) = \frac{1}{2}\varepsilon - \mu\,. \tag{B.10b}$$

B.4 Second Order Contribution from the Coupling

The last integral of Eq. (B.1) gives the energy due to the coupling of atoms to both of the molecular states. In this energy component, there is a $\xi^* D$ term with a second order part given by

$$\begin{aligned}
&\int'_{\mathbf{k},\mathbf{k}',\mathbf{k}''} \delta(\mathbf{k}''-\mathbf{k}+\mathbf{k}')v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{k}'\Big)\Big[\xi^{*(0)}(\mathbf{k}'',t)D^{(2)}(\mathbf{k},\mathbf{k}',t)+\xi^{*(1)}(\mathbf{k}'',t)D^{(1)}(\mathbf{k},\mathbf{k}',t)+\text{H. c.}\Big] \\
&\qquad = \int'_{\mathbf{k},\mathbf{k}'''} v(\mathbf{k})\xi\Big[\delta G^*(\mathbf{k}''',\mathbf{k},t)\,\frac{1}{4}G(\mathbf{k})^{-2}G(\mathbf{k}''')^{-1}\delta G(\mathbf{k},\mathbf{k}''',t) \\
&\qquad\qquad +\delta\Sigma^*(\mathbf{k}''',\mathbf{k},t)4G(\mathbf{k}''')\delta\Sigma(\mathbf{k},\mathbf{k}''',t)\Big] \\
&+\int'_{\mathbf{k},\mathbf{k}',\mathbf{k}''} \delta(\mathbf{k}''-\mathbf{k}+\mathbf{k}')v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{k}'\Big)\Big\{-\lambda\alpha\delta\phi^*(\mathbf{k}'',t)\Big[\frac{1}{4}G(\mathbf{k})^{-1}G(\mathbf{k}')^{-1}+1\Big]\delta G(\mathbf{k},\mathbf{k}',t) \\
&-g\delta\chi^*(\mathbf{k}'',t)\Big[\frac{1}{4}G(\mathbf{k})^{-1}G(\mathbf{k}')^{-1}+1\Big]\delta G(\mathbf{k},\mathbf{k}',t)-2\lambda\alpha\delta\omega^*(\mathbf{k}'',t)\Big[G(\mathbf{k})+G(\mathbf{k}')\Big]\delta\Sigma(\mathbf{k},\mathbf{k}',t) \\
&\qquad\qquad -2g\delta\nu^*(\mathbf{k}'',t)\Big[G(\mathbf{k})+G(\mathbf{k}')\Big]\delta\Sigma(\mathbf{k},\mathbf{k}',t)\Big\}\,,
\end{aligned} \tag{B.11}$$

which can be more compactly written as

$$\begin{aligned}
&\int'_{\mathbf{q},\mathbf{q}',\mathbf{P}} \Big[\delta G^*(\mathbf{q},\mathbf{P},t)D_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P})\delta G(\mathbf{q},\mathbf{P},t)+\delta\Sigma^*(\mathbf{q},\mathbf{P},t)D_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})\delta\Sigma(\mathbf{q},\mathbf{P},t)\Big] \\
&+\int_{\mathbf{q},\mathbf{P}} \Big[\delta\phi^*(\mathbf{P},t)D_{G\phi}(\mathbf{q},\mathbf{P})\delta G(\mathbf{q},\mathbf{P},t)+\delta\chi^*(\mathbf{P},t)D_{G\chi}(\mathbf{q},\mathbf{P},t)\delta G(\mathbf{q},\mathbf{P},t) \\
&\qquad +\delta\omega^*(\mathbf{P},t)D_{\Sigma\omega}(\mathbf{q},\mathbf{P})\delta\Sigma(\mathbf{q},\mathbf{P},t)+\delta\nu^*(\mathbf{P},t)D_{\Sigma\nu}(\mathbf{q},\mathbf{P})\delta\Sigma(\mathbf{q},\mathbf{P},t)\Big]\,,
\end{aligned} \tag{B.12}$$

where

$$D_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P})=\xi\left[v\Big(\mathbf{q}+\frac{1}{2}\mathbf{P}\Big)\frac{1}{8}G_+^{-2}\,G_-^{-1}+v\Big(\mathbf{q}-\frac{1}{2}\mathbf{P}\Big)\frac{1}{8}G_-^{-2}\,G_+^{-1}\right]\delta(\mathbf{q}-\mathbf{q}') \tag{B.13a}$$

$$D_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P})=\xi\left[v\Big(\mathbf{q}+\frac{1}{2}\mathbf{P}\Big)\,2\,G_-+v\Big(\mathbf{q}-\frac{1}{2}\mathbf{P}\Big)\,2\,G_+\right]\delta(\mathbf{q}-\mathbf{q}') \tag{B.13b}$$

$$D_{G\phi}(\mathbf{q},\mathbf{P}) = -\lambda\alpha v(\mathbf{q})\left(\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\right) \tag{B.13c}$$

$$D_{G\chi}(\mathbf{q},\mathbf{P}) = -gv(\mathbf{q})\left(\frac{1}{4}G_+^{-1}\,G_-^{-1}+1\right) \tag{B.13d}$$

$$D_{\Sigma\omega}(\mathbf{q},\mathbf{P}) = -2\lambda\alpha v(\mathbf{q})(G_+ + G_-) \tag{B.13e}$$

$$D_{\Sigma\nu}(\mathbf{q},\mathbf{P}) = -2gv(\mathbf{q})(G_+ + G_-)\,. \tag{B.13f}$$

In this compact notation we have used the definitions of $\mathbf{q}$ and $\mathbf{P}$ given by Eqs. (A.10) as well as the shorthand of (A.12). In a like manner, the second order part from the $\xi^*\psi\psi$ term is

$$\begin{aligned}
&\int'_{\mathbf{k},\mathbf{k}',\mathbf{k}''} \delta(\mathbf{k}''-\mathbf{k}+\mathbf{k}')v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{k}'\Big)\Big[\xi^{*(0)}(\mathbf{k}'',t)\psi\psi^{(2)}(\mathbf{k},\mathbf{k}',t)+\xi^{*(1)}(\mathbf{k}'',t)\psi\psi^{(1)}(\mathbf{k},\mathbf{k}',t)+\text{H. c.}\Big] \\
&\qquad = \int'_{\mathbf{k}} v(\mathbf{k})\xi\Big[\delta\psi(\mathbf{k},t)^2-\delta\pi(\mathbf{k},t)^2\Big] \\
&+ \int'_{\mathbf{k},\mathbf{k}',\mathbf{k}''} \delta(\mathbf{k}''-\mathbf{k}+\mathbf{k}')v\Big(\frac{1}{2}\mathbf{k}+\frac{1}{2}\mathbf{k}'\Big)\Big\{\Big[\lambda\alpha\delta\phi(\mathbf{k}'',t)+g\delta\chi(\mathbf{k}'',t)\Big]\Big[\psi\delta(\mathbf{k}')\delta\psi(\mathbf{k},t)+\psi\delta(\mathbf{k})\delta\psi(\mathbf{k}',t)\Big] \\
&\qquad\qquad \Big[\lambda\alpha\delta\omega(\mathbf{k}'',t)+g\delta\nu(\mathbf{k}'',t)\Big]\Big[\psi\delta(\mathbf{k}')\delta\pi(\mathbf{k},t)+\psi\delta(\mathbf{k})\delta\pi(\mathbf{k}',t)\Big]\Big\}\,.
\end{aligned} \tag{B.14}$$

After multiplying out the integrands, this becomes

$$\begin{aligned}
\int'_{\mathbf{P}} \Big[&\delta\psi^*(\mathbf{P},t)\psi^2_{\psi^2}(\mathbf{P})\delta\psi(\mathbf{P},t)+\delta\pi^*(\mathbf{P},t)\psi^2_{\pi^2}(\mathbf{P})\delta\pi(\mathbf{P},t)+\delta\phi^*(\mathbf{P},t)\psi^2_{\phi\psi}(\mathbf{P})\delta\psi(\mathbf{P},t) \\
&+\delta\chi^*(\mathbf{P},t)\psi^2_{\chi\psi}(\mathbf{P})\delta\psi(\mathbf{P},t)+\delta\omega^*(\mathbf{P},t)\psi^2_{\omega\pi}(\mathbf{P})\delta\pi(\mathbf{P},t)+\delta\nu^*(\mathbf{P},t)\psi^2_{\nu\pi}(\mathbf{P})\delta\pi(\mathbf{P},t)\Big]\,,
\end{aligned} \tag{B.15}$$

where

$$\psi^2_{\psi^2}(\mathbf{P}) = v(\mathbf{P})\xi \tag{B.16a}$$

$$\psi^2_{\pi^2}(\mathbf{P}) = -v(\mathbf{P})\xi \tag{B.16b}$$

$$\psi^2_{\phi\psi}(\mathbf{P}) = 2v\Big(\frac{1}{2}\mathbf{P}\Big)\psi\lambda\alpha \tag{B.16c}$$

$$\psi^2_{\chi\psi}(\mathbf{P}) = 2v\Big(\frac{1}{2}\mathbf{P}\Big)\psi\, g \tag{B.16d}$$

$$\psi^2_{\omega\pi}(\mathbf{P}) = 2v\Big(\frac{1}{2}\mathbf{P}\Big)\psi\lambda\alpha \tag{B.16e}$$

$$\psi^2_{\nu\pi}(\mathbf{P}) = 2v\Big(\frac{1}{2}\mathbf{P}\Big)\psi\, g\,. \tag{B.16f}$$

B.5 Matrix Form of RPA

Using the same matrix notation as in Sec. A.4, the second order grand canonical Hamiltonian of Eq. (B.1) can be written

$$\begin{aligned} K_{RPA} =& \frac{1}{2}\delta\mathcal{P}^\dagger(\mathbf{q},\mathbf{P}) \begin{bmatrix} \mathfrak{A}_{GG}(\mathbf{q},\mathbf{q}',\mathbf{P}) & \mathfrak{A}_{G\psi}(\mathbf{q},\mathbf{P}) & \mathfrak{A}_{G\phi}(\mathbf{q},\mathbf{P}) & \mathfrak{A}_{G\chi}(\mathbf{q},\mathbf{P}) \\ \mathfrak{A}_{\psi G}(\mathbf{q}',\mathbf{P}) & \mathfrak{A}_{\psi\psi}(\mathbf{P}) & \mathfrak{A}_{\psi\phi}(\mathbf{P}) & \mathfrak{A}_{\psi\chi}(\mathbf{P}) \\ \mathfrak{A}_{\phi G}(\mathbf{q}',\mathbf{P}) & \mathfrak{A}_{\phi\psi}(\mathbf{P}) & \mathfrak{A}_{\phi\phi}(\mathbf{P}) & \mathfrak{A}_{\phi\chi}(\mathbf{P}) \\ \mathfrak{A}_{\chi G}(\mathbf{q}',\mathbf{P}) & \mathfrak{A}_{\chi\psi}(\mathbf{P}) & \mathfrak{A}_{\chi\phi}(\mathbf{P}) & \mathfrak{A}_{\chi\chi}(\mathbf{P}) \end{bmatrix} \delta\mathcal{P}(\mathbf{q}',\mathbf{P}) \\ & + \frac{1}{2}\delta\mathcal{Q}^\dagger(\mathbf{q},\mathbf{P}) \begin{bmatrix} \mathfrak{B}_{\Sigma\Sigma}(\mathbf{q},\mathbf{q}',\mathbf{P}) & \mathfrak{B}_{\Sigma\pi}(\mathbf{q},\mathbf{P}) & \mathfrak{B}_{\Sigma\omega}(\mathbf{q},\mathbf{P}) & \mathfrak{B}_{\Sigma\nu}(\mathbf{q},\mathbf{P}) \\ \mathfrak{B}_{\pi\Sigma}(\mathbf{q}',\mathbf{P}) & \mathfrak{B}_{\pi\pi}(\mathbf{P}) & \mathfrak{B}_{\pi\omega}(\mathbf{P}) & \mathfrak{B}_{\pi\nu}(\mathbf{P}) \\ \mathfrak{B}_{\omega\Sigma}(\mathbf{q}',\mathbf{P}) & \mathfrak{B}_{\omega\pi}(\mathbf{P}) & \mathfrak{B}_{\omega\omega}(\mathbf{P}) & \mathfrak{B}_{\omega\nu}(\mathbf{P}) \\ \mathfrak{B}_{\nu\Sigma}(\mathbf{q}',\mathbf{P}) & \mathfrak{B}_{\nu\pi}(\mathbf{P}) & \mathfrak{B}_{\nu\omega}(\mathbf{P}) & \mathfrak{B}_{\nu\nu}(\mathbf{P}) \end{bmatrix} \delta\mathcal{Q}(\mathbf{q}',\mathbf{P})\,, \end{aligned} \tag{B.17}$$

with the coordinates, $\delta\mathcal{Q}$, and momenta, $\delta\mathcal{P}$, defined as

$$\delta\mathcal{Q}^\dagger(\mathbf{q},\mathbf{P}) = \begin{bmatrix} \delta\Sigma(\mathbf{q},\mathbf{P}) & \delta\pi(\mathbf{P}) & \delta\omega(\mathbf{P}) & \delta\nu(\mathbf{P}) \end{bmatrix} \tag{B.18a}$$

$$\delta\mathcal{P}^\dagger(\mathbf{q},\mathbf{P}) = \begin{bmatrix} \delta G(\mathbf{q},\mathbf{P}) & \delta\psi(\mathbf{P}) & \delta\phi(\mathbf{P}) & \delta\chi(\mathbf{P}) \end{bmatrix}\,. \tag{B.18b}$$

To find explicit expressions for the matrix elements, it is required to combine the results of (A.11), (A.14), (B.10), (B.13) and (B.16). Although this form appears somewhat more complicated than the 2×2 matrices found in A.4, it will be seen that the increased dimensionality is an equitable trade-off with the resulting simplification of the elements themselves.

B.5.1 $\mathfrak{A}$ Matrix Elements

Taking the step function $v(\mathbf{k})$ as defined in Eq. (2.111), the contributions from the expansion are read off, thus allowing the identifications

$$\begin{aligned} \mathfrak{A}_{GG}(\mathbf{q},\mathbf{q}',\mathbf{P}) &= 2\,R_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) + D_{G^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) \\ &= \frac{1}{8}\left[(q_+^2 - \mu + \xi)G_+^{-2}G_-^{-1} + (q_-^2 - \mu + \xi)G_-^{-2}G_+^{-1}\right]\delta(\mathbf{q}-\mathbf{q}') \\ &= s_K(\mathbf{q},\mathbf{P})\,\delta(\mathbf{q}-\mathbf{q}')\,. \end{aligned} \tag{B.19}$$

In the above case, for instance, the terms were obtained from (A.11a) and (B.13a). Similar matchings obtain the remaining elements:

$$\mathfrak{A}_{G\psi}(\mathbf{q},\mathbf{P}) = \mathfrak{A}_{\psi G}(\mathbf{q},\mathbf{P}) = 0 \tag{B.20}$$

$$\begin{aligned} \mathfrak{A}_{G\phi}(\mathbf{q},\mathbf{P}) = \mathfrak{A}_{\phi G}(\mathbf{q},\mathbf{P}) &= \frac{1}{2}D_{G\phi}(\mathbf{q},\mathbf{P}) \\ &= -\frac{\lambda\alpha}{2}\Big(\frac{1}{4}G_+^{-1}G_-^{-1} + 1\Big) \end{aligned} \tag{B.21}$$

$$\begin{aligned}\mathfrak{A}_{G\chi}(\mathbf{q},\mathbf{P}) = \mathfrak{A}_{\chi G}(\mathbf{q},\mathbf{P}) &= \frac{1}{2}D_{G\chi}(\mathbf{q},\mathbf{P}) \\ &= -\frac{g}{2}\Big(\frac{1}{4}G_+^{-1}G_-^{-1}+1\Big)\end{aligned} \tag{B.22}$$

$$\begin{aligned}\mathfrak{A}_{\psi\psi}(\mathbf{P}) &= 2(k^2-\mu)\psi^*\psi_{\,\psi^2}(\mathbf{P}) + \psi^2_{\psi^2}(\mathbf{P}) \\ &= P^2-\mu+\xi\end{aligned} \tag{B.23}$$

In Eq. (B.23), the expression for $(k^2-\mu)\psi^*\psi_{\,\psi^2}(\mathbf{P})$ was obtained from (A.14a).

$$\begin{aligned}\mathfrak{A}_{\psi\phi}(\mathbf{P}) = \mathfrak{A}_{\phi\psi}(\mathbf{P}) &= \frac{1}{2}\psi^2_{\phi\psi}(\mathbf{P}) \\ &= \lambda\alpha\psi\end{aligned} \tag{B.24}$$

$$\begin{aligned}\mathfrak{A}_{\psi\chi}(\mathbf{P}) = \mathfrak{A}_{\chi\psi}(\mathbf{P}) &= \frac{1}{2}\psi^2_{\chi\psi}(\mathbf{P}) \\ &= g\psi\end{aligned} \tag{B.25}$$

$$\begin{aligned}\mathfrak{A}_{\phi\phi}(\mathbf{P}) &= 2\phi^*\phi_{\,\phi^2}(\mathbf{P}) \\ &= \epsilon-2\mu\end{aligned} \tag{B.26}$$

$$\mathfrak{A}_{\phi\chi}(\mathbf{P}) = \mathfrak{A}_{\chi\phi}(\mathbf{P}) = 0 \tag{B.27}$$

$$\begin{aligned}\mathfrak{A}_{\chi\chi}(\mathbf{P}) &= 2\chi^*\chi_{\,\chi^2}(\mathbf{P}) \\ &= \varepsilon-2\mu\end{aligned} \tag{B.28}$$

B.5.2 $\mathfrak{B}$ Matrix Elements

$$\begin{aligned}\mathfrak{B}_{\Sigma\Sigma}(\mathbf{q},\mathbf{q}',\mathbf{P}) &= 2\,R_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) + D_{\Sigma^2}(\mathbf{q},\mathbf{q}',\mathbf{P}) \\ &= 2\left[(q_+^2-\mu+\xi)\,G_- + (q_-^2-\mu+\xi)\,G_+\right]\delta(\mathbf{q}-\mathbf{q}') \\ &= s_M(\mathbf{q},\mathbf{P})\,\delta(\mathbf{q}-\mathbf{q}')\,.\end{aligned} \tag{B.29}$$

Analogous to (B.19), the terms here were obtained from (A.11b) and (B.13b).

$$\mathfrak{B}_{\Sigma\pi}(\mathbf{q},\mathbf{P}) = \mathfrak{B}_{\pi\Sigma}(\mathbf{q},\mathbf{P}) = 0 \tag{B.30}$$

$$\begin{aligned}\mathfrak{B}_{\Sigma\omega}(\mathbf{q},\mathbf{P}) = \mathfrak{B}_{\omega\Sigma}(\mathbf{q},\mathbf{P}) &= \frac{1}{2}D_{\Sigma\omega}(\mathbf{q},\mathbf{P}) \\ &= -\lambda\alpha\,(G_+ + G_-)\end{aligned} \tag{B.31}$$

$$\begin{aligned}\mathfrak{B}_{\Sigma\nu}(\mathbf{q},\mathbf{P}) = \mathfrak{B}_{\nu\Sigma}(\mathbf{q},\mathbf{P}) &= \frac{1}{2} D_{\Sigma\nu}(\mathbf{q},\mathbf{P}) \\ &= -g\,(G_{+} + G_{-})\end{aligned} \tag{B.32}$$

$$\begin{aligned}\mathfrak{B}_{\pi\pi}(\mathbf{P}) &= 2(k^2-\mu)\psi^{*}\psi_{\,\pi^2}(\mathbf{P}) + \psi^2_{\,\pi^2}(\mathbf{P}) \\ &= P^2 - \mu - \xi\end{aligned} \tag{B.33}$$

In Eq. (B.33), the expression for $(k^2-\mu)\psi^{*}\psi_{\,\pi^2}(\mathbf{P})$ was obtained from (A.14b).

$$\begin{aligned}\mathfrak{B}_{\pi\omega}(\mathbf{P}) = \mathfrak{B}_{\omega\pi}(\mathbf{P}) &= \frac{1}{2}\psi^2_{\omega\pi}(\mathbf{P}) \\ &= \lambda\alpha\psi\end{aligned} \tag{B.34}$$

$$\begin{aligned}\mathfrak{B}_{\pi\nu}(\mathbf{P}) = \mathfrak{B}_{\nu\pi}(\mathbf{P}) &= \frac{1}{2}\psi^2_{\nu\pi}(\mathbf{P}) \\ &= g\psi\end{aligned} \tag{B.35}$$

$$\begin{aligned}\mathfrak{B}_{\omega\omega}(\mathbf{P}) &= 2\phi^{*}\phi_{\,\omega^2}(\mathbf{P}) \\ &= \epsilon - 2\mu\end{aligned} \tag{B.36}$$

$$\mathfrak{B}_{\omega\nu}(\mathbf{P}) = \mathfrak{B}_{\nu\omega}(\mathbf{P}) = 0 \tag{B.37}$$

$$\begin{aligned}\mathfrak{B}_{\nu\nu}(\mathbf{P}) &= 2\chi^{*}\chi_{\,\nu^2}(\mathbf{P}) \\ &= \varepsilon - 2\mu\end{aligned} \tag{B.38}$$

Note that unlike the previous case discussed in Sec. A.4, the $\mathfrak{A}$ and $\mathfrak{B}$ matrices have a diagonal continuum in $\mathbf{q}$ and $\mathbf{q}'$. Consequently, this leads to a simplification in the analysis that determines the continuous spectrum of $\mathfrak{A}\cdot\mathfrak{B}$.

Appendix C

Fluctuation Expansions

The purpose of this appendix is to expand the quantum fluctuations $\int D(\mathbf{k})$ and $\int R(\mathbf{k})$ for each of the three cases: (i) $|\xi| < |\gamma^2|$, (ii) $|\xi| \sim |\gamma^2|$ and (iii) $|\xi| > |\gamma^2|$, corresponding to sections 6.3.1, 6.3.2 and 6.3.3, respectively. In each case, the starting point is the expressions in (6.18).

C.1 Case (i): $|\xi| < |\gamma^2|$

In both the integrands of (6.18), the denominator is expanded in powers of ξ/γ^2:

$$\frac{1}{\sqrt{(k^2+\gamma^2)^2-\xi^2}} = \frac{1}{k^2+\gamma^2}\left[1+\frac{1}{2}\,\frac{\xi^2}{(k^2+\gamma^2)^2}+\frac{3}{8}\,\frac{\xi^4}{(k^2+\gamma^2)^4}+\frac{5}{16}\,\frac{\xi^6}{(k^2+\gamma^2)^6}+\ldots\right]. \quad \text{(C.1)}$$

Evaluation of $\int D(\mathbf{k})$ and $\int R(\mathbf{k})$ requires the integrals $\int (k^2+\gamma^2)^{-n} dk$, which can be found by induction:

$$\int_0^K \frac{dk}{k^2+\gamma^2} = \frac{1}{\gamma}\,\tan^{-1}\!\left(\frac{K}{\gamma}\right) \quad \text{(C.2a)}$$

$$\int_0^K \frac{dk}{(k^2+\gamma^2)^n} = -\frac{1}{n-1}\,\frac{d}{d\gamma^2}\int_0^K \frac{dk}{(k^2+\gamma^2)^{n-1}}\,. \quad \text{(C.2b)}$$

Using the expansion in (C.1) gives

$$
\begin{aligned}
\int_{\mathbf{k}}' D(\mathbf{k}) &= -\frac{\xi}{4\pi^2}\int_0^K \frac{k^2 dk}{\sqrt{(k^2+\gamma^2)^2-\xi^2}} \\
&= -\frac{\xi}{4\pi^2}\int_0^K \frac{k^2 dk}{k^2+\gamma^2}\left[1+\frac{1}{2}\,\frac{\xi^2}{(k^2+\gamma^2)^2}+\dots\right] \\
&= -\frac{\xi}{4\pi^2}\int_0^K \left[1-\frac{\gamma^2}{k^2+\gamma^2}+\frac{1}{2}\,\frac{\xi^2}{(k^2+\gamma^2)^2}-\frac{1}{2}\,\frac{\xi^2\gamma^2}{(k^2+\gamma^2)^3}+\dots\right]. \qquad \text{(C.3)}
\end{aligned}
$$

The integrals in this expansion are performed with Eqs. (C.2):

$$
\int_{\mathbf{k}}' D(\mathbf{k}) = \frac{\xi}{4\pi^2}\left[-K+\left(\gamma-\frac{1}{16}\,\frac{\xi^2}{\gamma^3}\right)\tan^{-1}\!\left(\frac{K}{\gamma}\right)-\frac{1}{16}\,\frac{\xi^2}{\gamma^2}\,\frac{K}{K^2+\gamma^2}+\frac{\xi^2}{8}\,\frac{K}{(K^2+\gamma^2)^2}+\dots\right]. \qquad \text{(C.4)}
$$

Assuming the cutoff K to be much larger than γ allows the following expansions

$$
\begin{aligned}
\tan^{-1}\!\left(\frac{K}{\gamma}\right) &= \frac{\pi}{2}-\frac{\gamma}{K}+\frac{1}{3K^3}\,\gamma^3-\frac{2}{15}\,\frac{1}{K^5}\,\gamma^4+\dots & \text{(C.5a)}\\
\frac{K}{K^2+\gamma^2} &= \frac{1}{K}-\frac{\gamma^2}{K^3}+\frac{\gamma^4}{K^5}-\dots & \text{(C.5b)}\\
\frac{K}{(K^2+\gamma^2)^2} &= \frac{1}{K^3}-\frac{2}{K^5}\,\gamma^2+\dots\,. & \text{(C.5c)}
\end{aligned}
$$

Substituting expansions (C.5) into (C.4) gives the desired result in (6.24b):

$$
\begin{aligned}
\int_{\mathbf{k}}' D(\mathbf{k}) = -\frac{\xi}{4\pi^2}K+\frac{1}{8\pi}\xi\gamma\left(1-\frac{1}{16}\,\frac{\xi^2}{\gamma^4}\right)-\frac{1}{4\pi^2}\,\frac{1}{K}\,\xi\gamma^2 \\
+\frac{1}{12\pi^2}\,\frac{1}{K^3}\,\xi\gamma^4\left(1+\frac{1}{2}\,\frac{\xi^2}{\gamma^4}\right)-\frac{1}{30\pi^2}\,\frac{1}{K^5}\,\xi\gamma^6\left(1+\frac{73}{32}\,\frac{\xi^2}{\gamma^4}\right)+\dots\,. \qquad \text{(C.6)}
\end{aligned}
$$

A similar procedure obtains $\int R(\mathbf{k})$. To order ξ^2/γ^4 we have

$$\begin{aligned}
\int_{\mathbf{k}}' R(\mathbf{k}) &\simeq \frac{\xi^2}{8\pi^2}\int_0^K \frac{k^2dk}{(k^2+\gamma^2)^2} \\
&= \frac{\xi^2}{8\pi^2}\int_0^K \frac{dk}{k^2+\gamma^2} - \frac{\xi^2\,\gamma^2}{8\pi^2}\int_0^K \frac{dk}{(k^2+\gamma^2)^2} \\
&= \frac{\xi^2}{16\pi^2}\,\frac{1}{\gamma}\,\tan^{-1}\!\left(\frac{K}{\gamma}\right) - \frac{\xi^2}{16\pi^2}\,\frac{K}{K^2+\gamma^2} \\
&= \frac{1}{32\pi}\,\frac{\xi^2}{\gamma} - \frac{\xi^2}{8\pi^2}\,\frac{1}{K}\,,
\end{aligned} \tag{C.7}$$

which is the same as (6.24a).

C.2 Case (ii): $|\xi| \sim |\gamma^2|$

Defining a dimensionless integration variable as $x = k/\gamma$, the fluctuations (6.18) become

$$\begin{aligned}
\int_{\mathbf{k}}' D(\mathbf{k}) &= -\frac{\xi\,\gamma}{4\pi^2}\int_0^{K/\gamma} \frac{x^2\,dx}{\sqrt{x^4+2x^2+\frac{\gamma^4-\xi^2}{\gamma^4}}} \\
&= -\frac{K}{4\pi^2}\,\xi - \frac{\xi\,\gamma}{4\pi^2}\int_0^{K/\gamma}\left(\frac{x^2}{\sqrt{x^4+2x^2+\frac{\gamma^4-\xi^2}{\gamma^4}}} - 1\right)dx
\end{aligned} \tag{C.8a}$$

$$\int_{\mathbf{k}}' R(\mathbf{k}) = \frac{\gamma^3}{4\pi^2}\int_0^{K/\gamma} x^2\,dx\left(\frac{x^2+1}{\sqrt{x^4+2x^2+\frac{\gamma^4-\xi^2}{\gamma^4}}} - 1\right). \tag{C.8b}$$

It is simpler to first examine the case of $\int D(\mathbf{k})$. For $K \gg |\gamma|$, the elliptic integral in (C.8a) can be approximated by

$$\begin{aligned}
\int_0^{K/\gamma}\left(\frac{x^2}{\sqrt{x^4+2x^2+\frac{\gamma^4-\xi^2}{\gamma^4}}} - 1\right)dx &= \int_0^{\infty}\left(\frac{x^2}{\sqrt{x^4+2x^2+\frac{\gamma^4-\xi^2}{\gamma^4}}} - 1\right)dx \\
&\quad + \lim_{\gamma\to 0}\left\{\frac{d}{d\gamma}\left[\int_0^{K/\gamma}\left(\frac{x^2}{\sqrt{x^4+2x^2+\frac{\gamma^4-\xi^2}{\gamma^4}}} - 1\right)dx\left(-\frac{K}{\gamma^2}\right)\right]\right\}\cdot\gamma \\
&= -\sqrt{1+\frac{\xi}{\gamma^2}}\,E\!\left(\sqrt{\frac{2\xi}{\xi+\gamma^2}}\right) + \frac{\gamma}{K} + O\!\left(\frac{\gamma^2}{K^2}\right).
\end{aligned} \tag{C.9}$$

Here, the first integral is expressed in terms of the complete elliptic integral of the second kind, E[1]. With this expression, $\int D(\mathbf{k})$ is

$$\int_{\mathbf{k}}' D(\mathbf{k}) = -\frac{K}{4\pi^2}\,\xi + \frac{1}{4\pi^2}\,\xi\,\gamma\sqrt{1+\frac{\xi}{\gamma^2}}\,E\left(\sqrt{\frac{2\xi}{\xi+\gamma^2}}\right) - \frac{1}{4\pi^2}\,\frac{\xi\,\gamma^2}{K} + O\left(\frac{\gamma^2}{K^2}\right). \tag{C.10}$$

Because $\xi \sim \gamma^2$, it follows that the quantity $\delta = 1 - 2\xi/(\xi+\gamma^2)$, is small compared to one. In this regime, the elliptic functions have the logarithmic expansion[2]

$$E(\sqrt{1-\delta}) = 1 - \frac{1}{4}\,\delta\,\ln(\delta) + \left(\ln 2 - \frac{1}{4}\right)\delta - \frac{3}{32}\,\delta^2\,\ln(\delta) + O(\delta^2) \tag{C.11a}$$

$$F(\sqrt{1-\delta}) = 2\,\ln 2 - \frac{1}{2}\,\ln(\delta) + \frac{1}{4}\,(2\ln 2 - 1)\,\delta - \frac{1}{8}\,\delta\,\ln(\delta) - \frac{9}{128}\,\delta^2\,\ln(\delta) + O(\delta^2) \tag{C.11b}$$

Since $\xi \sim \gamma^2$, which is a small parameter at low density, it is assumed that the higher order corrections can be accounted for in a series in powers of γ:

$$\xi = \xi_0\,\gamma^2 + \xi_1\,\gamma^3 + \xi_2\,\gamma^4 + \dots\,, \tag{C.12}$$

where the coefficients ξ_0, ξ_1, $\xi_2, \dots$ have yet to be determined.

Defining the parameters

$$\delta_0 = 1 - \frac{2\,\xi_0}{1+\xi_0} \tag{C.13a}$$

$$\delta_1 = \frac{2\,\xi_1}{(1+\xi_0)^2} \tag{C.13b}$$

$$\delta_2 = \frac{\xi_1}{\xi_0}\,\frac{1+\frac{3}{2}\xi_0}{1+\xi_0} \tag{C.13c}$$

it is convenient to expand the following quantities in powers of γ

$$\xi\,\gamma\sqrt{1+\frac{\xi}{\gamma^2}} = \xi_0\sqrt{1+\xi_0}(\gamma^3 + \delta_2\,\gamma^4 + \dots) \tag{C.14a}$$

$$\delta = 1 - \frac{2\xi}{\xi+\gamma^2} = \delta_0 - \delta_1\,\gamma + \dots\,. \tag{C.14b}$$

Assuming that $\delta_1\,\gamma \ll \delta_0$, the logarithm of δ may be approximated by

$$\ln(\delta_0 - \delta_1\,\gamma + \dots) \simeq \ln\delta_0 - \frac{\delta_1}{\delta_0}\,\gamma\,. \tag{C.15}$$

Substitution of this approximation into the elliptic functions gives expansions dependent only on γ and the coefficients in (C.13)

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[1] I. S. Gradshteyn and I. M. Ryzhik (2000), p. 277, 3.153.1.

[2] These expansions are given by 8.113.3 and 8.114.3 of Gradshteyn and Ryzhik (2000), p. 852.

$$\begin{aligned} E\big(\sqrt{1-\delta}\big) &= 1 + \delta_0\left(\ln 2 - \frac{1}{4}\right) - \frac{\delta_0}{4}\left(1 + \frac{3\delta_0}{8}\right)\ln\delta_0 \\ &\qquad + \frac{\delta_1}{4}\left[2 - 4\ln 2 + \frac{3\delta_0}{8} + \left(1 + \frac{3\delta_0}{4}\right)\ln\delta_0\right]\gamma + O\big[(\delta_0 - \delta_1\,\gamma)^2\big] \end{aligned} \tag{C.16a}$$

$$\begin{aligned} F\big(\sqrt{1-\delta}\big) &= 2\ln 2 + \delta_0\left(\ln\sqrt{2} - \frac{1}{4}\right) - \left[\frac{\delta_0}{8}\left(1 + \frac{9\delta_0}{16}\right) + \frac{1}{2}\right]\ln\delta_0 \\ &\qquad + \left[\frac{1}{2}\,\frac{\delta_1}{\delta_0} - \delta_1\left(\ln\sqrt{2} - \frac{1}{4}\right) + \frac{\delta_1}{8}\left(1 + \frac{9\delta_0}{16}\right)\right. \\ &\qquad \left. + \frac{\delta_1}{8}\left(1 + \frac{9\delta_0}{8}\right)\ln\delta_0\right]\gamma + O\big[(\delta_0 - \delta_1\,\gamma)^2\big] \end{aligned} \tag{C.16b}$$

Expressions (C.12), (C.14a) and (C.16a) are used in (C.10) to obtain $\int D(\mathbf{k})$ as an expansion in γ

$$\int_{\mathbf{k}}' D(\mathbf{k}) = -\frac{K}{4\pi^2}\,\xi_0\,\gamma^2 + \left(d_1 - \frac{K}{4\pi^2}\,\xi_1\right)\gamma^3 + \left(d_2 - \frac{K}{4\pi^2}\,\xi_2 - \frac{1}{4\pi^2}\,\frac{\xi_0}{K}\right)\gamma^4 + \dots\,, \tag{C.17}$$

where

$$d_1 = \frac{1}{4\pi^2}\,\xi_0\,\sqrt{1+\xi_0}\left[1 + \delta_0\left(\ln 2 - \frac{1}{4}\right) - \frac{\delta_0}{4}\left(1 + \frac{3\delta_0}{8}\right)\ln\delta_0\right] \tag{C.18a}$$

$$\begin{aligned} d_2 &= \frac{1}{4\pi^2}\,\xi_0\,\sqrt{1+\xi_0}\left\{\delta_2 + (\delta_0\delta_2 - \delta_1)\left(\ln 2 - \frac{1}{4}\right) + \frac{\delta_1}{4}\left(1 + \frac{3\delta_0}{8}\right)\right. \\ &\qquad \left. + \frac{1}{4}\left[\delta_1\left(1 + \frac{3\delta_0}{4}\right) - \delta_0\,\delta_2\left(1 + \frac{3\delta_0}{8}\right)\right]\ln\delta_0\right\}. \end{aligned} \tag{C.18b}$$

Similar calculations lead to the analogous expression for $\int R(\mathbf{k})$. For $K \gg |\gamma|$, (C.8b) can be approximated by

$$\begin{aligned} \int_0^{K/\gamma} x^2 dx\left(\frac{x^2+1}{\sqrt{x^4 + 2x^2 + \frac{\gamma^4-\xi^2}{\gamma^4}}} - 1\right) &= \int_0^{\infty} x^2 dx\left(\frac{x^2+1}{\sqrt{x^4 + 2x^2 + \frac{\gamma^4-\xi^2}{\gamma^4}}} - 1\right) \\ &\quad + \lim_{\gamma\to 0}\left\{\left[\frac{d}{d\gamma}\int_0^{K/\gamma} x^2 dx\left(\frac{x^2+1}{\sqrt{x^4 + 2x^2 + \frac{\gamma^4-\xi^2}{\gamma^4}}} - 1\right)\right]\left(-\frac{K}{\gamma^2}\right)\right\}\cdot\gamma\,. \end{aligned} \tag{C.19}$$

To express the first integral in terms of standard elliptic integrals, we use the decomposition

$$\begin{aligned}\int_0^\infty x^2dx\left(\frac{x^2+1}{\sqrt{x^4+2x^2+\frac{\gamma^4-\xi^2}{\gamma^4}}}-1\right) = \lim_{u\to\infty}\Bigg\{&\int_0^u \frac{x^4\,dx}{\sqrt{\left(x^2+1-\frac{\xi}{\gamma^2}\right)\left(x^2+1+\frac{\xi}{\gamma^2}\right)}} \\ &+\int_0^u \frac{x^2\,dx}{\sqrt{\left(x^2+1-\frac{\xi}{\gamma^2}\right)\left(x^2+1+\frac{\xi}{\gamma^2}\right)}}-\frac{1}{3}u^3\Bigg\}.\end{aligned} \tag{C.20}$$

Application of 3.154.1 and 3.153.1 of Gradshteyn and Ryzhik, p. 277, allows the expression of (C.20) in terms of the elliptic integrals of the first and second kind[1]:

$$\lim_{u\to\infty}\int_0^u \frac{x^4\,dx}{\sqrt{\left(x^2+1-\frac{\xi}{\gamma^2}\right)\left(x^2+1+\frac{\xi}{\gamma^2}\right)}} = \frac{1}{3}\sqrt{1+\frac{\xi}{\gamma^2}}\left[4E-\left(1-\frac{\xi}{\gamma^2}\right)F\right]+\frac{1}{3}u^3-u \tag{C.21a}$$

$$\lim_{u\to\infty}\int_0^u \frac{x^2\,dx}{\sqrt{\left(x^2+1-\frac{\xi}{\gamma^2}\right)\left(x^2+1+\frac{\xi}{\gamma^2}\right)}} = u-\sqrt{1+\frac{\xi}{\gamma^2}}\,E\,. \tag{C.21b}$$

Substitution of Eqs. (C.21) into (C.20) gives

$$\int_0^\infty x^2dx\left(\frac{x^2+1}{\sqrt{x^4+2x^2+\frac{\gamma^4-\xi^2}{\gamma^4}}}-1\right) = \frac{1}{3}\sqrt{1+\frac{\xi}{\gamma^2}}\left[E-\left(1-\frac{\xi}{\gamma^2}\right)F\right]. \tag{C.22}$$

Additionally, the second term on the right hand side of (C.19) is found to be $-\xi_0^2/(2K)$. Combining this with (C.22) then inserting the result into (C.8b) yields

$$\int_{\mathbf{k}}' R(\mathbf{k}) = \frac{\gamma^3}{12\pi^2}\sqrt{1+\frac{\xi}{\gamma^2}}\left[E-\left(1-\frac{\xi}{\gamma^2}\right)F\right]-\frac{1}{4\pi^2}\frac{\xi_0^2}{2K}\gamma^4+O(\gamma^5)\,. \tag{C.23}$$

Finally, Eqs. (C.14) and (C.16) are employed to obtain the required expansion in γ, which to lowest order is proportional to γ^3,

$$\int_{\mathbf{k}}' R(\mathbf{k}) = r_1\,\gamma^3\,, \tag{C.24}$$

where

$$\begin{aligned} r_1 = \frac{\sqrt{1+\xi_0}}{12\pi^2}\Bigg\{&1-\left(1-\xi_0\right)2\ln 2+\frac{1}{2}\left[\left(1+\xi_0\right)\ln 2-\frac{1}{2}\xi_0\right]\delta_0 \\ &+\frac{1}{2}\left[1-\xi_0-\frac{\delta_0}{4}\left(1+\xi_0\right)-\frac{3\delta_0^2}{128}\left(1+3\xi_0\right)\right]\ln\delta_0\Bigg\}\end{aligned} \tag{C.25}$$

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[1] For simplicity of notation, we drop the argument $\sqrt{\frac{2\xi}{\xi+\gamma^2}}$ in the elliptic integrals, E and F.

Arising in the expansion of the chemical potential, the combination, $r_1 + \xi_0 d_1$, depends on a single parameter, δ_0. This dependence is made explicit through the following algebraic simplifications. From (C.18a) and (C.25) we have

$$\begin{aligned} r_1 + \xi_0 d_1 = \frac{\sqrt{1+\xi_0}}{12\pi^2} \Bigg\{ & 1 - \big(1-\xi_0\big)\, 2\ln 2 + 3\,\xi_0^2 + \frac{1}{2}\Big[\big(1+\xi_0+6\,\xi_0^2\big)\ln 2 - \frac{1}{2}\xi_0\big(1+3\xi_0\big)\Big]\,\delta_0 \\ & + \frac{1}{2}\left[1 - \xi_0 - \frac{\delta_0}{4}\big(1+\xi_0\big) - \frac{3}{2}\,\xi_0^2\,\delta_0\left(1+\frac{3\delta_0}{8}\right) - \frac{3\,\delta_0^2}{128}\big(1+3\xi_0\big)\right]\ln\delta_0 \Bigg\} \end{aligned} \tag{C.26}$$

This can be more compactly written by first simplifying the following parts.

$$\xi_0 = \frac{1-\delta_0}{1+\delta_0} \tag{C.27a}$$

$$1+\xi_0 = \frac{2}{1+\delta_0} \tag{C.27b}$$

$$1-\xi_0 = \frac{2\delta_0}{1+\delta_0} \tag{C.27c}$$

$$1+3\xi_0 = \frac{4-2\delta_0}{1+\delta_0} \tag{C.27d}$$

$$1 - \big(1-\xi_0\big)2\ln 2 + 3\xi_0^2 = \frac{4}{(1+\delta_0)^2}\big[1 - \big(1+\ln 2\big)\delta_0 + \big(1-\ln 2\big)\delta_0^2\big] \tag{C.28}$$

$$\begin{aligned} \big(1+\xi_0+6\,\xi_0^2\big)\ln 2 - \frac{1}{2}\xi_0\big(1+3\,\xi_0\big) = & \frac{1}{\big(1+\delta_0\big)^2}\big[8\ln 2 - 2 \\ & + \big(3 - 10\ln 2\big)\delta_0 + \big(6\ln 2 - 1\big)\delta_0^2\big] \end{aligned} \tag{C.29}$$

$$1 - \xi_0 - \frac{\delta_0}{4}\big(1+\xi_0\big) = \frac{3}{2}\frac{\delta_0}{1+\delta_0} \tag{C.30}$$

$$-\frac{3}{2}\,\xi_0^2\,\delta_0\left(1+\frac{3\,\delta_0}{8}\right) - \frac{3\,\delta_0^2}{128}\big(1+3\,\xi_0\big) = -\frac{3}{64}\frac{\delta_0}{\big(1+\delta_0\big)^2}\big(32 - 50\,\delta_0 + 9\,\delta_0^2 + 11\,\delta_0^3\big)\,. \tag{C.31}$$

Combining Eqs. (C.27 - C.31) gives

$$\begin{aligned} r_1 + \xi_0 d_1 = \frac{\sqrt{2}}{12\pi^2}\,\frac{1}{\big(1+\delta_0\big)^{5/2}} \Bigg[& 4 - 5\,\delta_0 + \left(\frac{11}{2} - 9\ln 2\right)\delta_0^2 + \left(3\ln 2 - \frac{1}{2}\right)\delta_0^3 \\ & + \frac{3}{128}\big(82 - 9\,\delta_0 - 11\,\delta_0^2\big)\delta_0^2\ln\delta_0 \Bigg] \end{aligned} \tag{C.32}$$

C.3 Case (iii): $|\xi| > |\gamma^2|$

For this case, we let $\xi = i\eta$ then expand in γ^2/η. Defining $k = \sqrt{\eta}x$, $\int D(\mathbf{k})$ in (6.18) becomes

$$\int_{\mathbf{k}}' D(\mathbf{k}) = -\frac{i\eta}{4\pi^2}\int_0^{\frac{K}{\sqrt{\eta}}} \frac{\sqrt{\eta}\,x^2\,dx}{\sqrt{\left(x^2+\frac{\gamma^2}{\eta}\right)^2+1}}\,. \tag{C.33}$$

The integrand can be easily expanded as

$$\frac{1}{\sqrt{\left(x^2+\frac{\gamma^2}{\eta}\right)^2+1}} = \frac{1}{\sqrt{x^4+1}}-\frac{\gamma^2}{\eta}\,\frac{x^2}{\left(x^4+1\right)^{3/2}}+\frac{1}{2}\,\frac{\gamma^4}{\eta^2}\left[\frac{3\,x^4}{\left(x^4+1\right)^{5/2}}-\frac{1}{\left(x^4+1\right)^{3/2}}\right]+O\left(\frac{\gamma^6}{\eta^3}\right) \tag{C.34}$$

Inserting this into (C.33) obtains a result valid to order γ^6/η^3:

$$\begin{aligned}\int_{\mathbf{k}}' D(\mathbf{k}) = -i\,\frac{\eta^{3/2}}{4\pi^2}\Bigg\{&\int_0^{\frac{K}{\sqrt{\eta}}}\frac{x^2}{\sqrt{x^4+1}}\,dx-\frac{\gamma^2}{\eta}\int_0^{\frac{K}{\sqrt{\eta}}}\frac{x^4}{\left(x^4+1\right)^{3/2}}\,dx\\ &+\frac{1}{2}\,\frac{\gamma^4}{\eta^2}\left[\int_0^{\frac{K}{\sqrt{\eta}}}\frac{3\,x^6}{\left(x^4+1\right)^{5/2}}\,dx-\int_0^{\frac{K}{\sqrt{\eta}}}\frac{x^2}{\left(x^4+1\right)^{3/2}}\,dx\right]\Bigg\}.\end{aligned} \tag{C.35}$$

Since $\int D(\mathbf{k})$ is required up to order $\eta^{5/2}$, each integral must be expanded up to order η. Because the first integral is divergent as $\eta \to 0$, it can be handled by splitting the range into two pieces:

$$\begin{aligned}\int_0^{\frac{K}{\sqrt{\eta}}}\frac{x^2}{\sqrt{x^4+1}}\,dx &= \int_0^{C}\frac{x^2}{\sqrt{x^4+1}}\,dx+\int_C^{\frac{K}{\sqrt{\eta}}}\frac{x^2}{\sqrt{x^4+1}}\,dx\\ &= \int_0^{C}\frac{x^2}{\sqrt{x^4+1}}\,dx+\int_0^{\frac{K}{\sqrt{\eta}}}\left(1-\frac{1}{2}\,\frac{1}{x^4}+\frac{3}{8}\,\frac{1}{x^8}-\frac{5}{16}\,\frac{1}{x^{12}}+\ldots\right)dx\\ &= \int_0^{C}\frac{x^2}{\sqrt{x^4+1}}\,dx+\frac{K}{\sqrt{\eta}}-C+\frac{1}{6}\,\frac{\eta^{3/2}}{K^3}-\frac{1}{6\,C^3}-\ldots\\ &= \int_0^{C}\left(\frac{x^2}{\sqrt{x^4+1}}-1\right)dx+\frac{K}{\sqrt{\eta}}+\frac{1}{6}\,\frac{\eta^{3/2}}{K^3}-\frac{1}{6\,C^3}-\ldots\,.\end{aligned} \tag{C.36}$$

Allowing the cutoff go to infinity obtains

$$\int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^2}{\sqrt{x^4+1}}\,dx = \int_0^{\infty}\left(\frac{x^2}{\sqrt{x^4+1}} - 1\right) dx + \frac{K}{\sqrt{\eta}} + \frac{1}{6}\,\frac{1}{K^3}\,\eta^{3/2} + O\big(\eta^{3/2}\big)\,. \tag{C.37}$$

The remaining integrals are expanded in order of their appearance in expression (C.35). Each integral is differentiated the appropriate number of times to obtain terms to linear order in η.

$$\frac{d}{d\sqrt{\eta}} \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4}{\big(x^4+1\big)^{3/2}}\,dx = -\frac{K^5}{\big(K^4+\eta^2\big)^{3/2}} \tag{C.38a}$$

$$\frac{d^2}{d\sqrt{\eta}^2} \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4}{\big(x^4+1\big)^{3/2}}\,dx = 6\,\frac{K^5}{\big(K^4+\eta^2\big)^{5/2}}\,\eta^{3/2} \tag{C.38b}$$

$$\Rightarrow \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4}{\big(x^4+1\big)^{3/2}}\,dx = \int_0^{\infty} \frac{x^4}{\big(x^4+1\big)^{3/2}}\,dx - \frac{1}{K}\sqrt{\eta} + O\big(\eta^{5/2}\big)\,. \tag{C.38c}$$

$$\frac{d}{d\sqrt{\eta}} \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^6}{\big(x^4+1\big)^{5/2}}\,dx = -\frac{K^7}{\big(K^4+\eta^2\big)^{5/2}}\,\eta \tag{C.39a}$$

$$\Rightarrow \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^6}{\big(x^4+1\big)^{5/2}}\,dx = \int_0^{\infty} \frac{x^6}{\big(x^4+1\big)^{5/2}}\,dx + O\big(\eta^{3/2}\big)\,. \tag{C.39b}$$

$$\frac{d}{d\sqrt{\eta}} \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^2}{\big(x^4+1\big)^{3/2}}\,dx = -\frac{K^3}{\big(K^4+\eta^2\big)^{3/2}}\,\eta \tag{C.40a}$$

$$\Rightarrow \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^2}{\big(x^4+1\big)^{3/2}}\,dx = \int_0^{\infty} \frac{x^2}{\big(x^4+1\big)^{3/2}}\,dx + O\big(\eta^{3/2}\big)\,. \tag{C.40b}$$

It is convenient to define the above integrals as

$$I_1 \equiv \frac{1}{4\pi^2} \int_0^\infty \left(\frac{x^2}{\sqrt{x^4+1}} - 1 \right) dx \tag{C.41a}$$

$$I_2 \equiv \frac{1}{4\pi^2} \int_0^\infty \frac{x^4}{\left(x^4+1\right)^{3/2}}\, dx \tag{C.41b}$$

$$I_3 \equiv \frac{1}{4\pi^2} \int_0^\infty \frac{x^6 - \frac{1}{2}x^2}{\left(x^4+1\right)^{5/2}}\, dx \tag{C.41c}$$

$$I \equiv I_1 - \frac{\gamma^2}{\eta}\, I_2 + \frac{\gamma^4}{\eta^2}\, I_3 \,. \tag{C.41d}$$

Substitution of (C.37 - C.41) into (C.35) gives $\int D(\mathbf{k})$ to order η^3:

$$\int_{\mathbf{k}}' D(\mathbf{k}) = -\frac{K}{4\pi^2}\, i\eta - I\, i\eta^{3/2} - \frac{1}{4\pi^2}\, \frac{1}{K}\, \frac{\gamma^2}{\eta}\, i\eta^2 + O\left(\eta^3\right) . \tag{C.42}$$

By first decomposing it in terms of $\int D(\mathbf{k})$, the other fluctuation, $\int R(\mathbf{k})$, is calculated in a similar way. Again using $\xi = i\eta$, we have

$$\begin{aligned}
\int_{\mathbf{k}}' R(\mathbf{k}) &= \frac{1}{4\pi^2} \int_0^K k^2\, dk \left[\frac{k^2+\gamma^2}{\sqrt{\left(k^2+\gamma^2\right)^2 + \eta^2}} - 1 \right] \\
&= \frac{1}{4\pi^2} \int_0^K \frac{k^4\, dk}{\sqrt{\left(k^2+\gamma^2\right)^2+\eta^2}} + i\frac{\gamma^2}{\eta} \int_{\mathbf{k}}' D(\mathbf{k}) - \frac{K^3}{12\pi^2} \\
&= \frac{\eta^{3/2}}{4\pi^2} \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4\, dx}{\sqrt{\left(x^2+\frac{\gamma^2}{\eta}\right)^2+1}} + \frac{K}{4\pi^2}\, \gamma^2 + \frac{\gamma^2}{\eta}\, I_1\, \eta^{3/2} - \frac{\gamma^4}{\eta^2}\, I_2\, \eta^{3/2} \\
&\qquad - \frac{K^3}{12\pi^2} + \frac{1}{4\pi^2}\, \frac{1}{K}\, \frac{\gamma^4}{\eta^2}\, \eta^2 \,.
\end{aligned} \tag{C.43}$$

Using (C.34), the integrand of the first integral is expanded to order γ^4/η^2:

$$\int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4\,dx}{\sqrt{\left(x^2+\frac{\gamma^2}{\eta}\right)^2+1}} = \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4}{\sqrt{x^4+1}}\,dx - \frac{\gamma^2}{\eta}\int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^6}{\left(x^4+1\right)^{3/2}}\,dx$$
$$+\frac{1}{2}\frac{\gamma^4}{\eta^2}\left[\int_0^{\frac{K}{\sqrt{\eta}}} \frac{3\,x^8}{\left(x^4+1\right)^{5/2}}\,dx - \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4}{\left(x^4+1\right)^{3/2}}\,dx\right]. \tag{C.44}$$

On the right-hand side of (C.44), the last integral given by (C.38c), whereas the first three can be calculated as was done in (C.36):

$$\begin{aligned}\int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4}{\sqrt{x^4+1}}\,dx &= \int_0^{C} \frac{x^4}{\sqrt{x^4+1}}\,dx + \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4}{\sqrt{x^4+1}}\,dx \\ &= \int_0^{C} \frac{x^4}{\sqrt{x^4+1}}\,dx + \int_0^{\frac{K}{\sqrt{\eta}}} \left(x^2 - \frac{1}{2}\frac{1}{x^2} + \frac{3}{8}\frac{1}{x^6} - \dots\right) dx \\ &= \int_0^{\infty} \left(\frac{x^4}{\sqrt{x^4+1}} - x^2\right) dx + \frac{1}{3}\frac{K^3}{\eta^{3/2}} + O\big(\eta^{3/2}\big) \end{aligned} \tag{C.45}$$

$$\begin{aligned}\int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^6}{\left(x^4+1\right)^{3/2}}\,dx &= \int_0^{C} \frac{x^6}{\left(x^4+1\right)^{3/2}}\,dx + \int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^6}{\left(x^4+1\right)^{3/2}}\,dx \\ &= \int_0^{C} \frac{x^6}{\left(x^4+1\right)^{3/2}}\,dx + \int_0^{\frac{K}{\sqrt{\eta}}} \left(1 - \frac{3}{2}\frac{1}{x^4} - \dots\right) dx \\ &= \int_0^{\infty} \left[\frac{x^6}{\left(x^4+1\right)^{3/2}} - 1\right] dx + \frac{K}{\sqrt{\eta}} + O\big(\eta^{3/2}\big) \end{aligned} \tag{C.46}$$

$$\int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^8}{\left(x^4+1\right)^{5/2}}\,dx = \int_0^{\infty} \frac{x^8}{\left(x^4+1\right)^{5/2}}\,dx + O\big(\eta^{3/2}\big)\,. \tag{C.47}$$

Hence, the expansion (C.44) becomes

$$\int_0^{\frac{K}{\sqrt{\eta}}} \frac{x^4\, dx}{\sqrt{\left(x^4 + \frac{\gamma^2}{\eta}\right)^2 + 1}} = \int_0^\infty \left(\frac{x^4}{\sqrt{x^4+1}} - x^2 \right) dx + \frac{1}{3} \frac{K^3}{\eta^{3/2}} - \frac{\gamma^2}{\eta} \int_0^\infty \left[\frac{x^6}{\left(x^4+1\right)^{3/2}} - 1 \right] dx$$
$$- \frac{\gamma^2}{\eta} \frac{K}{\sqrt{\eta}} + \frac{\gamma^4}{\eta^2} \int_0^\infty \frac{x^8 - \frac{1}{2}x^4}{\left(x^4+1\right)^{5/2}}\, dx + O\left(\eta^{3/2}\right) \tag{C.48}$$

Substituting this along with the explicit expressions of I_1, I_2 and I_3 [see Eqs. (C.41)], $\int R(\mathbf{k})$ is obtained to order η^3:

$$\int_{\mathbf{k}}' R(\mathbf{k}) = J\, \eta^{3/2} + \frac{1}{4\pi^2} \frac{1}{K} \frac{\gamma^4}{\eta^2}\, \eta^2 + O\left(\eta^3\right), \tag{C.49}$$

where we define

$$J_1 \equiv \frac{1}{4\pi^2} \int_0^\infty \left(\frac{x^4}{\sqrt{x^4+1}} - x^2 \right) dx \tag{C.50a}$$

$$J_2 \equiv \frac{1}{4\pi^2} \int_0^\infty \frac{x^2}{\left(x^4+1\right)^{3/2}}\, dx \tag{C.50b}$$

$$J_3 \equiv \frac{1}{4\pi^2} \int_0^\infty \frac{x^4}{\left(x^4+1\right)^{5/2}}\, dx \tag{C.50c}$$

$$J \equiv J_1 + \frac{\gamma^2}{\eta} J_2 - \frac{3}{2} \frac{\gamma^4}{\eta^2} J_3\,. \tag{C.50d}$$

Bibliography

[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell. Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor. *Science*, **269**:198, 1995.

[2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer. Theory of Superconductivity. *Phys. Rev.*, **108**:1175, 1957.

[3] M. Bartenstein, A. Altmeyer, S. Riedl, R. Geursen, S. Jochim, C. Chin, J. Hecker Denschlag, R. Grimm, A. Simoni, E. Tiesinga, C. J. Williams, and P. S. Julienne. Precise Determination of ^{6}Li Cold Collision Parameters by Radio-Frequency spectroscopy on Weakly Bound Molecules. arXiv:cond-mat/0408673v1, 2004.

[4] P. F. Bedaque, E. Braaten, and H.-W. Hammer. Three-Body Recombination in Bose Gases with Large Scattering Length. *Phys. Rev. Lett.*, **85**:908, 2000.

[5] John M. Blatt and Victor F. Weisskopf. *Theoretical Nuclear Physics*. John Wiley & Sons, Inc., 1952.

[6] C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet. Evidence of Bose-Einstein Condensation in an Atomic Gas with Attractive Interactions. *Phys. Rev. Lett.*, **75**:1687, 1995.

[7] Y. Castin and R. Dum. Bose-Einstein Condensates in Time Dependent Traps. *Phys. Rev. Lett.*, **77**:5315, 1996.

[8] Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë. *Quantum Mechanics*. John Wiley & Sons, Inc., 1977.

[9] E. A. Cornell, J. R. Ensher, and C. E. Wieman. Experiments in dilute atomic Bose-Einstein condensation. In S. Stringari M. Inguscio and C. E. Wieman, editors, *Bose-Einstein Condensation in Atomic Gases*, pages 15–66, 1998. Proceedings of the International School of Physics.

[10] S. L. Cornish, N. R. Claussen, J. L. Roberts, E. A. Cornell, and C. E. Wieman. Stable ^{85}Rb Bose-Einstein Condensates with Widely Tunable Interactions. *Phys. Rev. Lett.*, **85**:1795, 2000.

[11] G. E. Cragg and A. K. Kerman. Complex Chemical Potential: Signature of Decay in a Bose-Einstein Condensate. *Phys. Rev. A*, **94**:190402, 2005.

[12] A. Das and A. C. Melissinos. *Quantum Mechanics: A Modern Introduction.* Gordon and Breach, Fourth edition, 1990.

[13] K. B. Davis, M-O. Mewes, M.R Andrews, N. J. van Druten, D. M. Kurn D. S. Durfee, and W. Ketterle. Bose-Einstein Condensation in a Gas of Sodium Atoms. *Phys. Rev. Lett.*, **75**:3969, 1995.

[14] L. P. H. de Goey, H. T. C. Stoof, B. J. Verhaar, and W. Glöckle. Role of Three-Body Correlations in Recombination of Spin-Polarized Atomic Hydrogen. *Phys. Rev. B*, **38**:646, 1988.

[15] E. A. Donley, N. R. Claussen, S. T. Thompson, and C. E. Wieman. Atom-Molecule Coherence in a Bose-Einstein Condensate. *Nature*, **417**:529, 2002.

[16] A. Eleftheriou and K. Huang. Instability of a Bose-Einstein condensate with an attractive interaction. *Phys. Rev. A*, **61**:043601, 2000.

[17] P. O. Fedichev, M. W. Reynolds, and G. V. Shlyapnikov. Three-Body Recombination of Ultracold Atoms to a Weakly Bound s Level. *Phys. Rev. Lett.*, **77**:2921, 1996.

[18] H. Feshbach. A Unified Theory of Nuclear Reactions, II. *Annals of Physics*, **281**:519, 2000.

[19] A. L. Fetter and J. D. Walecka. *Quantum Theory of Many-Particle Systems.* Dover, 2003.

[20] I. S. Gradshteyn and I. M. Ryzhik. *Table of Integrals, Series and Products.* Academic Press, sixth edition, 2000.

[21] A. Griffin. A brief history of our understanding of BEC: From Bose to Beliaev. In S. Stringari M. Inguscio and C. E. Wieman, editors, *Bose-Einstein Condensation in Atomic Gases*, pages 1–13, 1998. Proceedings of the International School of Physics.

[22] E. P. Gross. Hydrodynamics of a Superfluid Condensate. *J. Math. Phys.*, **4**:195, 1963.

[23] H. F. Hess, D. A. Bell, G. P. Kochanski, and R. W. Cline. Observation of Three-Body Recombination in Spin-Polarized Hydrogen. *Phys. Rev. Lett.*, **51**:483, 1983.

[24] M. Holland, J. Park, and R. Walser. Formation of Pairing Fields in Resonantly Coupled Atomic and Molecular Bose-Einstein Condensates. *Phys. Rev. Lett.*, **86**:1915, 2001.

[25] K. Huang and C. N. Yang. Quantum-Mechanical Many-Body Problem with Hard-Sphere Interaction. *Phys. Rev.*, **105**:767, 1957.

[26] S. Inouye, M. R. Andrews, J. Stenger, H.-J. Miesner, D. M. Stamper-Kurn, and W. Ketterle. Observation of Feshbach resonances in a Bose-Einstein condensate. *Nature*, **392**:151, 1998.

[27] D. Jaksch, V. Venturi, J. I. Cirac, C. J. Williams, and P. Zoller. Creation of a Molecular Condensate by Dynamically Melting a Mott Insulator. *Phys. Rev. Lett.*, **89**:040402, 2002.

[28] T. Mukaiyama K. Xu, J. R. Abo-Shaeer, J. K. Shin, D. E. Miller, and W. Ketterle. Formation of Quantum-Degenerate Sodium Molecules. *Phys. Rev. Lett.*, **91**:210402, 2003.

[29] A. K. Kerman and P. Tommasini. Gaussian Time-Dependent Variational Principle for Bosons. *Annals of Physics*, **260**:250, 1997.

[30] S. J. J. M. F. Kokkelmans and M. J. Holland. Ramsey Fringes in a Bose-Einstein Condensate between Atoms and Molecules. *Phys. Rev. Lett.*, **89**:180401, 2002.

[31] S. J. J. M. F. Kokkelmans, J. N. Milstein, M. L. Chiofalo, R. Walser, and M. J. Holland. Resonance Superfluidity: Renormalization of Resonance Scattering Theory. *Phys. Rev. A*, **65**:053617, 2002.

[32] S. J. J. M. F. Kokkelmans, H. M. S. Vissers, and B. J. Verhaar. Formation of a Bose condensate of stable molecules via a Feshbach resonance. *Phys. Rev. A*, **63**:031601, 2001.

[33] A. J. Leggett. Diatomic Molecules and Cooper Pairs. In A. Pekalski and J. Przystawa, editors, *Modern Trends in the Theory of Condensed Matter*, pages 14–27, 1979. Proceedings of the XVI Karpacz Winter School of Theoretical Physics.

[34] A. J. Leggett. Topics in the Theory of the Ultracold Dilute Alkali Gases. In Craig M. Savage and Mukunda P. Das, editors, *Bose-Einstein Condensation: From Atomic Physics to Quantum Fluids*, pages 1–42, 2000. Proceedings of the Thirteenth Physics Summer School.

[35] A. J. Leggett. Bose-Einstein Condensation in the Akali Gases: Some Fundamental Concepts. *Rev. Mod. Phys.*, **73**:307, 2001.

[36] E. H. Lieb and J. Yngvason. Ground State Energy of the Low Density Bose Gas. *Phys. Rev. Lett.*, **80**:2504, 1998.

[37] Elliott H. Lieb and Werner Liniger. Exact Analysis of an Interacting Bose Gas. I. the General Solution and the Ground State. *Physical Review*, **130**:1605, 1963.

[38] G. Modugno, G. Ferrari, G. Roati, R. J. Brecha, A. Simoni, and M. Inguscio. Bose-Einstein Condensation of Potassium Atoms by Sympathetic Cooling. *Science*, **294**:1320, 2001.

[39] A. J. Moerdijk, H. M. J. M. Boesten, and B. J. Verhaar. Decay of Trapped Ultracold Alkali Atoms by Recombination. *Phys. Rev. A*, **53**:916, 1996.

[40] John W. Negele and Henri Orland. Frontiers in Physics. In Allan M. Wylde, editor, *Quantum Many-Particle Systems*, 1988.

[41] Roger G. Newton. *Scattering Theory of Waves and Particles.* Dover, Second edition, 2002.

[42] J. Oitmaa. Statistical Mechanics of Bosonic Systems. In Craig M. Savage and Mukunda P. Das, editors, *Bose-Einstein Condensation: From Atomic Physics to Quantum Fluids*, pages 43–63, 2000. Proceedings of the Thirteenth Physics Summer School.

[43] R. K. Pathria. *Statistical Mechanics.* Butterworth-Heinemann, Second edition, 1996.

[44] David Porter and David S. G. Stirling. *Integral Equations: A Practical Treatment, from Spectral Theory to Applications.* Cambridge University Press, 1990.

[45] C. A. Regal, M. Greiner, and D. S. Jin. Observation of Resonance Condensation of Fermionic Atom Pairs. *Phys. Rev. Lett.*, **92**:040403, 2003.

[46] A. Robert, O. Sirjean, , A. Browaeys, J. Poupard, S. Nowak, D. Boiron, C. I. Westbrook, and A. Aspect. A Bose-Einstein Condensate of Metastable Atoms. *Science*, **292**:461, 2001.

[47] J. L. Roberts, N. R. Claussen, S. L. Cornish, E. A. Donley, E. A. Cornell, and C. E. Wieman. Controlled Collapse of a Bose-Einstein Condensate. *Phys. Rev. Lett.*, **86**:4211, 2001.

[48] J. L. Roberts, N. R. Claussen, S. L. Cornish, and C. E. Wieman. Magnetic Field Dependence of Ultracold Inelastic Collisions near a Feshbach Resonance. *Phys. Rev. Lett.*, **85**:728, 2000.

[49] M. W. J. Romans, R. A. Duine, S. Sachdev, and H. T. C. Stoof. Quantum Phase Transition in an Atomic Bose Gas with a Feshbach Resonance. *Phys. Rev. Lett.*, **93**:020405, 2004.

[50] J. J. Sakurai. *Modern Quantum Mechanics.* Addison-Wesley, Revised edition, 1994.

[51] T. Schumm, S. Hofferberth, L. M. Anderson, S. Wildermuth, S. Groth, I. Bar-Joseph, J. Schmiedmayer, and P. Krüger. Matter-wave interferometry in a double well on an atom chip. *Nature Physics*, **1**:57, 2005.

[52] J. Schwinger. On Gauge Invariance and Vacuum Polarization. *Phys. Rev.*, **82**:664, 1951.

[53] J. Söding, D. Guéry-Odelin, P. Desbiolles, F. Chevy, H. Inamori, and J. Dalibard. Three-Body Decay of a Rubidium Bose-Einstein Condensate. *Appl. Phys. B*, **69**:257, 1999.

[54] John R. Taylor. *Scattering Theory: The Quantum Theory on Nonrelativistic Collisions.* John Wiley & Sons, Inc., 1972.

[55] E. Timmermans, K. Furuya, P. Milonni, and A. K. Kerman. Prospect of Creating a Composite Fermi-Bose Superfluid. *Phys. Lett. A*, **285**:228, 2001.

[56] E. Timmermans, P. Tommasini, R Côté, M. Hussein, and A. K. Kerman. Rarified Liquid Properties of Hybrid Atomic-Molecular Bose-Einstein Condensates. *Phys. Rev. Lett.*, **83**:2691, 1999.

[57] M. Ueda and A. J. Leggett. Macroscopic Quantum Tunneling of a Bose-Einstein Condensate with Attractive Interaction. *Phys. Rev. Lett.*, **80**:1576, 1998.

[58] D. van Oosten, P. van der Straten, and H. T. C. Stoof. Quantum Phases in an Optical Lattice. *Phys. Rev. A*, **63**:053601, 2001.

[59] T. Weber, J. Herbig, M. Mark, H.-C. Nägerl, and R. Grimm. Three-Body Recombination at Large Scattering Lengths in an Ultracold Atomic Gas. *Phys. Rev. Lett.*, **91**:123201, 2003.

[60] Steven Weinberg. *The Quantum Theory of Fields I.* Cambridge University Press, 1995.

[61] V. A. Yurovsky and A. Ben-Reuven. Three-body loss of trapped ultracold ^{87}Rb atoms due to a Feshbach resonance. *Phys. Rev. A*, **67**:050701, 2003.

[62] V. A. Yurovsky, A. Ben-Reuven, P. S. Julienne, and C. J. Williams. Atom loss from Bose-Einstein condensates due to Feshbach resonance. *Phys. Rev. A*, **60**:R765, 1999.