Cold Bose Gases at Unitarity

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Abstract

We consider a cold Bose gas in the unitarity limit. The unitarity limit corresponds to the limit where the scattering length goes to infinity. In this thesis we first review basic quantum-mechanical scattering theory and explain the physics of Feshbach resonances. After that we discuss a many-body theory, which exactly incorporates the two-body physics of a Feshbach resonance. In a mean-field approximation we obtain a divergence of the energy per particle in the unitarity limit. Beyond mean field the spectral function is ill behaved. To get more insight into these problems, we also discuss a model of linearly coupled atoms and phonons. A generalized Bogoliubov transformation is used to obtain expressions for the quantized atomic and phonon field operators. Finally, we use these operators to calculate some correlation functions.

Contents

1 Introduction

Strong interaction is an interesting aspect of quantum gases. In this regime, in contrast to the weakly interacting case, we cannot use perturbation methods. An important step forward in the study of these strongly interacting systems, was the discovery of Feshbach resonances in 1993 by Eite Tiesinga, Boudewijn Verhaar and Henk Stoof [11]. This allowed us to alter the interaction strength between atoms, by tuning the external magnetic field. Thus by changing this magnetic field, we can explore both the weakly interacting and strongly interacting regime for cold gases.

In the last couple of years strongly interacting fermions have been intensively studied, both theoretically and experimentally. More recently, also the strongly interacting atomic Bose gas has gained theoretical interest [2]. Also the number of experiments for Bose gases in this regime increases [7],[13]. However, these experiments are rather difficult since at low temperatures the three-body losses rapidly increase. This is in contrast to fermions, where the three-body losses are suppressed by the Pauli exclusion principle. In this thesis we are particularly interested in these strongly interacting cold Bose gases.

For cold gases, the dimensionless interaction strength is determined by the density and the s-wave scattering length a. If a is negative, the gas is attractive and for positive a the gas is repulsive. Bose gases with attractive interactions are unstable. Therefore most studies focus on repulsive Bose gases. Also in this thesis, we will consider repulsive Bose gases. If the scattering length a tends to infinity, we are in the so-called unitarity limit. In this limit the properties of the gas become universal, which means that the properties are independent of the details of the system. By only using dimensional arguments, we only have one energy scale for cold quantum gases in the unitarity limit [12]. This energy scale is defined as the Fermi energy and is proportional to $n^{2/3}$, where n is the particle density. For ultracold fermions in the unitarity limit, we have for instance that $\mu = (1 + \beta)\epsilon_F \simeq 0.42\epsilon_F$ [1]. In this thesis we will try to obtain a similar expression for ultracold Bose gases at unitarity.

This thesis is organized as follows. In chapter 2 we discuss basic two-body scattering and the principle of a Feshbach resonance is explained. Subsequently, in chapter 3 we consider an effective theory that correctly incorporates the two-atom physics of a Feshbach resonance. Hereafter, this effective action is used for a mean-field theory which describes the equilibrium properties of the atomic and molecular condensates. Chapter 4 gives a discussion of the problems that arise in the Green's function formalism, if we go beyond mean field. To get more insight into these problems, we consider a model consisting of linearly coupled atoms and phonons in chapter 5. We determine expressions for the quantized atomic and phonon field operators, in order to make a comparison with the spectral function obtained in the Green's function and operator formalism. Hereafter, the field operators are used to calculate some correlation functions. Finally, this thesis is concluded in Chapter 6.

2 Quantum-mechanical scattering

In this chapter we discuss quantum-mechanical scattering. Since we consider dilute gases, two-body interactions are most important. Therefore we consider the scattering properties of two cold atoms. The material covered in this chapter is primarily based on [9], [3] and [10].

2.1 Two-body scattering

If two particles interact via an interacting potential $V(\mathbf{r}_1, \mathbf{r}_2)$ that only depends on the distance between their positions $\mathbf{r}_1$ and $\mathbf{r}_2$, we can split the Hamiltonian in a center-of-mass and a relative part. In this case both parts are described by separate Schrödinger equations. Because the Schrödinger equation that describes the relative motion incorporates the scattering physics, we focus on this part. The relative Schrödinger equation is given by

$$\left\{ \frac{-\hbar^2 \nabla^2}{m} + V(\mathbf{r}_1 - \mathbf{r}_2) \right\} \psi(\mathbf{r}_1 - \mathbf{r}_2) = E \psi(\mathbf{r}_1 - \mathbf{r}_2). \tag{1}$$

For elastic scattering processes, where E is given by the kinetic energy of the incoming wave $2\epsilon_\mathbf{p} = \mathbf{p}^2/m$ with p the incoming relative momentum and m the mass of the atoms, the time-independent Schrödinger equation reads

$$\left\{ 2\epsilon_\mathbf{p} - \hat{H}_0 \right\} |\psi_\mathbf{p}\rangle = \hat{V} |\psi_\mathbf{p}\rangle. \tag{2}$$

Here $\hat{H}_0 = \hbar^2 \nabla^2/m$ and $|\psi_\mathbf{p}\rangle$ is the base-independent notation for the scattering state. To formally solve this equation, we first assume that the interaction potential is zero. In this case the solution is a simple plain wave $|\mathbf{p}\rangle$. If we slowly turn on the interaction potential, the wave function will slowly change too. Therefore, the solution to the relative Schrödinger equation is given by

$$|\psi_\mathbf{p}^\pm\rangle = |\mathbf{p}\rangle + \frac{1}{2\epsilon_\mathbf{p} - \hat{H}_0 \pm i\epsilon} \hat{V} |\psi_\mathbf{p}^\pm\rangle, \tag{3}$$

where ϵ tends to zero. This equation is known as the Lippmann-Schwinger equation. Here, the $i\epsilon$ is introduced to handle the pole of $1/(2\epsilon_\mathbf{p} - \hat{H}_0)$. The difference between adding $i\epsilon$ or $-i\epsilon$, will be explained at the end of this section. By multiplying this equation with $\langle \mathbf{r}|$ from the left, we obtain

$$\langle \mathbf{r}|\psi_\mathbf{p}^\pm\rangle = \langle \mathbf{r}|\mathbf{p}\rangle + \int d\tilde{\mathbf{r}} \langle \mathbf{r}| \frac{1}{2\epsilon_\mathbf{p} - \hat{H}_0 \pm i\epsilon} |\tilde{\mathbf{r}}\rangle \langle \tilde{\mathbf{r}}|\hat{V}|\psi_\mathbf{p}^\pm\rangle. \tag{4}$$

Because,

$$\langle \tilde{\mathbf{r}}|\tilde{\mathbf{p}}\rangle = \frac{e^{i\tilde{\mathbf{p}}\cdot\tilde{\mathbf{r}}/\hbar}}{(2\pi\hbar)^{3/2}}, \tag{5}$$

we can rewrite (4) into

$$\begin{aligned}
\langle \mathbf{r}|\psi_\mathbf{p}^\pm\rangle &= \frac{e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}}{(2\pi\hbar)^{3/2}} + \int d\tilde{\mathbf{r}} \int d\tilde{\mathbf{p}} \int d\tilde{\mathbf{q}} \langle \mathbf{r}|\tilde{\mathbf{p}}\rangle \langle \tilde{\mathbf{p}}| \frac{1}{2\epsilon_\mathbf{p} - \hat{H}_0 \pm i\epsilon} |\tilde{\mathbf{q}}\rangle \langle \tilde{\mathbf{q}}|\tilde{\mathbf{r}}\rangle \langle \tilde{\mathbf{r}}|\hat{V}|\psi_\mathbf{p}^\pm\rangle \\
&= \frac{e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}}{(2\pi\hbar)^{3/2}} + \int d\tilde{\mathbf{r}} \int d\tilde{\mathbf{p}} \int d\tilde{\mathbf{q}} \langle \mathbf{r}|\tilde{\mathbf{p}}\rangle \langle \tilde{\mathbf{q}}|\tilde{\mathbf{r}}\rangle \frac{1}{2\epsilon_\mathbf{p} - 2\epsilon_{\tilde{\mathbf{q}}} \pm i\epsilon} \langle \tilde{\mathbf{p}}|\tilde{\mathbf{q}}\rangle \langle \tilde{\mathbf{r}}|\hat{V}|\psi_\mathbf{p}^\pm\rangle \\
&= \frac{e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}}{(2\pi\hbar)^{3/2}} + \int d\tilde{\mathbf{r}} \int \frac{d\tilde{\mathbf{p}}}{(2\pi\hbar)^3} \frac{e^{i\tilde{\mathbf{p}}\cdot(\mathbf{r}-\tilde{\mathbf{r}})/\hbar}}{2\epsilon_\mathbf{p} - 2\epsilon_{\tilde{\mathbf{p}}} \pm i\epsilon} \langle \tilde{\mathbf{r}}|\hat{V}|\psi_\mathbf{p}^\pm\rangle,
\end{aligned} \tag{6}$$

where the following orthonormality condition is used

$$\langle \tilde{\mathbf{p}}|\tilde{\mathbf{q}}\rangle = \delta(\tilde{\mathbf{p}} - \tilde{\mathbf{q}}). \tag{7}$$

The result of the momentum integral in (6) is well known, and is for example given in table 3.1 of [10]. By inserting this result, (6) simplifies to

$$\langle \mathbf{r} | \psi_{\mathbf{p}}^{\pm} \rangle = \frac{e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}}{(2\pi\hbar)^{3/2}} - \frac{m}{\hbar^2} \int d\tilde{\mathbf{r}} \frac{e^{\pm i\tilde{\mathbf{p}}\cdot|\mathbf{r}-\tilde{\mathbf{r}}|/\hbar}}{4\pi|\mathbf{r}-\tilde{\mathbf{r}}|} \langle \tilde{\mathbf{r}} | \hat{V} | \psi_{\mathbf{p}}^{\pm} \rangle. \tag{8}$$

By assuming that the potential is short ranged, we are especially interested at distances which are larger than the range of this potential. Therefore, we now consider the behaviour of the scattering wavefunction at distances $r \gg \tilde{r}$. In this case (8) changes into

$$\langle \mathbf{r} | \psi_{\mathbf{p}}^{\pm} \rangle = \frac{e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}}{(2\pi\hbar)^{3/2}} - \frac{m}{\hbar^2} \frac{e^{\pm ipr/\hbar}}{4\pi r} \int d\tilde{\mathbf{r}} \langle \tilde{\mathbf{r}} | \hat{V} | \psi_{\mathbf{p}}^{\pm} \rangle e^{\mp i\tilde{\mathbf{p}}\cdot\tilde{\mathbf{r}}/\hbar}, \tag{9}$$

where $\tilde{\mathbf{p}} := p\mathbf{r}/r$ and we used that

$$|\mathbf{r} - \tilde{\mathbf{r}}| = \sqrt{r^2 - 2r\tilde{r}\cos(\theta) + \tilde{r}^2} = r\sqrt{1 - 2\frac{\tilde{r}}{r}\cos(\theta) + \frac{\tilde{r}^2}{r^2}} \approx r - \tilde{r}\cos(\theta) = r - \frac{\mathbf{r}\cdot\tilde{\mathbf{r}}}{r}. \tag{10}$$

Furthermore, we recognize a Fourier transform in the integral of (9). Hence

$$\psi_{\mathbf{p}}^{\pm}(\mathbf{r}) = \langle \mathbf{r} | \psi_{\mathbf{p}}^{\pm} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} \left\{ e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} + \frac{e^{\pm ipr/\hbar}}{r} f(\pm\tilde{\mathbf{p}}, \mathbf{p}) \right\}, \tag{11}$$

where

$$f(\tilde{\mathbf{p}}, \mathbf{p}) := -\frac{m}{4\pi\hbar^2} (2\pi\hbar)^3 \langle \pm\tilde{\mathbf{p}} | \hat{V} | \psi_{\mathbf{p}}^{\pm} \rangle, \tag{12}$$

is the scattering amplitude. At this moment we see the difference between the $i\epsilon$ or $-i\epsilon$. In the first case the total wavefunction is a sum of an incoming plane wave and an outgoing spherical wave. However, if we add $-i\epsilon$, we would have an incoming spherical wave. This is a time-reversed process. In this thesis we focus on $\psi_{\mathbf{p}}^{+}(\mathbf{r})$.

2.2   T matrix

For many purposes we do not need the full wavefunction but only the scattering amplitude. Therefore we introduce the operator $\hat{T}^{2B}$. This operator is known as the two-body transition or T matrix, and is defined by

$$\hat{V} | \psi_{\mathbf{p}}^{+} \rangle := \hat{T}^{2B} | \mathbf{p} \rangle. \tag{13}$$

With the help of this definition, the scattering amplitude reads

$$f(\tilde{\mathbf{k}}, \mathbf{k}) = -\frac{m}{4\pi\hbar^2} \langle \tilde{\mathbf{k}} | \hat{T}^{2B} | \mathbf{k} \rangle. \tag{14}$$

Here we introduced the wavevector $\mathbf{k} := \frac{\mathbf{p}}{\hbar}$, since wavevectors are more convenient for generalization to many-body scattering. Also for many-body physics the following normalization condition

$$\langle \tilde{\mathbf{r}} | \tilde{\mathbf{k}} \rangle = e^{i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{r}}}, \tag{15}$$

is more convenient. Note that this condition is slightly different from the one defined in (5). Furthermore by multiplying (3) with $\hat{V}$ from the left, the Lippmann-Schwinger equation changes into

$$\hat{T}^{2B} | \mathbf{k} \rangle = \hat{V} | \mathbf{k} \rangle + \hat{V} \frac{1}{E - \hat{H}_0 + i\epsilon} \hat{T}^{2B} | \mathbf{k} \rangle. \tag{16}$$

Since this equation holds for any incoming plane wave $| \mathbf{k} \rangle$, we can drop $| \mathbf{k} \rangle$. The equation for the T matrix can be solved in an iterative way. This leads to the Born series, which in the limit of $\epsilon \downarrow 0$ is given by

$$\hat{T}^{2B} = \hat{V} + \hat{V} \frac{1}{E - \hat{H}_0} \hat{V} + \hat{V} \frac{1}{E - \hat{H}_0} \hat{V} \frac{1}{E - \hat{H}_0} \hat{V} + \dots. \tag{17}$$

From this equation the physical meaning of the T matrix is clear. Since $1/(E - \hat{H}_0)$ is equal to the non-interacting atomic propagator at energy E, each term in the Born series corresponds to a collision process. If the operator $\hat{V}$ enters n times, this corresponds to scattering viewed as a n-step process. Thus the T matrix describes the outcome of a collision process, by summing over elementary interaction processes. In the Born approximation we only consider the first term of the Born series. Now define $\hat{H} = \hat{H}_0 + \hat{V}$, whose complete set of eigenstates are denoted by $|\psi_\alpha\rangle$. Then the formal solution for the transition matrix is given by

$$T^{2\mathrm{B}}(z) = \hat{V} + \hat{V}\frac{1}{z - \hat{H}}\hat{V}. \tag{18}$$

By inserting a completeness relation

$$T^{2\mathrm{B}}(z) = \hat{V} + \sum_{\mathbf{p}} \hat{V}\frac{|\psi_{\mathbf{p}}\rangle\langle\psi_{\mathbf{p}}|}{z - \epsilon_{\mathbf{p}}}\hat{V} + \int \frac{d\mathbf{q}}{(2\pi)^3}\hat{V}\frac{|\psi_{\mathbf{q}}^+\rangle\langle\psi_{\mathbf{q}}^+|}{z - \epsilon_{\mathbf{q}}}\hat{V}. \tag{19}$$

Note that there is a summation over possible bound states energies, since these energies $\epsilon_{\mathbf{p}} < 0$ are discrete. Furthermore, there is an integration over the energies $\epsilon_{\mathbf{q}} > 0$ due to the continuum of the scattering states. This expression shows that the T matrix has poles in the complex energy plane at the energy values of bound states of the potential. Also, there is a branch cut on the positive real axis due to the continuum of scattering states.

To find an explicit expression for the T matrix, we expand the wave functions in (11) in terms of spherical harmonics. Note that this expansion is unique, since the spherical harmonics form a complete orthonormal basis in the Hilbert space of square-integrable functions. So we write

$$f(\tilde{\mathbf{k}}, \mathbf{k}) = \sum_{l=0}^{\infty}(2l + 1)f_l(k)P_l(\cos(\theta)). \tag{20}$$

Note that the left-hand side does not depend on $\tilde{\mathbf{k}}$. This is because $\tilde{\mathbf{k}}$ and $\mathbf{k}$ have the same length. Therefore we only have dependence on $k = |\mathbf{k}|$, and the angle between $\mathbf{k}$ and $\mathbf{r}$. Furthermore we write

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty}(2l + 1)i^l j_l(kr)P_l(\cos(\theta)), \tag{21}$$

which asymptotically equals

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty}(2l + 1)P_l(\cos(\theta))\left\{\frac{e^{ikr} - e^{-i(kr - l\pi)}}{2ikr}\right\}. \tag{22}$$

From these expansions we observe that for $\hat{V} = 0 = f(\tilde{\mathbf{k}}, \mathbf{k})$, the scattering state is a sum of the an outgoing wave e^{ikr} and an incoming spherical wave $e^{-i(kr - l\pi)}$. The effect of turning on the potential is changing the coefficient in front of the outgoing wave. This coefficient changes as follows

$$1 \rightarrow 1 + 2ikf_l(k). \tag{23}$$

Because of unitarity or probability conservation, the magnitude of the coefficient in front of outgoing and incoming wave must be equal. Furthermore, because of rotational invariance we have angular-momentum conservation, and therefore $|1 + 2ikf_l(k)| = 1$ holds for every l. Hence

$$1 + 2ikf_l(k) = \frac{1 + ikg(k)}{1 - ikg(k)}, \tag{24}$$

or

$$f_l(k) = \frac{g(k)}{1 - ikg(k)}, \tag{25}$$

where $g(k)$ is some function of k. For cold gases the dominant amplitude is $f_0(l)$. This can be understood classically, since at low energies the particle cannot overcome the centrifugal barrier for $l \neq 0$. Furthermore, at low energies we can neglect terms which are quadratic in k. So for low energies

$$f(\tilde{\mathbf{k}}, \mathbf{k}) \approx f_0(k) = -\frac{a}{1 + ika}. \tag{26}$$

Here we used (20), the fact that $P_0(\cos(\theta)) = 1$ and the s-wave scattering length a is defined as

$$a = -\lim_{k \to 0} f_0. \tag{27}$$

Thus for low energies the T matrix reads

$$\langle \tilde{\mathbf{k}} | \hat{T}^{2B} | \mathbf{k} \rangle = T^{2B}(k) = \frac{4\pi\hbar^2}{m} \frac{a}{1 + ika}, \tag{28}$$

where (14) is used. In terms of a small positive energy E, the T matrix is given by

$$T^{2B}(E) = \frac{4\pi\hbar^2}{m} \frac{a}{1 + ia\sqrt{mE/\hbar^2}}. \tag{29}$$

And by analytic continuation

$$T^{2B}(z) = \frac{4\pi\hbar^2}{m} \frac{a}{1 - a\sqrt{-mz/\hbar^2}}, \tag{30}$$

where z is an arbitrary complex number. Clearly, for positive a the T matrix has a pole at $E_m = -\hbar^2/ma^2$ corresponding to a two-body bound state. This result does not depend on the details of the interaction potential. This is expected, since at low temperatures the thermal de Broglie wavelength is large and therefore the particle does not feel the details of the potential. Thus at low temperatures, any potential with a large positive scattering length a has a bound state slightly below to the atomic continuum.

2.3 Alkali atoms

Most experimentalists use alkali atoms to perform all kinds of experiments at low temperatures. Therefore, in this section the internal structure of alkali atoms is briefly discussed. An alkali atom can be considered as a hydrogen core with charge e and a single outer electron with charge $-e$. So to good approximation the Hamiltonian is given by

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 \hat{r}}. \tag{31}$$

Here the core is assumed to be fixed in space. This is a reasonable assumption, since the core is much heavier than the electron. Apart from the Coulomb interaction there are also other interactions. First of all, there is the spin-orbit coupling. This coupling of the spin $\hat{\mathbf{S}}$ and the orbital angular momentum $\hat{\mathbf{L}}$ of the outer electron is via the following spin-orbit Hamiltonian

$$\hat{H}_{so} = \frac{\alpha_{so}}{\hbar^2} \hat{\mathbf{L}} \cdot \hat{\mathbf{S}}. \tag{32}$$

This coupling splits the energy levels of the atom, which is known as the fine-structure splitting. Besides this spin-orbit coupling, there is also the coupling of the nuclear spin $\hat{\mathbf{I}}$ with the electron spin $\hat{\mathbf{S}}$, which is described by

$$\hat{H}_{hf} = \frac{\alpha_{hf}}{\hbar^2} \hat{\mathbf{I}} \cdot \hat{\mathbf{S}}. \tag{33}$$

This interaction leads to the so-called hyperfine splitting of the energy levels and is usually much smaller than the fine splitting. However, for cold gases most atoms are in the ground state with

$l = 0$ and therefore the fine-structure splitting is absent for cold atoms. Thus for cold gases the hyperfine splitting is the dominant effect.

Finally, there is also the coupling of the magnetic moments of the nucleus and electron to the external magnetic field. This shift is known as the Zeeman shift. Clearly this coupling is of experimental relevance as by tuning the magnetic field, the energy levels can be changed. The coupling to an external magnetic field $\mathbf{B}$ shifts the hyperfine states. By assuming the the magnetic field is directed along the z-axis, this Zeeman coupling changes the hyperfine Hamiltonian into

$$\hat{H} = \hat{H}_{\text{hf}} - \gamma_{\text{N}} B \hat{I}_z + \gamma B \hat{S}_z. \tag{34}$$

Here γ_{N} corresponds to the coupling of the nucleur spin with the magnetic field and γ is the coupling strength of the electronic spin with the external magnetic field. These coupling constants are proportional to the inverse mass and therefore $\gamma_{\text{N}} << \gamma$. Thus the coupling of the electron to the external magnetic field is the dominant Zeeman effect.

2.4 Feshbach resonance

As mentioned before in the introduction, the interaction strength of a cold Bose gases can be controlled by means of a Feshbach resonance. In order to explain these Feshbach resonances, we consider two cold alkali atoms. These atoms can be in different internal states or so-called channels. The channels are distinguished by the different quantum numbers of the internal states of the atoms. At low temperatures these channels are completely described by the spin degrees of freedom. Because alkali atoms only have one valence electron, the two cold alkali atoms can be approximately described by a two-channel model. Roughly speaking, there is one channel where the two valence electrons are in the singlet state and there is a channel where the two electrons are in the triplet state. Note that generally the singlet potential is deeper than the triplet potential. This is because in the singlet state the electrons are allowed to be on top of each other and for the triplet state this is forbidden.

The total spin in the singlet and triplet state is different, and therefore both potentials differ by a factor of $\Delta \mu B$ due to the Zeeman effect. Here $\Delta \mu$ is the difference in magnetic moment. Two cold atoms who scatter with energy $E \approx k_{\text{b}} T \ll \Delta \mu B$, in the channel with the smallest continuum energy, cannot leave this channel due to energy conservation. Therefore this channel is referred as the open channel and the other is referred as the closed channel. The two channels
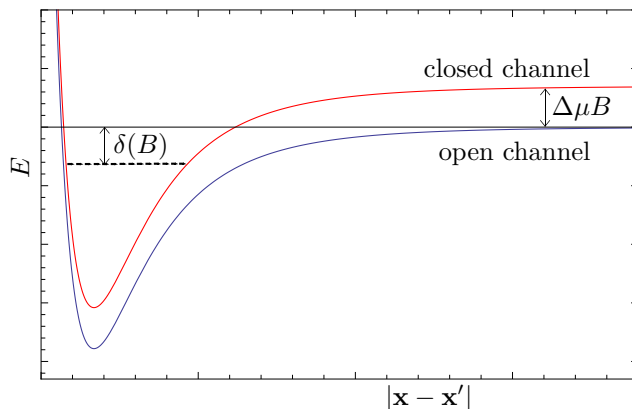

Figure 1: Schematic picture of a Feshbach resonance. The blue line is the open channel interaction potential and the red line denotes the closed channel interaction potential. The latter contains the bound state, which is denoted by the dashed line, that is responsible for the Feshbach resonance.

are coupled due to the hyperfine interaction. The closed channel is assumed to have a bound

state close to the continuum threshold of the atoms. In general the closed channel contains more than one bound state. However, by assuming that the energy difference between the bound states is larger than the thermal energy, near resonance only one bound state is important. For most atomic gases of interest this condition is satisfied. Furthermore, the difference between the energy of that bound state and the continuum threshold is denoted by $\delta(B)$. If $\delta(B)$ is equal to zero, we are on resonance. Note that δ depends linearly on the magnetic field because of the Zeeman effect. Therefore we can change the difference between the energy of the bound state and the continuum threshold of the atoms, by tuning the applied magnetic field. The situation is depicted in Figure 1.

Now consider that we have two colliding alkali atoms in the open channel. Those atoms can scatter and stay in the open channel, or they can temporarily form a molecule in the closed channel. Note that for the latter the spin state changes and therefore the outgoing particles are in a different channel then the incoming particles. Therefore this process corresponds to multi-channel scattering. The concept of the Feshbach resonance is that by tuning the external magnetic field, $\delta(B)$ can be changed and thereby the scattering properties of the atoms in the open channel can be tuned. To see that the T matrix and thus the scattering properties depend on $\delta(B)$, we start with the following microscopic action

$$S[a^*,a,b^*,b] = \sum_{\mathbf{k},n}(-i\hbar\omega_n + \epsilon_\mathbf{k} - \mu)a_{\mathbf{k},n}a^*_{\mathbf{k},n} \tag{35}$$

$$+ \sum_{\mathbf{k},n}(-i\hbar\omega_n + \epsilon_\mathbf{k}/2 + \delta(B) - 2\mu)b_{\mathbf{k},n}b^*_{\mathbf{k},n}$$

$$+ \frac{T^{2B}_{\text{bg}}}{2\hbar\beta V} \sum_{\mathbf{K},\mathbf{k},\mathbf{q},n,m,l} a^*_{\mathbf{K}/2+\mathbf{k},n/2+m}a^*_{\mathbf{K}/2-\mathbf{k},n/2-m}a_{\mathbf{K}/2+\mathbf{q},n/2+l}a_{\mathbf{K}/2-\mathbf{q},n/2-l}$$

$$+ \frac{g}{(\hbar\beta V)^{1/2}} \sum_{\mathbf{K},\mathbf{k},n,m} b^*_{\mathbf{K},n}a_{\mathbf{K}/2+\mathbf{k},n/2+m}a_{\mathbf{K/2}-\mathbf{k},n/2-m}$$

$$+ \frac{g}{(\hbar\beta V)^{1/2}} \sum_{\mathbf{K},\mathbf{k},n,m} b_{\mathbf{K},n}a^*_{\mathbf{K}/2+\mathbf{k},n/2+m}a^*_{\mathbf{K/2}-\mathbf{k},n/2-m}.$$

This action can be obtained by starting from an microscopic action which describes atoms in the open channel and the closed channel. By making a Hubbard-Stratonovich transformation to a pairing field, which describes two atoms in the closed channel and can be related to the field which describes the molecular bound state in the closed channel, we end up with the action given in (35).

The coefficients $a_{\mathbf{k},n}$ and their complex conjugates describe the atoms in the open channel. So the first part of this action corresponds to the noninteracting atoms in the open channel. The second part of the action describes the noninteracting molecules. The third term accounts for the background scattering, the interaction of the atoms in the open channel. The fourth term describes the creation of a molecule by annihilating two atoms and the last term describes the creation of two atoms by annihilating a molecule. Note that in general the coupling constant g has energy-dependence. However, the energy dependence is proportional to a_{bg}. As we will prove in a moment, close to resonance this background scattering length can be neglected. Since we are especially interested in this regime, we can take g energy independent.

To obtain the interatomic scattering properties, we have to eliminate the molecules. By performing the Gaussian integral over the molecular field, we put $i\hbar\omega_n - \epsilon_\mathbf{K}/2 + 2\mu$ equal to zero. This is allowed, since the scattering length is a property at zero energy and momentum. After performing the integration, we end up with

$$\frac{4\pi a_{\text{bg}}\hbar^2}{m} - \frac{2g^2}{\delta(B)} = \frac{4\pi a(B)\hbar^2}{m}. \tag{36}$$

where $a(B)$ is the effective interatomic scattering length. From this equation it is clear that by tuning $\delta(B)$, also the scattering properties can be varied. Thus the consequence of a Feshbach

resonance is a magnetic field dependent scattering length. This shows the experimental relevance of a Feshbach resonance. Namely, by changing the magnetic field, the interatomic interaction can be controlled. Therefore, both the weakly and strongly interacting regime can be investigated. To make contact with experiments, we write

$$a(B) = a_{\text{bg}} \left(1 - \frac{\Delta B}{B - B_0} \right), \tag{37}$$

where B_0 and ΔB are experimentally characterized. Here B_0 is defined as the position and ΔB is the so-called width of the resonance. This formula is actually confirmed experimentally and the first experimental proof is given in [4].

3   Mean-field theory of a Feshbach resonance

In the last section of the previous chapter, we wrote down a field-theoretical description of a Feshbach resonance. In this chapter we use this action to perform a mean-field theory. However, at the quadratic level the action given in (35) does not incorporate the right physics. Namely, we obtain for the molecular propagator

$$G_{\mathrm{m}}(\mathbf{k}, \omega) = \frac{\hbar}{\hbar\omega - \epsilon_{\mathbf{k}}/2 - \delta(B) + 2\mu}. \tag{38}$$

The energy of the molecular bound state is determined by the poles of this propagator. So the energy reads

$$\hbar\omega = \epsilon_{\mathbf{k}}/2 + \delta(B) - 2\mu. \tag{39}$$

As can be seen from this result, the energy of the bound state is proportional to δ. However, recall from the T-matrix formalism that the bound state energy scales as a^{-2}. Therefore, by using (36) we obtain that the energy of the bound state should be proportional to δ^2. Thus the action in (35) is not a good description of the atom-molecule system. For a better description we already have to include some interaction effects into the microscopic action, and start from that effective action. In this chapter we first consider a correction to the microscopic action, such that the effective action incorporates the physics of a Feshbach resonance. Hereafter, a mean-field theory will be discussed.

3.1   Molecular selfenergy

The molecular selfenergy is a correction to the non-interacting molecular propagator. This self-energy shifts the molecular bound-state energy due to the coupling between the open and closed channel. To derive a expression for the molecular selfenergy, we start with the action given in (35) in real space

$$
\begin{aligned}
S[\phi_{\mathrm{m}}^*, \phi_{\mathrm{m}}, \phi_{\mathrm{a}}^*, \phi_{\mathrm{a}}] = {} & \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\, \phi_{\mathrm{m}}^*(\mathbf{x}, \tau)\Big[\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\nabla^2}{4m} + \delta - 2\mu\Big]\phi_{\mathrm{m}}(\mathbf{x}, \tau) \\
& + \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\, \phi_{\mathrm{a}}^*(\mathbf{x}, \tau)\Big[\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\nabla^2}{2m} - \mu\Big]\phi_{\mathrm{a}}(\mathbf{x}, \tau) \\
& + \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\, g\Big[\phi_{\mathrm{m}}^*(\mathbf{x}, \tau)\phi_{\mathrm{a}}(\mathbf{x}, \tau)\phi_{\mathrm{a}}(\mathbf{x}, \tau) + \phi_{\mathrm{m}}(\mathbf{x}, \tau)\phi_{\mathrm{a}}^*(\mathbf{x}, \tau)\phi_{\mathrm{a}}^*(\mathbf{x}, \tau)\Big].
\end{aligned} \tag{40}
$$

Note that we neglected the background scattering, since we are interested in regions close to resonance. Diagrammatically the molecular selfenergy, up to second order in g, is given in Figure 2. Hence

$$\hbar\Sigma(\mathbf{x} - \tilde{\mathbf{x}}; \tau - \tilde{\tau}) = -\frac{g^2}{\hbar}G_0(\mathbf{x} - \tilde{\mathbf{x}}; \tau - \tilde{\tau})G_0(\mathbf{x} - \tilde{\mathbf{x}}; \tau - \tilde{\tau}), \tag{41}$$

where $G_0(\mathbf{x} - \tilde{\mathbf{x}}; \tau - \tilde{\tau})$ is the non-interacting propagator for the atoms. In Fourier space

$$
\begin{aligned}
\hbar\Sigma(\mathbf{K}; i\Omega_n) &= \frac{1}{\hbar\beta V}\int_0^{\hbar\beta} d\tau\, d\tilde{\tau}\int d\mathbf{x}\, d\tilde{\mathbf{x}}\ \hbar\Sigma(\mathbf{x} - \tilde{\mathbf{x}}; \tau - \tilde{\tau})e^{-i\mathbf{K}\cdot(\mathbf{x} - \tilde{\mathbf{x}})}e^{i\Omega_n(\tau - \tilde{\tau})} \\
&= \frac{-g^2}{\hbar^2\beta V}\sum_{\mathbf{k}, m}G_0(\mathbf{k}, i\omega_m)G_0(\mathbf{K} - \mathbf{k}, i\Omega_n - i\omega_m) \\
&= \frac{-g^2}{\hbar\beta V}\sum_{\mathbf{k}, m}\frac{G_0(\mathbf{k}, i\omega_m) + G_0(\mathbf{K} - \mathbf{k}, i\Omega_n - i\omega_m)}{-i\hbar\Omega_n + \epsilon_{\mathbf{K}-\mathbf{k}} + \epsilon_{\mathbf{k}} - 2\mu} \\
&= \frac{g^2}{V}\sum_{\mathbf{k}}\frac{1 + N_{\mathrm{BE}}(\epsilon_{\mathbf{K}-\mathbf{k}}) + N_{\mathrm{BE}}(\epsilon_{\mathbf{k}})}{-i\hbar\Omega_n - \epsilon_{\mathbf{K}-\mathbf{k}} - \epsilon_{\mathbf{k}} + 2\mu}.
\end{aligned} \tag{42}
$$

11

where in the last step contour integration is used to obtain the Bose-Einstein distribution $N_{BE}(\epsilon_{\mathbf{k}}) = 1/(e^{\beta(\epsilon_{\mathbf{k}}-\mu)} - 1)$. By setting N_{BE} equal to zero, we neglect many-body effects and obtain the two-atom molecular selfenergy in vacuum. Furthermore, by defining $\mathbf{q} = \mathbf{K}/2 - \mathbf{k}$, we
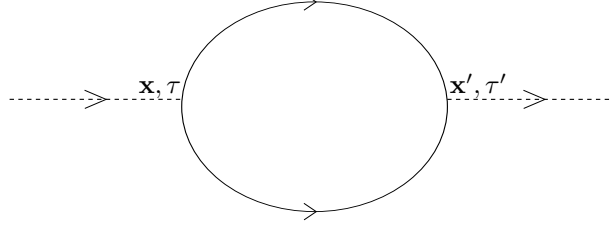

Figure 2: Feynman diagram of the molecular selfenergy. The solid lines correspond to atomic propagators and the dashed lines represent molecules.

obtain in the continuum limit

$$
\begin{aligned}
\hbar\Sigma(\mathbf{K};\Omega_n) &= \frac{g^2}{V}\sum_{\mathbf{q}}\frac{1}{-i\hbar\Omega_n - \epsilon_{\mathbf{K}/2-\mathbf{q}} - \epsilon_{\mathbf{K}/2+\mathbf{q}} + 2\mu} \\
&= g^2\int\frac{d\mathbf{q}}{(2\pi)^3}\frac{1}{-i\hbar\Omega_n - \epsilon_{\mathbf{K}/2} - 2\epsilon_{\mathbf{q}} + 2\mu}.
\end{aligned}
\tag{43}
$$

Now define $z = i\hbar\Omega_n - \epsilon_{\mathbf{K}/2} + 2\mu$. Then

$$
\hbar\Sigma(z) = \int\frac{d\mathbf{q}}{(2\pi)^3}\frac{g^2}{z - 2\epsilon_{\mathbf{q}}}.
\tag{44}
$$

As explained in the previous chapter, we are at resonance if $\delta(B)$ is equal to zero. However, the molecular selfenergy shifts the bound-state energy of the molecule and we are no longer at resonance if $\delta(B) = 0$. Therefore, we shift the molecular selfenergy with $\hbar\Sigma(0)$. Then we regain the normal resonance condition and the two-body molecular selfenergy is given by

$$
\begin{aligned}
\hbar\Sigma_{\mathrm{m}}^{2B}(z) &:= \hbar\Sigma(z) - \hbar\Sigma(0) \\
&= g^2\int\frac{d\mathbf{q}}{(2\pi)^3}\left(\frac{1}{z - 2\epsilon_{\mathbf{q}}} + \frac{1}{2\epsilon_{\mathbf{q}}}\right) \\
&= \frac{mg^2}{2\hbar^2\pi^2}z\int_0^\infty\frac{dq}{z - \frac{\hbar^2q^2}{m}}.
\end{aligned}
\tag{45}
$$

By using the method of contour integration, we obtain

$$
\hbar\Sigma_{\mathrm{m}}^{2B}(z) = \frac{m^{\frac{3}{2}}g^2}{2\pi\hbar^3}\sqrt{-z},
\tag{46}
$$

where z is an arbitrary complex number. In the following we use (46) as a definition for the molecular selfenergy. To properly account for the background scattering we should substitute $g^2 \to \frac{g^2}{1+q^2a_{bg}^2}$ in (44), see [3]. Again by using the method of contour integration, we then obtain for the two-body molecular selfenergy

$$
\hbar\Sigma_m^{2B}(z) = \frac{m^{\frac{3}{2}}g^2}{2\pi\hbar^3}\frac{\sqrt{-z}}{1 + |a_{bg}|\sqrt{-mz/\hbar^2}}.
\tag{47}
$$

3.2 Effective action

By incorporating the molecular selfenergy, the effective action reads

$$S^{\text{eff}}[a^*, a, b^*, b] = \sum_{\mathbf{k},n}(-i\hbar\omega_n + \epsilon_{\mathbf{k}} - \mu)a_{\mathbf{k},n}a^*_{\mathbf{k},n} \tag{48}$$

$$+ \sum_{\mathbf{k},n}(-i\hbar\omega_n + \epsilon_{\mathbf{k}}/2 + \delta(B) - 2\mu + \hbar\Sigma^{2\text{B}}_{\text{m}}(i\hbar\omega_n - \epsilon_{\mathbf{k}}/2 + 2\mu))b_{\mathbf{k},n}b^*_{\mathbf{k},n}$$

$$+ \frac{g^{2\text{B}}}{(\hbar\beta V)^{1/2}}\sum_{\mathbf{K},\mathbf{k},n,m}b^*_{\mathbf{K},n}a_{\mathbf{K}/\mathbf{2}+\mathbf{k},n/2+m}a_{\mathbf{K}/\mathbf{2}-\mathbf{k},n/2-m}$$

$$+ \frac{g^{2\text{B}}}{(\hbar\beta V)^{1/2}}\sum_{\mathbf{K},\mathbf{k},n,m}b_{\mathbf{K},n}a^*_{\mathbf{K}/\mathbf{2}+\mathbf{k},n/2+m}a^*_{\mathbf{K}/\mathbf{2}-\mathbf{k},n/2-m},$$

Note that (48) is an effective action in the sense that all two-body ladder diagrams are taken into account. Also the coupling $g^{2\text{B}}$ is renormalized, by taking into account all two-body ladder diagrams. For the details we refer to [3]. By including this molecular selfenergy, the retarded molecular propagator changes into

$$G^+_{\text{m}}(\mathbf{k}, \omega) = \frac{\hbar}{\hbar\omega + i\epsilon - \epsilon_{\mathbf{k}}/2 - \delta(B) + 2\mu - \hbar\Sigma^{2\text{B}}_{\text{m}}(\hbar\omega - \epsilon_{\mathbf{k}}/2 + 2\mu + i\epsilon)}, \tag{49}$$

where ϵ goes to zero. Note that the molecular selfenergy only contains diagrams up to order g^2, but by writing

$$\begin{aligned}
G^+_{\text{m}} &= \frac{1}{G^{-1}_0 - \hbar\Sigma^{2\text{B}}_{\text{m}}} \tag{50}\\
&= G_0\frac{1}{1 - \hbar\Sigma^{2\text{B}}_{\text{m}}G_0}\\
&= G_0 + G_0\hbar\Sigma^{2\text{B}}_{\text{m}}G_0 + G_0\hbar\Sigma^{2\text{B}}_{\text{m}}G_0\hbar\Sigma^{2\text{B}}_{\text{m}}G_0 + \dots,
\end{aligned}$$

we see that the two-body molecular ladder diagrams are indeed incorporated. Here the argument of the molecular selfenergy is omitted for notational convenience. Furthermore $G^{-1}_0 = \hbar\omega - \epsilon_{\mathbf{k}}/2 - \delta(B) + 2\mu$ denotes the non-interacting molecular propagator. The energy of the molecular state is determined by solving the following equation for x

$$x - \delta(B) - \hbar\Sigma^{2\text{B}}_{\text{m}}(x) = 0. \tag{51}$$

First note that for positive detunings $\delta(B)$, this equation only has a solution with a nonzero negative imaginary part. This is expected, since for positive detunings the energy of the molecule is larger than the two-atom continuum threshold. Therefore this solution corresponds to the decay of a molecule into two atoms, where the negative imaginary part is related to the lifetime of the molecule. In contrast, for negative detunings there is a real negative solution corresponding to the bound-state energy of the molecule. By substituting $y = \sqrt{-x}$, (51) changes into

$$y^2 + \delta(B) + \alpha y = 0. \tag{52}$$

Here $\alpha = m^{\frac{3}{2}}g^2/2\pi\hbar^3$. Hence

$$\begin{aligned}
y &= \frac{\alpha}{2}\left(-1 \pm \sqrt{1 - \frac{4\delta}{\alpha^2}}\right) \tag{53}\\
&= \frac{\alpha}{2}\left(-1 + \sqrt{1 + \frac{8\pi\hbar^4}{m^2g^2a(B)}}\right),
\end{aligned}$$

where we used (36) for $a_{\text{bg}} = 0$. Note that in the second step we have to choose the solution with the plus-sign, because $y = \sqrt{-x} > 0$. In the experimentally interesting case of broad Feshbach

resonances, when $\delta \to \infty$ and $g^2 \to \infty$, this expression simplifies to

$$y = \frac{1}{2}\left(-\alpha + \left(\alpha + \frac{2\hbar}{a(B)\sqrt{m}}\right)\right). \tag{54}$$

So in the limit of $\delta \to \infty$ and $g^2 \to \infty$, the solution for the bound state reads

$$E_b = -\frac{\hbar^2}{ma(B)^2}. \tag{55}$$

Thus instead of the microscopic action described in the previous section, the effective action of (48) correctly describes the molecular bound state. In the next section this effective action is used to obtain the mean-field equations.

3.3 Mean-field equations

The mean-field equations describe the equilibrium properties of the atomic and the molecular condensate. To obtain these equations, we should substitute $a_{\mathbf{0},0} \to a_{\mathbf{0},0} + \phi_a \sqrt{\hbar \beta V}$ and $b_{\mathbf{0},0} \to b_{\mathbf{0},0} + \phi_m \sqrt{\hbar \beta V}$ into the action and demand that the linear terms in the fluctuations $a_{\mathbf{k},n}$ and $b_{\mathbf{k},n}$ vanish. Here ϕ_m and ϕ_a describe respectively the molecular and atomic condensate. By using the action in (48), we obtain the following mean-field equations

$$\mu \phi_a = 2g^{2\mathrm{B}} \phi_a^* \phi_m, \tag{56}$$
$$2\mu \phi_m = (\delta(B) + \hbar \Sigma_m^{2\mathrm{B}}(2\mu - 2\hbar \Sigma^{\mathrm{HF}}))\phi_m + g^{2B} \phi_a^2. \tag{57}$$

Here the Hartree-Fock selfenergy of the non-condensed atoms is introduced. This selfenergy is the mean-field energy felt by the non-condensed atoms due to the presence of the atomic condensate. Due to this effect the argument of the molecular selfenergy should be evaluated at $2\mu - 2\hbar \Sigma^{\mathrm{HF}}$. This is because by looking at (44), the Hartree-Fock selfenergy shifts the internal energy of the non-condensed atoms from $\epsilon_{\mathbf{k}}$ to $\epsilon_{\mathbf{k}} + \hbar \Sigma^{\mathrm{HF}}$. Thus for the condensate, where $\omega_n = \epsilon_{\mathbf{k}} = 0$, we
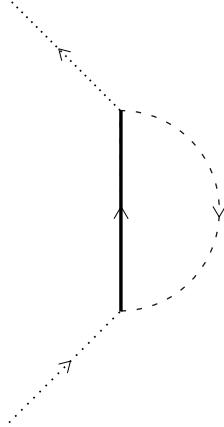

Figure 3: Diagrammatic representation of the Hartree-Fock selfenergy of the atoms. The dotted lines are non-condensed atoms. The dashed line is the propagator of condensed atoms. Furthermore the solid line correspond to the full molecular propagator.

have to evaluate the molecular selfenergy at $2\mu - 2\hbar \Sigma^{\mathrm{HF}}$. Diagrammatically this Hartree-Fock selfenergy is shown in Figure 3. Thus the Hartree-Fock selfenergy is given by

$$\hbar \Sigma^{\mathrm{HF}} = \frac{4n_a |g^{2\mathrm{B}}|^2}{\hbar \Sigma^{\mathrm{HF}} + \mu - \delta(B) - \hbar \Sigma_m^{2\mathrm{B}}(\mu - \hbar \Sigma^{\mathrm{HF}})}, \tag{58}$$

where $n_{\mathrm{a}} = |\phi_{\mathrm{a}}|^2$ is the density of condensed atoms. Note that the argument of the molecular selfenergy is different from the first factor in the numerator. To explain this, we first recall that the molecular propagator is given by

$$\hbar G_{\mathrm{m}} = \frac{1}{E - \delta(B) - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(E)}. \tag{59}$$

As we want to describe a Feshbach resonance, the Hartree-Fock selfenergy is evaluated at the continuum energy. Therefore, the energy of a non-condensed atom is equal to $\hbar\Sigma^{\mathrm{HF}}$. Because the energy of a condensed atom is μ, we should evaluate the molecular propagator at $\mu + \hbar\Sigma^{\mathrm{HF}}$. However, the molecular selfenergy contains an integral over internal energy. This internal energy is shifted with the Hartree-Fock selfenergy, $\epsilon_{\mathbf{k}} \to \epsilon_{\mathbf{k}} + \hbar\Sigma^{\mathrm{HF}}$ in (45), and therefore the molecular selfenergy is evaluated at $\mu - \hbar\Sigma^{\mathrm{HF}}$.

There is also a physical reason to include this Hartree-Fock selfenergy. The molecular bound state is only stable if the energy of a condensed molecule is smaller than the continuum threshold of two atoms in vacuum. A condensed molecule has energy 2μ. Because for the Bose-condensed phase the chemical potential is larger than zero, the energy of the molecular condensate is also larger than zero. Without the incorporation of the Hartree-Fock selfenergy, the energy of the condensed molecule is larger than the continuum threshold of the atoms. Therefore the molecule decays into two atoms and this is not a stable solution of the mean-field equations. However, by including the Hartree-Fock selfenergy the continuum threshold is shifted by an amount of $2\hbar\Sigma^{\mathrm{HF}}$. Because this Hartree-Fock selfenergy appears to be larger than the chemical potential, which will be shown in section 3.5, the energy of the condensed molecule is smaller than the continuum threshold of two atoms. So by including the Hartree-Fock selfenergy, we also expect a (meta)stable solution of the mean-field equations consisting of an atomic condensate.

3.4 Densities

In this section we have a closer look at the different equilibrium solutions of the mean-field equations. So, we determine the density of condensed molecules and atoms as a function of the chemical potential. For a fixed chemical potential, (56) and (57) have the following solutions

1. $n_{\mathrm{a}} = 0$ and $n_{\mathrm{m}} = 0$.

2. $n_{\mathrm{a}} = 0$ and $2\mu - \delta - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(2\mu - 2\hbar\Sigma^{\mathrm{HF}}) = 0$.

3. $n_{\mathrm{a}} = \frac{\mu}{2g^2}\left(2\mu - \delta - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(2\mu - 2\hbar\Sigma^{\mathrm{HF}})\right)$ and $n_{\mathrm{m}} = \frac{\mu^2}{4g^2}$.

Here we assumed that $g \neq 0$ and in the third case $2\mu - \delta - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(2\mu - 2\hbar\Sigma^{\mathrm{HF}}) \neq 0$. The first case is the trivial solution. In the second case $2\mu - \delta - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(2\mu - 2\hbar\Sigma^{\mathrm{HF}}) = 0$. First notice that $n_a = 0$ implies that $\Sigma^{\mathrm{HF}} = 0$ according to (58). Thus $2\mu - \delta - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(2\mu - 2\hbar\Sigma^{\mathrm{HF}}) = 0$ simplifies to

$$2\mu - \delta(B) - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(2\mu) = 0, \tag{60}$$

which is the same equation as we already solved in section 3.2. Recall that this equation only has a real solution if the detuning δ is negative. For negative detunings

$$\mu = -\frac{\hbar^2}{2m(a(B))^2} = \frac{1}{2}E_{\mathrm{b}}, \tag{61}$$

in the limit of $g^2 \to \infty$. Again for positive detuning we get an imaginary chemical potential, corresponding to the instability of the molecules. This case corresponds to the situation where we have a molecular condensate and there are no condensed atoms. Because the chemical potential of the molecules is the same as the molecular bound state, the number of condensed molecules is macroscopically large. This is the real ground state of our system, since for negative detunings the energy of condensed molecules is lower than the energy of condensed atoms.

To get a better understanding of this atom-molecule system, we focus now on Figure 4. This figure shows the energy as a function of the detuning. For negative detunings there is a molecular branch at negative energy and an atomic continuum at positive energy. By looking at Figure 4, we expect that there are two solutions of the mean-field equations. The first solution is the real groundstate of the system where there is a condensate of molecules. Furthermore, since we included this Hartree-Fock selfenergy, we also expect a metastable solution where we have a condensate of atoms. Because the chemical potential determines the density, since at low temperatures particles with energies far above the chemical potential get exponentially suppressed, we expect two different chemical potentials that satisfy the mean-field equations. There should be a chemical potential around the molecular branch and the other one is around the atomic continuum. In the next section we show that there indeed is a solution of the chemical
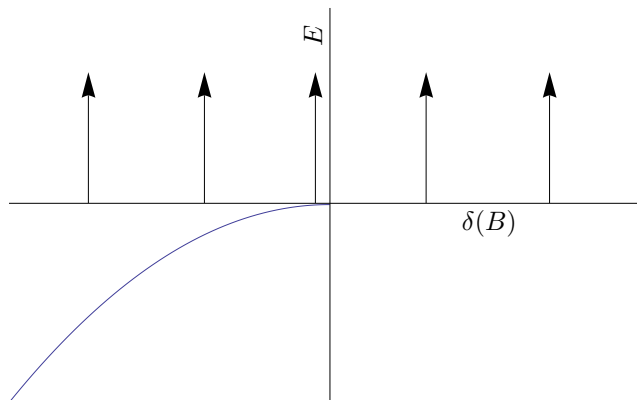

Figure 4: The energy as a function of the detuning δ. The blue curve corresponds to the molecular bound state energy and the arrows denote that there is a atomic continuum for positive energies.

potential which is around the atomic continuum. In this section we found the solution where the chemical potential is at the molecular branch, which corresponds to the solution of a condensate of molecules. Thus, there are indeed two different solutions of the mean-field equations. Also in case 3

$$\frac{n_{\mathrm{m}}}{n_{\mathrm{a}}} = \frac{\mu}{2} \frac{1}{2\mu - \delta - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(2\mu - 2\hbar\Sigma^{\mathrm{HF}})}. \tag{62}$$

By using (46), we observe that this ratio goes to zero for a fixed chemical potential and $g^2 \to \infty$ and $\delta \to \infty$. Therefore the molecular density is zero in the limit of a broad Feshbach resonance and the two-channel model reduces to a single-channel model. Still the situation is different from a normal single-channel model, because for a broad Feshbach resonance the molecular bound state causes a magnetic-field dependent scattering length.

3.5 Chemical potential

In the previous section we found that the true ground state of the system is a condensate of molecules. However, we are interested in the metastable situation of an atomic condensate. Thus we consider case 3, where $2\mu - \delta(B) - \Sigma_{\mathrm{m}}^{2\mathrm{B}}(2\mu - 2\hbar\Sigma^{\mathrm{HF}}) \neq 0$, and obtain the following coupled equations

$$\mu = \frac{2n_a(g^{2\mathrm{B}})^2}{2\mu - \delta(B) - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(2\mu - 2\hbar\Sigma^{\mathrm{HF}})}, \tag{63}$$

$$\hbar\Sigma^{\mathrm{HF}} = \frac{4n_a(g^{2\mathrm{B}})^2}{\hbar\Sigma^{\mathrm{HF}} + \mu - \delta(B) - \hbar\Sigma_{\mathrm{m}}^{2\mathrm{B}}(\mu - \hbar\Sigma^{\mathrm{HF}})}, \tag{64}$$

16

where the molecular selfenergy is given in equation (46). In this thesis we are especially interested in the experimentally relevant broad Feshbach resonances, where $g^2 \to \infty$. However, because of (36) we can only take this limit if we also send $\delta(B) \to \infty$ and keep the ratio g^2/δ constant. Furthermore, to compare the results with experiments it is more convenient to solve the mean-field equations for the chemical potential at fixed molecular and atomic densities. Therefore, (63) and (64) are solved for the Hartree-Fock selfenergy and the chemical potential at fixed densities. Thus we define a Fermi momentum k_F and energy ϵ_F, such that $n_a = k_F^3/6\pi^2$ and $m/\hbar^2 = k_F^2/2\epsilon_F$. Then in the limit of a broad Feshbach resonance, the mean-field equations change into

$$\mu = \frac{\epsilon_F}{3\pi} \frac{4k_F a}{1 - k_F a \sqrt{-(\mu - \hbar\Sigma^{HF})/\epsilon_F}}, \tag{65}$$

$$\hbar\Sigma^{HF} = \frac{\epsilon_F}{3\pi} \frac{8k_F a}{1 - k_F a \sqrt{-(\mu - \hbar\Sigma^{HF})/2\epsilon_F}}. \tag{66}$$

To proceed further, these equations are rewritten as one equation for $z := (\hbar\Sigma^{HF} - \mu)/\epsilon_F$

$$z = \frac{4k_F a}{3\pi} \cdot \frac{2(1 - k_F a\sqrt{z}) - (1 - k_F a\sqrt{z/2})}{(1 - k_F a\sqrt{z})(1 - k_F a\sqrt{z/2})}. \tag{67}$$

This equation is solved numerically and subsequently this solution is substituted into (65) and (66), to obtain the mean-field chemical potential and Hartree-Fock selfenergy. These mean-field quantities are given in Figure 5. Note that the chemical potential is positive and the Hartree-Fock
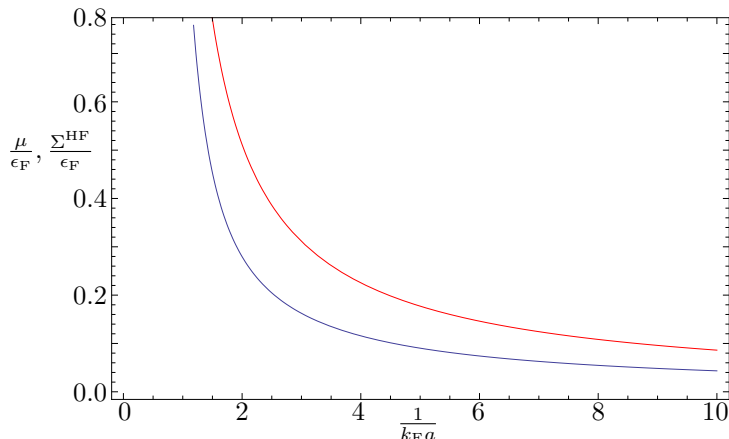
Figure 5: The chemical potential μ and the Hartree-Fock selfenergy Σ^{HF} in units of the Fermi energy ϵ_F as a function of the inverse scattering length $1/k_F a$. The red and the blue curve correspond to respectively the Hartree-Fock selfenergy and the chemical potential μ.

selfenergy is larger than the chemical potential. Hence, this is an equilibrium solution of the mean-field equations. There is also another well-known mean-field result for the energy of a cold Bose gas. This result for the energy per particle is given

$$e = \frac{4\pi\hbar^2}{ma^2} na^3 \Big(1 + \frac{128}{15\pi}\sqrt{na^3} + ...\Big). \tag{68}$$

The first term is the Gross-Pitaevskii result and the second term is the Lee-Huang-Yang correction [5]. This correction is due to the depletion of the condensate. The result of (68) is obtained from a ϕ^4-theory, which describes Bose-Einstein condensation. In contrast to our theory, this theory only consists of atoms. As we can see from Figure 6, the result of our mean-field theory coincides with this result for small $k_F a$. For large $k_F a$ both diverge, but there difference between both curves increases. This shows that the incorporation of the molecules is important for large scattering lengths. By using the definitions of the density and mass, we obtain that the Gross-Pitaevskii
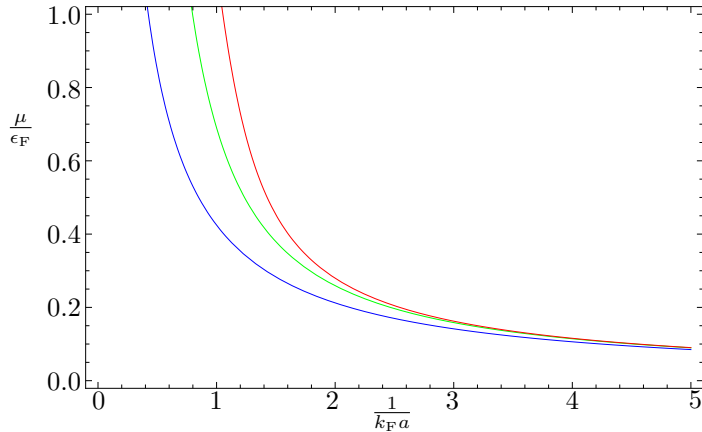
17

Figure 6: The red line shows the chemical potential μ in units of the Fermi energy ϵ_F as a function of the inverse scattering length $1/k_\mathrm{F}a$. The green curve corresponds to the Bogoliubov result from equation 68 with the LHY correction and the blue curve is without this correction. Just as the Bogoliubov result, our two-channel mean-field result diverges in the unitary limit.

result for the energy per particle in units of the Fermi energy ϵ_F, diverges as $4k_\mathrm{F}a/3\pi$.

Now the question arises if we can determine the divergence of our mean field result. By looking at Figure 7, we observe that $p := z(k_\mathrm{F}a)^2 = (k_\mathrm{F}a)^2(\hbar\Sigma^{\mathrm{HF}} - \mu)/\epsilon_\mathrm{F}$ is constant for large $k_\mathrm{F}a$. Thus (67) can be rewritten as

$$\frac{p}{(k_\mathrm{F}a)^3} = \frac{4}{3\pi} \cdot \frac{2(1 - \sqrt{z}) - (1 - \sqrt{z/2})}{(1 - \sqrt{z})(1 - \sqrt{z/2})}. \tag{69}$$

Because p is constant for large $k_\mathrm{F}a$, the left-handside of this equation tends to zero as $k_\mathrm{F}a \to \infty$. Thus by solving for which z the right-handside is equal to zero, we can determine the value of z in the unitarity limit. By substituting this result into (65), we obtain

$$\mu = \frac{4k_\mathrm{F}a}{3\pi}(3 + \sqrt{2}), \tag{70}$$

for large $k_\mathrm{F}a$. Thus our mean-field chemical potential diverges even faster than the Gross-Pitaevskii result. The divergence of the energy for large $k_\mathrm{F}a$ is unphysical. However, in our in a mean-field
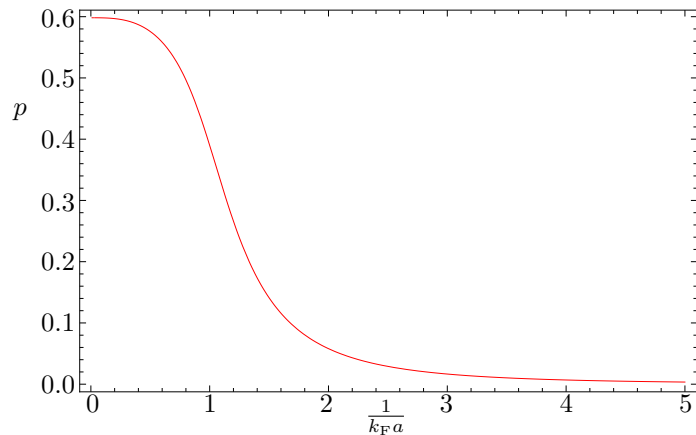

Figure 7: The quantity $p := (k_\mathrm{F}a)^2(\hbar\Sigma^{\mathrm{HF}} - \mu)$ as a function of the inverse scattering length $1/k_\mathrm{F}a$. The value of p is constant in the limit of $1/k_\mathrm{F}a \to 0$.

theory this divergence maybe an artifact of taking the limit of $g^2 \to \infty$ and $\delta(B) \to \infty$. Therefore

18

we will now have a look at the case when g is finite. This corresponds to realistic cases, since g is finite in all experiments. First define
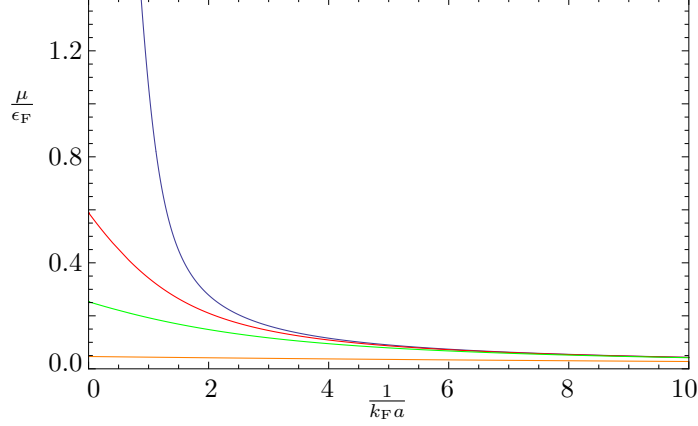

Figure 8: The chemical potential μ as a function of the inverse scattering length $1/k_{\mathrm{F}}a$ for different values for η. The values for η are $10, 1, 0.5, 0.1$ for respectively the blue, red, green and orange lines.

$$\eta^2 = \frac{g^2 m^{3/2}}{4\pi\hbar^3} = \sqrt{\frac{\epsilon_{\mathrm{F}}}{2}} \frac{g^2 m^2}{2\pi\hbar^4} (6\pi^2 n_a)^{-1/3} := \sqrt{\frac{\epsilon_{\mathrm{F}}}{2}} \tilde{\eta}^2, \tag{71}$$

where $\tilde{\eta}^2$ is dimensionless. Furthermore

$$\frac{1}{k_{\mathrm{F}}a} = -\frac{\bar{\delta}}{\tilde{\eta}^2}. \tag{72}$$

where (36) is used and the bar means a division through ϵ_{F}, thus $\bar{x} = x/\epsilon_{\mathrm{F}}$ for a variable x. Hence

$$\bar{\mu} = \frac{4}{3\pi} \frac{\tilde{\eta}^2}{2\bar{\mu} + \frac{\tilde{\eta}^2}{k_{\mathrm{F}}a} - \tilde{\eta}^2\sqrt{-(\mu - \Sigma^{\mathrm{HF}})}}, \tag{73}$$

$$\hbar\bar{\Sigma}^{\mathrm{HF}} = \frac{8}{3\pi} \frac{\tilde{\eta}^2}{\bar{\Sigma}^{\mathrm{HF}} + \bar{\mu} + \frac{\tilde{\eta}^2}{k_{\mathrm{F}}a} - \frac{1}{\sqrt{2}}\tilde{\eta}^2\sqrt{-(\mu - \Sigma^{\mathrm{HF}})}}.$$

These equations are solved numerically and the result is given in Figure 9. For small η the chemical potential remains finite in the unitary limit. However, in the limit of $g^2 \to \infty$ or similarly $\tilde{\eta}^2 \to \infty$, we regain the divergence of the chemical potential.

4 Bogoliubov Theory

In the mean-field theory described in the previous chapter, we have a divergence of the chemical potential at resonance. However, in this calculation depletion of the condensate is not incorporated. Note that this depletion of the condensate is due to quantum and thermal fluctuations. Thus to improve on the mean-field result, we consider the effective action in (48) up to second order in Gaussian fluctuations. This is known as the Bogoliubov approximation.

4.1 Collective excitation spectrum

In this Bogoliubov approximation, we first study the collective excitation spectrum over the ground state. The quadratic part of the action can be written as

$$S^{\text{eff}}[a^*, a, b^*, b] = \sum_{\mathbf{k},n}(-i\hbar\omega_n + \epsilon_\mathbf{k} - \mu)a_{\mathbf{k},n}a^*_{\mathbf{k},n} \tag{74}$$

$$+ \sum_{\mathbf{k},n}(-i\hbar\omega_n + \epsilon_\mathbf{k}/2 + \delta(B) - 2\mu + \hbar\Sigma^{\text{2B}}_{\text{m}}(i\hbar\omega_n - \epsilon_\mathbf{k}/2 + 2\mu - 2\hbar\Sigma^{\text{HF}}))b_{\mathbf{k},n}b^*_{\mathbf{k},n}$$

$$+ g^{\text{2B}} \sum_{\mathbf{k},n} \left(\phi^*_\text{m}a_{\mathbf{k},n}a_{-\mathbf{k},-n} + 2\phi_\text{a}b^*_{\mathbf{k},n}a_{\mathbf{k},n} \right)$$

$$+ g^{\text{2B}} \sum_{\mathbf{k},n} \left(\phi_\text{m}a^*_{\mathbf{k},n}a^*_{-\mathbf{k},-n} + 2\phi^*_\text{a}b_{\mathbf{k},n}a^*_{\mathbf{k},n} \right).$$

Recall that we obtained this part of this action, quadratic in the fluctuations, by substituting $a_{\mathbf{0},0} \to a_{\mathbf{0},0} + \phi_\text{a}\sqrt{\hbar\beta V}$ and $b_{\mathbf{0},0} \to b_{\mathbf{0},0} + \phi_\text{m}\sqrt{\hbar\beta V}$ in (48). Note that we also incorporated the Hartree-Fock selfenergy. Now define

$$\begin{aligned} G^{-1}_\text{a}(\mathbf{k}, i\omega_n) &= -i\hbar\omega_n + \epsilon_\mathbf{k} - \mu, \\ G^{-1}_\text{m}(\mathbf{k}, i\omega_n) &= i\hbar\omega_n - \epsilon_\mathbf{k}/2 + 2\mu - \delta(B) - \hbar\Sigma^{\text{2B}}_\text{m}(i\hbar\omega_n - \epsilon_\mathbf{k}/2 + 2\mu - 2\hbar\Sigma^{\text{HF}}). \end{aligned} \tag{75}$$

For simplicity, we integrate out the molecules and end up with

$$S_\text{B}[a^*, a] = \sum_{\mathbf{k},n} u^\dagger_{\mathbf{k},n} \cdot G^{-1}_\text{B}(\mathbf{k}, i\omega_n) \cdot u_{\mathbf{k},n}, \tag{76}$$

where

$$u_{\mathbf{k},n} := \left[\begin{array}{c} a_{\mathbf{k},n} \\ a^*_{-\mathbf{k},-n} \end{array} \right], \tag{77}$$

and

$$G^{-1}_\text{B}(\mathbf{k}, i\omega_n) = \frac{1}{2}\left[\begin{array}{cc} G^{-1}_\text{a}(\mathbf{k}, i\omega_n) & 0 \\ 0 & G^{-1}_\text{a}(\mathbf{k}, -i\omega_n) \end{array} \right] \tag{78}$$

$$+ \frac{1}{2}\left[\begin{array}{cc} 4|\phi_\text{a}|^2(g^{\text{2B}})^2 G_\text{m}(\mathbf{k}, i\omega_n) & 2\phi^2_\text{a}(g^{\text{2B}})^2 G_\text{m}(\mathbf{0}, 0) \\ 2(\phi^*_\text{a})^2(g^{\text{2B}})^2 G_\text{m}(\mathbf{0}, 0) & 4|\phi_\text{a}|^2(g^{\text{2B}})^2 G_\text{m}(\mathbf{k}, -i\omega_n) \end{array} \right].$$

From these equations, we see that integrating out the molecular field results in an effective T matrix for the atoms in the open channel of the form

$$T^{\text{MB}} = 4|\phi_\text{a}|^2(g^{\text{2B}})^2 G_\text{m}(\mathbf{k}, i\omega_n) \tag{79}$$

As we already proved in chapter 3, close to resonance the molecular Green's function has a pole at the bound state energy given by (55). Therefore, for large scattering lengths also the effective T matrix has a pole at the bound-state energy. Recall that this is expected from the formal definition of the T matrix in (19). Also note that in the expressions above, the chemical potential is equal to the mean-field result given in (63) and as a first approximation we use $n = n_a = k^3_\text{F}/6\pi^2$. Thus we neglect the contribution of the non-condensed particles.

Again we are interested in the limit of $g \to \infty$ and $\delta \to \infty$, while keeping the ratio g^2/δ constant. The spectrum of the collective excitations over the ground state is determined by the quasi-particle dispersion relations. This system has roughly two different dispersions. There is a Bogoliubov dispersion of the form

$$\hbar\omega \approx \pm\sqrt{\epsilon_{\mathbf{k}}^2 + \frac{8\pi a\hbar^2 n_{\mathrm{a}}}{m}\epsilon_{\mathbf{k}}}, \tag{80}$$

where a is equal to the full scattering length $a(B)$. Physically, this dispersion corresponds to phonon-like excitations. Furthermore, we also have a solution of the form

$$\hbar\omega \approx \pm\left(-\frac{2}{(k_{\mathrm{F}}a)^2} + \epsilon_{\mathbf{k}}/2\right). \tag{81}$$

This corresponds to atom-molecule oscillations, for example pairs of atoms moving between the atomic and molecular condensate. In the discussion above we focused on the real part of the dispersions. However, the dispersions also have a nonzero imaginary part. This imaginary part can be negative and positive, where the former corresponds to decay and the latter to exponential growth. As a final remark, also note the action before and after integrating out the molecules contain the same dispersions. Namely, by writing the action before integrating out the molecules as a 4×4-matrix structure, we obtain that this determinant is proportional to the determinant of $G_{\mathrm{B}}^{-1}(\mathbf{k}, \omega)$.

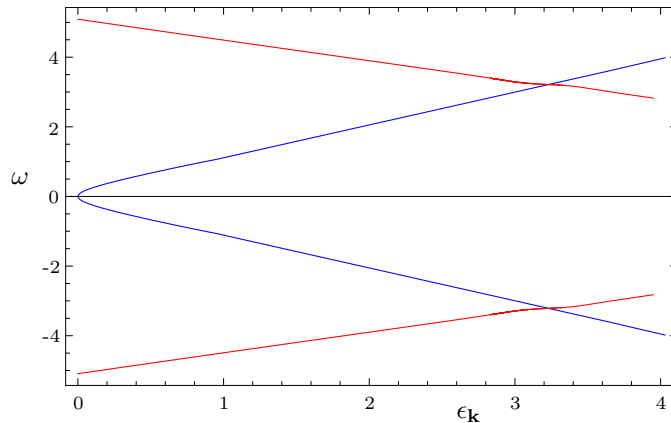Figure 9: The two dispersions, given in (80) and (81), as a function of $\epsilon_{\mathbf{k}}$ for $1/k_{\mathrm{F}}a = 1.51$.

4.2 The spectral-weight function

To calculate some physical quantities we have to determine the spectral-weight function. This function is also often called the spectral function and is defined by

$$\rho(\mathbf{k}, \omega) = \frac{1}{\hbar\pi}\mathrm{Im}[G^{\mathrm{ret}}(\mathbf{k}, \omega^+)], \tag{82}$$

where $\omega^+ = \omega + i\epsilon$ and ϵ goes to zero. The spectral function can be seen as the single-particle density of states as it gives the energies, amplitudes and lifetimes of the states accessible to a particle with momentum $\mathbf{k}$ in the presence of a medium. Note that this definition is only valid for systems without spin, but it can also be generalized to systems with spin. By using the Lehmann representation [10], we have that for bosons the spectral function should be positive for $\omega > 0$ and negative for $\omega < 0$. There is also an intuitive argument, why the spectral function should satisfy this condition. Namely, the expectation value of the number of particles can be obtained by multiplying the spectral function with the Bose-Einstein distribution function, followed by

an integration over ω. Since the Bose-Einstein distribution function is positive for $\omega > 0$ and negative for $\omega < 0$, the spectral function should have the same behaviour. Otherwise we can get the unphysical result of a negative density. Furthermore, for the atoms the spectral-weight function should satisfy

$$\int d(\hbar\omega)\rho(\mathbf{k},\omega) = 1, \tag{83}$$

which is known as the frequency sum-rule. This rule is a consequence of the canonical commutation relations. In this case we can obtain the retarded Green's function by substituting $i\omega_n = \omega + i\epsilon$ in (78), where ϵ goes to zero. Note that we are only interested in G_{11}, since this corresponds to the normal average. Numerical plots of the spectral function of the Bogoliubov theory is given in Figure 10.

In these figures we can see some general features of the excitation spectrum over the ground state. First of all, for small momenta, we clearly have the four different contributions already discussed in the previous section. Furthermore, there is also another contribution between roughly $\hbar\omega = \epsilon_{\mathrm{F}}$ and $\hbar\omega = 2\,\epsilon_{\mathrm{F}}$. This corresponds to a contribution of the molecular density of states of the two-atom continuum [3]. There is also a similar contribution at the corresponding negative values for ω, but this contribution is so small that it is not visible in the figure. For larger momenta,
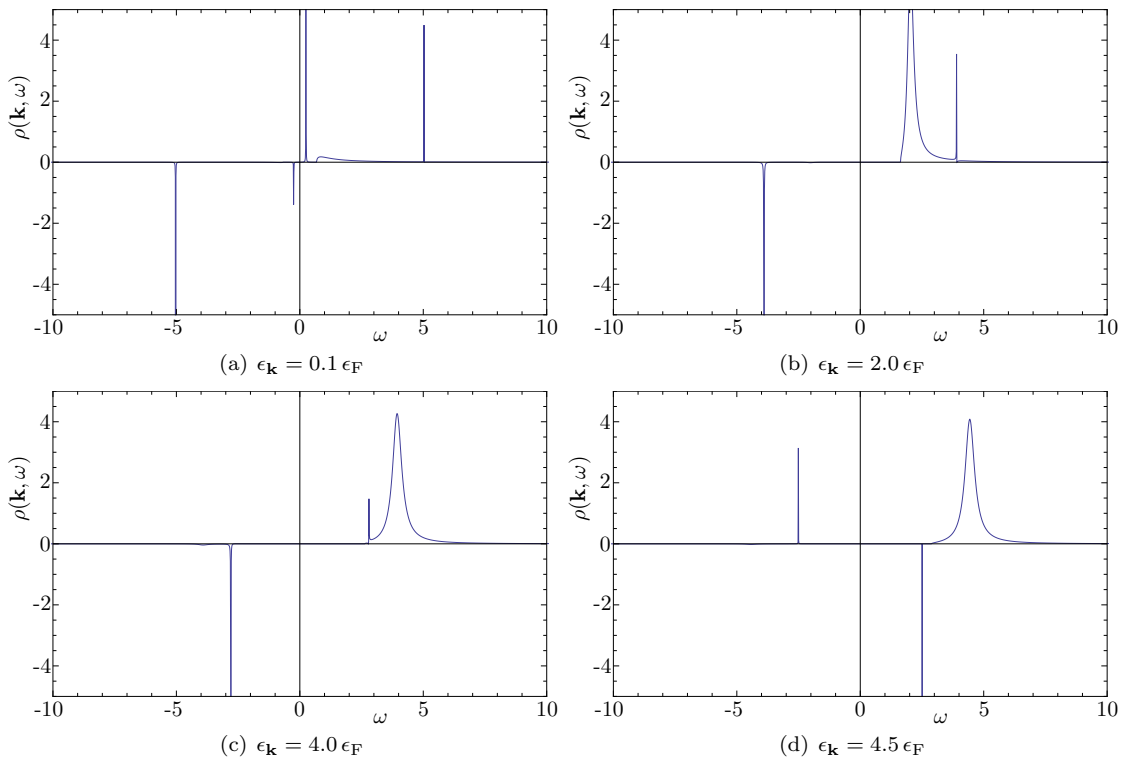

Figure 10: Numerical plots of the spectral function of the atom-molecule system over the ground-state in the limit of $g \to \infty$, $\delta \to \infty$ while keeping the ratio constant. In the plots $\epsilon = 10^{-4}$, $1/k_{\mathrm{F}}a = 1.51$ and the value of $\epsilon_{\mathbf{k}}/\epsilon_{\mathrm{F}}$ varies from 0.1 to 4.5.

this contribution merges with the contribution of the Bogoliubov dispersions. Furthermore, the contribution of the pole at the molecular bound-state energy moves through this phonon-like contribution. After they have crossed, the molecular contribution switches sign. This means that there is a region where the spectral function becomes negative for $\omega > 0$ and positive for $\omega < 0$. Furthermore, this spectral function also does not satisfy the sum rule. This is a direct

consequence of the fact that we have a dispersion with a positive imaginary part. Namely, the sum rule follows from the fact that for large ω, the spectral function behaves as $1/\omega$. Therefore, by using contour integration where the contour is closed in the upper complex plane, we have that the spectral function only satisfies the sum rule, if there are no poles in the upper complex plane.

5 Phonon model

In the previous chapter we found a spectral function for which the peaks of the spectral function have the wrong sign. Furthermore, we did not always satisfy the sum-rule. As explained before, this has to do with the complex dispersions with positive imaginary part. To get a better understanding of this problem we therefore now consider another model, where also dispersions with positive imaginary parts arise. This is a model consisting of atoms and phonons, which are linearly coupled.

5.1 Dispersion relations

The system of linearly coupled atoms and phonons is described by the following action

$$
\begin{aligned}
S[\psi^*, \psi, \phi] &= \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\, \psi^*(\mathbf{x}, \tau)\Big[\hbar\frac{\partial}{\partial\tau} - \nabla^2 + \Delta\Big]\psi(\mathbf{x}, \tau) \\
&+ \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\, \phi(\mathbf{x}, \tau)\Big[-\hbar^2\frac{\partial^2}{\partial\tau^2} - c^2\nabla^2\Big]\phi(\mathbf{x}, \tau) \\
&+ g\sqrt{2}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\Big[\psi^*(\mathbf{x}, \tau) + \psi(\mathbf{x}, \tau)\Big]\phi(\mathbf{x}, \tau).
\end{aligned}
\tag{84}
$$

Here c is a constant and $\hbar/2m$ is put equal to one. The phonon field is real, because it originates from a classical field that describes displacements of atoms. Furthermore, $-\Delta$ plays the role of a chemical potential. For non-interacting Bose gases the chemical potential is non-positive and therefore only cases with $\Delta > 0$ are considered. Notice that there is no chemical potential for the phonons. This is because phonons can be created or annihilated by random energy fluctuations and therefore there is no energy cost to add or remove a phonon from the system. Finally, g is the coupling between the phonons and the atoms, and the factor $\sqrt{2}$ is introduced for notational convenience. Now define

$$
\psi(\mathbf{x}, t) := \frac{1}{\sqrt{\hbar\beta V}}\sum_{\mathbf{k}, n} a_{\mathbf{k}, n}e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_n\tau)},
\tag{85}
$$

$$
\phi(\mathbf{x}, t) := \frac{1}{\sqrt{\hbar\beta V}}\sum_{\mathbf{k}, n} b_{\mathbf{k}, n}e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_n\tau)},
\tag{86}
$$

where $\omega_n = \pi(2n)/\hbar\beta$ are the bosonic Matsubara frequencies. Then in Fourier space the action reads

$$
\begin{aligned}
S[a^*, a, b^*, b] &= \sum_{\mathbf{k}, n}(-i\hbar\omega_n + \mathbf{k}^2 + \Delta)a_{\mathbf{k}, n}^* a_{\mathbf{k}, n} \\
&+ \sum_{\mathbf{k}, n}((\hbar\omega_n)^2 + c^2\mathbf{k}^2)b_{\mathbf{k}, n}^* b_{\mathbf{k}, n} + g\sqrt{2}\sum_{\mathbf{k}, n}(a_{\mathbf{k}, n}b_{\mathbf{k}, n}^* + a_{\mathbf{k}, n}^* b_{\mathbf{k}, n}).
\end{aligned}
\tag{87}
$$

By considering the partition sum we can integrate out the phonons and end up with an effective action for the atoms. Thus

$$
\begin{aligned}
Z[a^*, a] &= \prod_{\mathbf{k}, n}\int d[b_{\mathbf{k}, n}]e^{-S[a^*, a, b]/\hbar} \\
&= \prod_{\mathbf{k}\geq 0, n\geq 0}'\int d[b_{\mathbf{k}, n}]d[b_{\mathbf{k}, n}^*]d[b_{\mathbf{0}, 0}]e^{-S[a^*, a, b^*, b]/\hbar} \\
&:= e^{-S^{\text{eff}}[a^*, a]/\hbar},
\end{aligned}
\tag{88}
$$

where we used that $b_{-\mathbf{k},-n} = b^*_{\mathbf{k},n}$, since ϕ is real. Furthermore, the prime indicates that in the product there is no term with $\mathbf{k}$ and n equal to zero. Now write

$$
\begin{aligned}
S[a^*, a, b^*, b] &= \frac{1}{2} \sum_{\mathbf{k},n} \left((-i\hbar\omega_n + \mathbf{k}^2 + \Delta) a^*_{\mathbf{k},n} a_{\mathbf{k},n} + (i\hbar\omega_n + \mathbf{k}^2 + \Delta) a^*_{-\mathbf{k},-n} a_{-\mathbf{k},-n} \right) \quad (89) \\
&+ 2 \sideset{}{'}\sum_{\mathbf{k}\geq 0, n\geq 0} ((\hbar\omega_n)^2 + c^2\mathbf{k}^2) b^*_{\mathbf{k},n} b_{\mathbf{k},n} \\
&+ g\sqrt{2} \sideset{}{'}\sum_{\mathbf{k}\geq 0, n\geq 0} (a_{\mathbf{k},n} b^*_{\mathbf{k},n} + b_{\mathbf{k},n} a_{-\mathbf{k},-n} + a^*_{\mathbf{k},n} b_{\mathbf{k},n} + b^*_{\mathbf{k},n} a^*_{-\mathbf{k},-n}) \\
&+ g\sqrt{2}(a_{\mathbf{0},0} b_{\mathbf{0},0} + a^*_{\mathbf{0},0} b_{\mathbf{0},0}),
\end{aligned}
$$

where the prime again indicates that we do not sum over the term with $\mathbf{k}$ and n equal to zero. From now on we will neglect this zero mode. Then by performing the Gaussian integral we end up with

$$
S^{\text{eff}}[a^*, a] = \frac{1}{2} \sideset{}{'}\sum_{\mathbf{k},n} u^*_{\mathbf{k},n} \mathbf{G}^{-1} u_{\mathbf{k},n}, \quad (90)
$$

where

$$
u_{\mathbf{k},n} := \begin{bmatrix} a_{\mathbf{k},n} \\ a^*_{-\mathbf{k},-n} \end{bmatrix}, \quad (91)
$$

and

$$
\mathbf{G}^{-1}(\mathbf{k}, i\omega_n) = \begin{bmatrix} -i\hbar\omega_n + \mathbf{k}^2 + \Delta - \frac{g^2}{(\hbar\omega_n)^2 + c^2\mathbf{k}^2} & -\frac{g^2}{(\hbar\omega_n)^2 + c^2\mathbf{k}^2} \\ -\frac{g^2}{(\hbar\omega_n)^2 + c^2\mathbf{k}^2} & i\hbar\omega_n + \mathbf{k}^2 + \Delta - \frac{g^2}{(\hbar\omega_n)^2 + c^2\mathbf{k}^2} \end{bmatrix}. \quad (92)
$$

Because we neglected the zero mode, there is no term with $\mathbf{k} = 0$ and $n = 0$ in the effective action. Furthermore, there is also a constant coming from the Gaussian integration. However, in the end we are always interested in thermodynamic quantities which are independent of this constant. Therefore, this constant is neglected. The poles of this interacting Green's function
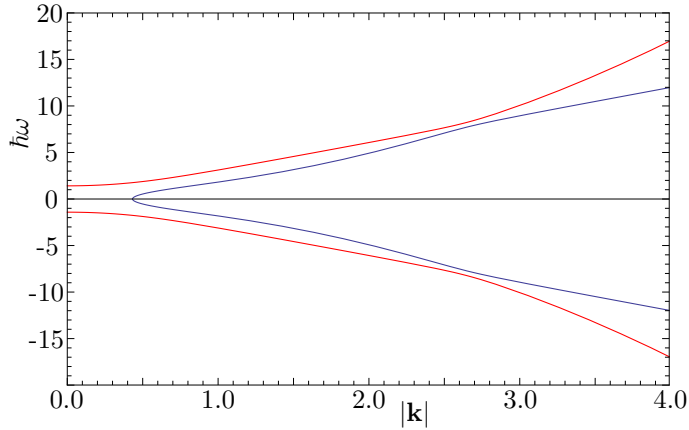

Figure 11: The dispersions of the atom-phonon model for $c = 3$, $g = 1$ and $\Delta = 1$. The blue curves correspond to $\pm\hbar\omega_-$ and the red lines denote $\pm\hbar\omega_+$. Furthermore, if $|\mathbf{k}|$ is smaller than roughly 0.4 the former becomes purely imaginary.

$G(\mathbf{k}, \omega)$ correspond to energies of the quasiparticle excitations of the many-body system. Thus the quasiparticle dispersion relations are determined by solving $\det[G^{-1}(\mathbf{k}, \omega)] = 0$ for $\hbar\omega$. The four solutions are given by

$$
\hbar\omega_{\sigma',\sigma} = \frac{\sigma'}{\sqrt{2}} \sqrt{c^2\mathbf{k}^2 + (\mathbf{k}^2 + \Delta)^2 + \sigma\sqrt{8g^2(\mathbf{k}^2 + \Delta) + (-c^2\mathbf{k}^2 + (\mathbf{k}^2 + \Delta)^2)^2}} := \sigma'\hbar\omega_\sigma, \quad (93)
$$

where σ and σ' are equal to ± 1. The dispersion relations are shown in Figure 11 for certain values of c, g and Δ.

In the limit of $g \to 0$ there are two phonon dispersion relations $\hbar\omega = \pm c|\mathbf{k}|$ and two atomic dispersions $\hbar\omega = \pm(\mathbf{k}^2 + \Delta)$. However, for some finite g the situation is different. In this case, the dispersions for large $|\mathbf{k}|$ are close to the dispersion for the decoupled system, but for small $|\mathbf{k}|$ the picture is different. Apart from the avoided crossing that normally occurs for a system with non-zero coupling between two internal states, there is a region where the dispersions $\hbar\omega_-$ are purely imaginary. This means that there is some instability in this system.

To understand this instability we first consider the classical situation of a harmonic oscillator which is linear coupled to a free particle. Schematically the potential of that system will look like

$$V(x, y) = \alpha x^2 + \beta x \cdot y, \tag{94}$$

for some non-trivial constants $\alpha > 0$ and β. Clearly the only extremum of this potential occurs at the origin. Whether this extremum is a maximum, minimum or saddle point, determines if this extremum is stable or unstable. By completing the square, the potential in (94) can be rewritten as

$$V(x, y) = \alpha \left(x + \frac{\beta}{2\alpha} y \right)^2 - \frac{\beta^2}{4\alpha} y^2. \tag{95}$$

Thus we end up with two harmonic oscillators. Due to this minus sign in front of the second term, the potential has a saddle point at the origin and therefore there is instability. In our field-theoretical model of the atom-phonon model there is a similar situation. The phonons are harmonic oscillators coupled to some other field, in this case a field describing atoms. By rewriting (87)

$$
\begin{aligned}
S[a^*, a, b^*, b] &= \sum_{\mathbf{k},n} \left\{ \mathbf{k}^2 + \Delta \right\} \left| a_{\mathbf{k},n} + \frac{g\sqrt{2}}{\mathbf{k}^2 + \Delta} b_{\mathbf{k},n} \right|^2 + \sum_{\mathbf{k},n} -i\hbar\omega_n a^*_{\mathbf{k},n} a_{\mathbf{k},n} \\
&+ \sum_{\mathbf{k},n} \left\{ (\hbar\omega_n)^2 + c^2 \mathbf{k}^2 - \frac{2g^2}{\mathbf{k}^2 + \Delta} \right\} |b_{\mathbf{k},n}|^2,
\end{aligned}
\tag{96}
$$

we observe that if

$$(\mathbf{k}^2 + \Delta)c^2\mathbf{k}^2 < 2g^2, \tag{97}$$

or equivalently for

$$\mathbf{k}^2 < \frac{1}{2} \left\{ -\Delta + \sqrt{\Delta^2 + \frac{8g^2}{c^2}} \right\}, \tag{98}$$

there is a minus-sign in front of the harmonic potential of the phonons. As explained before this corresponds to an instability. Therefore, this explains why for small $|\mathbf{k}|$ there are imaginary solutions. The exact analytic expressions for the dispersions, given by the $\hbar\omega_{\pm,-}$ in (93), show that (98) is indeed the criterium for the dispersions to become purely imaginary. Notice that in the limit of $g \to 0$ the above condition is never satisfied and all dispersions are real. Therefore, these imaginary dispersions are an effect of the coupling between the phonons and atoms.

5.2 Solving the quantum field theory

From Figure 11 it is clear that there are two different regions. For small $|\mathbf{k}|$ there are imaginary dispersions and for large $|\mathbf{k}|$ all dispersion are real. Therefore, we write

$$
\begin{aligned}
\psi(\mathbf{x}, t) &= \psi_<(\mathbf{x}, t) + \psi_>(\mathbf{x}, t) \tag{99} \\
\phi(\mathbf{x}, t) &= \phi_<(\mathbf{x}, t) + \phi_>(\mathbf{x}, t) \tag{100}
\end{aligned}
$$

for respectively the atomic and phonon field. Here the subscript $<$ denotes the low-momentum part with $|\mathbf{k}| < |\mathbf{k_1}|$, and the subscript $>$ corresponds to the high-momentum part with $|\mathbf{k}| > |\mathbf{k_1}|$. Furthermore, $\mathbf{k_1}$ is the momentum for which $\hbar\omega_- = 0$. Now we first focus on the region where all dispersions are real.

5.2.1 Real dispersions

In the region where all dispersions are real, the effective action of the atom-phonon model can be diagonalized by a Bogoliubov transformation. Therefore, new fields $d_{\mathbf{k},n}$ and $d^*_{\mathbf{k},n}$ are introduced via the transformation

$$\begin{bmatrix} d_{\mathbf{k},n} \\ d^*_{-\mathbf{k},-n} \end{bmatrix} := \begin{bmatrix} u^*_{\mathbf{k}} & -v^*_{\mathbf{k}} \\ -v_{\mathbf{k}} & u_{\mathbf{k}} \end{bmatrix} \cdot \begin{bmatrix} a_{\mathbf{k},n} \\ a^*_{-\mathbf{k},-n} \end{bmatrix}. \tag{101}$$

In the corresponding operator formalism $d_{\mathbf{k},n}$ and $a_{\mathbf{k},n}$ are bosonic operators. Therefore, both should satisfy the standard bosonic commutation relations. Hence,

$$\begin{aligned} 1 &= [\hat{d}_{\mathbf{k},n}, \hat{d}^*_{-\mathbf{k},-n}] \tag{102}\\ &= [u^*_{\mathbf{k}}\hat{a}_{\mathbf{k},n} - v^*_{\mathbf{k}}\hat{a}^*_{-\mathbf{k},-n}, -v_{\mathbf{k}}\hat{a}_{\mathbf{k},n} + u_{\mathbf{k}}\hat{a}^*_{-\mathbf{k},-n}] \\ &= (|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2)[\hat{a}_{\mathbf{k},n}, \hat{a}^*_{-\mathbf{k},-n}] \\ &= |u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2. \end{aligned}$$

Thus the fact that the operators must satisfy the normal bosonic commutation relations gives a normalization condition on the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. These coefficients are the non-trivial solution to the following equation

$$\mathbf{G}^{-1}(\mathbf{k},\omega) \begin{bmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{bmatrix} = 0, \tag{103}$$

where the inverse Green's function on the left-hand side is evaluated at $i\hbar\omega_n = \sigma'\hbar\omega_\sigma$. The non-trivial solution is given by

$$u_{\mathbf{k},\sigma',\sigma} = \alpha(\mathbf{k}^2 + \Delta + \sigma'\hbar\omega_\sigma), \tag{104}$$
$$v_{\mathbf{k},\sigma',\sigma} = \alpha(\mathbf{k}^2 + \Delta - \sigma'\hbar\omega_\sigma), \tag{105}$$

where α is a normalization constant. This constant is determined by the normalization constraint stated in (102). Hence,

$$2|\alpha|^2(\mathbf{k}^2 + \Delta)(\sigma'\hbar\omega_\sigma + \sigma'\hbar\omega^*_\sigma) = 1. \tag{106}$$

Clearly, if $\sigma'\hbar\omega_\sigma$ is negative this normalization equation cannot be satisfied and therefore these solutions are neglected in first instance. Thus from now on we only consider $\sigma'\hbar\omega_\sigma := \hbar\omega_\sigma$. Before we go to the operator formalism, we need a completeness relation to make a mode expansion. Therefore we first discuss some properties of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. Note that $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are found by solving (103) or

$$\begin{bmatrix} \mathbf{k}^2 + \Delta + \frac{g^2}{(\hbar\omega)^2 - c^2\mathbf{k}^2} & \frac{g^2}{(\hbar\omega)^2 - c^2\mathbf{k}^2} \\ \frac{g^2}{(\hbar\omega)^2 - c^2\mathbf{k}^2} & \mathbf{k}^2 + \Delta + \frac{g^2}{(\hbar\omega)^2 - c^2\mathbf{k}^2} \end{bmatrix} \begin{bmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{bmatrix} = \hbar\omega \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{bmatrix}, \tag{107}$$

where $\hbar\omega$ is equal to one of the four possibilities of $\hbar\omega_{\sigma,\sigma'}$. Due to the fact that on the right-hand side of this equation there is a matrix unequal to the identity matrix, an inner product is defined as

$$\begin{aligned} (k,l) &:= \int d^3\mathbf{x}\, k^\dagger(\mathbf{x})l(\mathbf{x}) \tag{108}\\ &= \int d^3\mathbf{x} \begin{bmatrix} k_1(\mathbf{x}) \\ k_2(\mathbf{x}) \end{bmatrix}^\dagger \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} l_1(\mathbf{x}) \\ l_2(\mathbf{x}) \end{bmatrix} \\ &= \int d^3\mathbf{x} \left\{ k^*_1(\mathbf{x})l_1(\mathbf{x}) - k^*_2(\mathbf{x})l_2(\mathbf{x}) \right\}. \end{aligned}$$

Mathematically this cannot be seen as a proper inner product. This is because (k, k) can be negative and therefore this inner product is called an indefinite inner product. Also (k, k) can be zero if $k(\mathbf{x})$ is non-zero. Nevertheless it is convenient for our purposes. Now define

$$
x_{\mathbf{k},\sigma}(\mathbf{x}) = \begin{bmatrix} u_{\mathbf{k},\sigma} \\ v_{\mathbf{k},\sigma} \end{bmatrix} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}}, \tag{109}
$$

$$
y_{\mathbf{k},\sigma}(\mathbf{x}) = \begin{bmatrix} v_{\mathbf{k},\sigma}^* \\ u_{\mathbf{k},\sigma}^* \end{bmatrix} \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}}. \tag{110}
$$

By using this definition, we observe that if $x_{\mathbf{k},\sigma}(\mathbf{x})$ is an eigenvector with eigenvalue $\hbar\omega_\sigma$, then $y_{\mathbf{k},\sigma}(\mathbf{x})$ is an eigenvector with eigenvalue $-\hbar\omega_\sigma^*$. Furthermore, by using (102) the orthogonality condition of the eigenvectors reads

$$
(x_{\mathbf{k},\sigma}, y_{\mathbf{k}',\sigma}) = 0, \tag{111}
$$

$$
(x_{\mathbf{k},\sigma}, x_{\mathbf{k}',\sigma}) = \delta_{\mathbf{k}\mathbf{k}'}, \tag{112}
$$

$$
(y_{\mathbf{k},\sigma}, y_{\mathbf{k}',\sigma}) = -\delta_{\mathbf{k}\mathbf{k}'}. \tag{113}
$$

And the completeness relation equals

$$
\sum_{\mathbf{k}>|\mathbf{k}_1|} \left\{ u_{\mathbf{k},\sigma}(\mathbf{x}_1) u_{\mathbf{k},\sigma}^*(\mathbf{x}_2) - v_{\mathbf{k},\sigma}^*(\mathbf{x}_1) v_{\mathbf{k},\sigma}(\mathbf{x}_2) \right\} = \sum_{\mathbf{k}>|\mathbf{k}_1|} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}}{\sqrt{V}}. \tag{114}
$$

Notice that there is a completeness relation for both pairs of eigenvectors. By integrating out the phonons, the Fourier transformed Hamiltonian depends on ω. However, we switch to a Hamiltonian where ω is replaced by ω_σ. This corresponds to expanding the Hamiltonian in terms of eigenstates. Because substituting ω_+ or ω_- results in different Hamiltonians, there are two Hamiltonians. In the operator formalism the solution is given by a linear superposition of the eigenstates of both Hamiltonians. Thus,

$$
\begin{bmatrix} \hat{\psi}_>(\mathbf{x}, t) \\ \hat{\psi}_>^\dagger(\mathbf{x}, t) \end{bmatrix} := \sum_{\mathbf{k}>|\mathbf{k}_1|,\sigma\in\{+,-\}} E_{\mathbf{k},\sigma} \left\{ \hat{d}_{\mathbf{k},\sigma}(t) \begin{bmatrix} u_{\mathbf{k},\sigma}(\mathbf{x}) \\ v_{\mathbf{k},\sigma}(\mathbf{x}) \end{bmatrix} + \hat{d}_{\mathbf{k},\sigma}^\dagger(t) \begin{bmatrix} v_{\mathbf{k},\sigma}^*(\mathbf{x}) \\ u_{\mathbf{k},\sigma}^*(\mathbf{x}) \end{bmatrix} \right\}. \tag{115}
$$

Here, $\hat{d}_{\mathbf{k},\sigma}$ and $\hat{d}_{\mathbf{k},\sigma}^\dagger$ are bosonic creation and annihilation operators. Note that for a complex field, the operators in front of the two terms do not have to be related. However, in this case they are related by complex conjugates, which follows from (101). Furthermore, the explicit time dependence of the creation and annihilation operators is obtained from the Heisenberg equation of motion, which reads

$$
\frac{d}{dt}\hat{A}(t) = \frac{i}{\hbar}[\hat{H}, \hat{A}(t)], \tag{116}
$$

for any observable $\hat{A}(t)$. By performing the Bogoliubov transformation the action and thereby the Hamiltonian of the system becomes diagonal in the new operators $\hat{d}_{\mathbf{k},\sigma}$ and $\hat{d}_{\mathbf{k},\sigma}^*$. Thus

$$
[\hat{H}, \hat{d}_{\mathbf{p},\sigma}^\dagger] = \sum_{\mathbf{k}>|\mathbf{k}_1|} \hbar\omega_\sigma \left[\hat{d}_{\mathbf{k},\sigma}^\dagger \hat{d}_{\mathbf{k},\sigma}, \hat{d}_{\mathbf{p},\sigma}^\dagger \right] = \hbar\omega_\sigma \hat{d}_{\mathbf{p},\sigma}^\dagger, \tag{117}
$$

and

$$
[\hat{H}, \hat{d}_{\mathbf{p},\sigma}] = \sum_{\mathbf{k}>|\mathbf{k}_1|} \hbar\omega_\sigma \left[\hat{d}_{\mathbf{k},\sigma}^\dagger \hat{d}_{\mathbf{k},\sigma}, \hat{d}_{\mathbf{p},\sigma} \right] = -\hbar\omega_\sigma \hat{d}_{\mathbf{p},\sigma}. \tag{118}
$$

Hence

$$
\hat{d}_{\mathbf{p},\sigma}^\dagger(t) = \hat{d}_{\mathbf{p},\sigma}^\dagger e^{i\omega_\sigma t}, \tag{119}
$$

$$
\hat{d}_{\mathbf{p},\sigma}(t) = \hat{d}_{\mathbf{p},\sigma} e^{-i\omega_\sigma t}. \tag{120}
$$

Thus

$$\left[\begin{array}{c} \hat{\psi}_>(\mathbf{x}, t) \\ \hat{\psi}_>^\dagger(\mathbf{x}, t) \end{array} \right] := \sum_{\mathbf{k} > |\mathbf{k}_1|, \sigma \in \{+, -\}} E_{\mathbf{k}, \sigma} \left(\hat{d}_{\mathbf{k}, \sigma} e^{-i\omega_\sigma t} \left[\begin{array}{c} u_{\mathbf{k}, \sigma}(\mathbf{x}) \\ v_{\mathbf{k}, \sigma}(\mathbf{x}) \end{array} \right] + \hat{d}_{\mathbf{k}, \sigma}^\dagger e^{i\omega_\sigma t} \left[\begin{array}{c} v_{\mathbf{k}, \sigma}^*(\mathbf{x}) \\ u_{\mathbf{k}, \sigma}^*(\mathbf{x}) \end{array} \right] \right). \quad (121)$$

Recall that in this expression

$$u_{\mathbf{k}, \sigma}(\mathbf{x}) = \alpha_{\mathbf{k}, \sigma}(\mathbf{k}^2 + \Delta + \hbar\omega_\sigma) \frac{e^{i\mathbf{k} \cdot \mathbf{x}}}{\sqrt{V}} := u_{\mathbf{k}, \sigma} \frac{e^{i\mathbf{k} \cdot \mathbf{x}}}{\sqrt{V}}, \quad (122)$$

$$v_{\mathbf{k}, \sigma}(\mathbf{x}) = \alpha_{\mathbf{k}, \sigma}(\mathbf{k}^2 + \Delta - \hbar\omega_\sigma) \frac{e^{i\mathbf{k} \cdot \mathbf{x}}}{\sqrt{V}} := v_{\mathbf{k}, \sigma} \frac{e^{i\mathbf{k} \cdot \mathbf{x}}}{\sqrt{V}}. \quad (123)$$

Here

$$\alpha_{\mathbf{k}, \sigma} = \frac{1}{\sqrt{4\hbar\omega_\sigma((\mathbf{k}^2 + \Delta))}}, \quad (124)$$

such that (106) is satisfied. To solve the whole model we also have to find an expression for the phonon field operator. However, due to the fact that we integrated out the phonons, this information is lost. Therefore, we now interchange the role of the atoms and phonons. So we start from the action given in (87) and integrate out the atoms. By performing this Gaussian integral we end up with the following effective action for the phonons

$$\begin{aligned} S^{\text{eff}}[b^*, b] &:= \frac{1}{2} \sum_{\mathbf{k}, n} G_{\text{ph}}^{-1} b_{\mathbf{k}, n} b_{-\mathbf{k}, -n} \quad (125) \\ &= \sum_{\mathbf{k}, n} \left\{ -(i\hbar\omega_n)^2 + c^2 \mathbf{k}^2 + \frac{2g^2(\mathbf{k}^2 + \Delta)}{(i\hbar\omega_n)^2 - (\mathbf{k}^2 + \Delta)^2} \right\} b_{\mathbf{k}, n} b_{-\mathbf{k}, -n}, \end{aligned}$$

where again the constant $\text{Tr}[\log(\mathbf{G}^{-1})]$ is neglected. Furthermore the poles of G_{ph} are the same as the poles of the Green's function of the theory where the atoms were integrated out. In the operator formalism

$$\hat{\phi}_>(\mathbf{x}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k} > |\mathbf{k}_1|, \sigma \in \{+, -\}} F_{\mathbf{k}, \sigma} \left(\hat{d}_{\mathbf{k}, \sigma} e^{i(\mathbf{k} \cdot \mathbf{x} - \omega_\sigma t)} + \hat{d}_{\mathbf{k}, \sigma}^\dagger e^{-i(\mathbf{k} \cdot \mathbf{x} - \omega_\sigma t)} \right). \quad (126)$$

Note that in this mode expansion the same operators as in (121), the operator expansion for the atomic field, are used. This is because in both cases the dispersions are the same, and therefore both field operators create or annihilate the same excitations. Hence, both mode expansions consist of the same operators.

5.2.2 Imaginary dispersions

Now we consider the region in which there are two imaginary solutions. Again we switch to the operator formalism. First recall that for an imaginary dispersion, the normalization constant $K_{\mathbf{k}, \sigma', \sigma}$, which follows from (106), cannot be chosen such that the new operators $d_{\mathbf{k}, n}^*$ and $d_{\mathbf{k}, n}$ still satisfy bosonic commutation relations. This is because for an imaginary dispersion, the norm of the eigenvectors $x_{\mathbf{k}, \sigma, -}$ is equal to zero. This fact can be proved mathematically. Namely, solving our eigenvalue equation corresponds to solving

$$W_{\mathbf{k}} z_{\mathbf{k}} = \sigma' \hbar\omega_\sigma z_{\mathbf{k}}, \quad (127)$$

where the matrix $W_{\mathbf{k}}$ is of the form

$$W_{\mathbf{k}} = \left[\begin{array}{cc} L & -M \\ M & -L \end{array} \right], \quad (128)$$

and

$$z_{\mathbf{k}} = \left[\begin{array}{c} u_{\mathbf{k}} \\ -v_{\mathbf{k}} \end{array} \right]. \quad (129)$$

For the exact expression of L and M we refer to (107). We find

$$(\sigma' \hbar \omega_\sigma)^*(z, z) = (Wz, z) = (z, Wz) = \sigma' \hbar \omega_\sigma(z, z). \tag{130}$$

Here we used that

$$(Wz, z) = \int d^3\mathbf{x} (W(\mathbf{x})z(\mathbf{x}))^\dagger \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} z(\mathbf{x}) \tag{131}$$

$$= z_\mathbf{k}^\dagger \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} W_\mathbf{k}^\dagger \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} z_\mathbf{k} \tag{132}$$

$$= z_\mathbf{k}^\dagger \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} W_\mathbf{k} z_\mathbf{k} = (z, Wz). \tag{133}$$

Because $\sigma' \hbar \omega_\sigma \neq \sigma' \hbar \omega_\sigma^*$ we have that $(z, z) = 0$. This proves that a normal Bogoliubov transformation cannot diagonalize our action. Therefore we have to come up with a different approach, which is based on [6].

For a mode expansion of the field operators we need a completeness relation. To obtain the completeness relation we adjust the normalization condition as follows

$$(z_{\mathbf{k},+,-}, z_{\mathbf{k},-,-}) = 1. \tag{134}$$

Recall that the imaginary part of the eigenvalue of the eigenvector $z_{\mathbf{k},+,-}$ is positive, while it is negative for $z_{\mathbf{k},-,-}$. This implies for the normalization constants $K_{\mathbf{k},\sigma',-}$

$$K_{\mathbf{k},+,-}^* K_{\mathbf{k},-,-} \left\{ 4(\mathbf{k}^2 + \Delta)\hbar\omega_- \right\} = 1, \tag{135}$$

where the definition of $x_{\mathbf{k},\sigma',\sigma}$ in (109) is used. So we choose

$$K_{\mathbf{k},-,-} = K_{\mathbf{k},+,-}^* = \frac{1}{\sqrt{4(\mathbf{k}^2 + \Delta)\hbar\omega_-}} = \frac{e^{i\frac{\pi}{4}}}{\sqrt{4(\mathbf{k}^2 + \Delta)|\hbar\omega_-|}}. \tag{136}$$

With this normalization condition the completeness relation for the complex modes is given by

$$\frac{1}{2} \sum_{\mathbf{k} < |\mathbf{k}_1|} \left\{ u_{\mathbf{k},+,-}(\mathbf{x}_1) u_{\mathbf{k},-,-}^*(\mathbf{x}_2) - v_{\mathbf{k},+,-}^*(\mathbf{x}_1) v_{\mathbf{k},-,-}(\mathbf{x}_2) + \right. \tag{137}$$

$$\left. u_{\mathbf{k},-,-}(\mathbf{x}_1) u_{\mathbf{k},+,-}^*(\mathbf{x}_2) - v_{\mathbf{k},-,-}^*(\mathbf{x}_1) v_{\mathbf{k},+,-}(\mathbf{x}_2) \right\} = \sum_{\mathbf{k} < |\mathbf{k}_1|} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_1 - \mathbf{x}_2)}}{\sqrt{V}}.$$

Furthermore,

$$\frac{1}{2} \sum_{\mathbf{k} < |\mathbf{k}_1|} \left\{ u_{\mathbf{k},+,-}(\mathbf{x}_1) v_{\mathbf{k},-,-}^*(\mathbf{x}_2) - v_{\mathbf{k},+,-}^*(\mathbf{x}_1) u_{\mathbf{k},-,-}(\mathbf{x}_2) + \right. \tag{138}$$

$$\left. u_{\mathbf{k},-,-}(\mathbf{x}_1) v_{\mathbf{k},+,-}^*(\mathbf{x}_2) - v_{\mathbf{k},-,-}^*(\mathbf{x}_1) u_{\mathbf{k},+,-}(\mathbf{x}_2) \right\} = 0.$$

The completeness relation can be checked by subtracting (138) multiplied by $v_{\mathbf{k},+,-}(\mathbf{x}_2)$ from (137) multiplied with $u_{\mathbf{k},+,-}(\mathbf{x}_2)$, followed by integration over $\mathbf{x}_2$. To verify the whole completeness relation, we have to do this trick for all different $u_{\mathbf{k},\sigma',-}(\mathbf{x}_2)$ and $u_{\mathbf{k},\sigma',-}(\mathbf{x}_2)$. Recall that in these expressions $u_{\mathbf{k},\sigma',-}(\mathbf{x})$ and $v_{\mathbf{k},\sigma',-}(\mathbf{x})$ are given by

$$u_{\mathbf{k},\sigma',-}(\mathbf{x}) = K_{\mathbf{k},\sigma',-}(\mathbf{k}^2 + \Delta + \sigma'\hbar\omega_-)\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} := \tilde{u}_{\mathbf{k},\sigma'}\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} = \tilde{u}_{\mathbf{k},\sigma'}(\mathbf{x}), \tag{139}$$

$$v_{\mathbf{k},\sigma',-}(\mathbf{x}) = K_{\mathbf{k},\sigma',-}(\mathbf{k}^2 + \Delta - \sigma'\hbar\omega_-)\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} := \tilde{v}_{\mathbf{k},\sigma'}\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} = \tilde{v}_{\mathbf{k},\sigma'}(\mathbf{x}). \tag{140}$$

Therefore,

$$\tilde{v}_{\mathbf{k},\sigma'}^*(\mathbf{x}) = \pm e^{i\frac{\pi}{2}} \tilde{u}_{-\mathbf{k},\sigma'}(\mathbf{x}). \tag{141}$$

30

Thus the completeness relation can be rewritten as

$$-i \sum_{\mathbf{k}<|\mathbf{k}_1|} \left\{ \tilde{u}_{\mathbf{k},+}(\mathbf{x}_1)\tilde{v}_{-\mathbf{k},-}(\mathbf{x}_2) - \tilde{v}^*_{-\mathbf{k},-}(\mathbf{x}_1)\tilde{u}^*_{\mathbf{k},+}(\mathbf{x}_2) \right\} = \sum_{\mathbf{k}<|\mathbf{k}_1|} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}}{\sqrt{V}}. \tag{142}$$

In addition,

$$\sum_{\mathbf{k}<|\mathbf{k}_1|} \left\{ \tilde{u}_{\mathbf{k},+}(\mathbf{x}_1)\tilde{v}^*_{\mathbf{k},-}(\mathbf{x}_2) - \tilde{v}^*_{\mathbf{k},-}(\mathbf{x}_1)\tilde{u}_{\mathbf{k},+}(\mathbf{x}_2) \right\} = 0. \tag{143}$$

For the real dispersions we can just use the Bogoliubov transformation from the last section, so we can write

$$\hat{\psi}_<(\mathbf{x},t) := \hat{\psi}_{<,\mathrm{at}}(x) + \hat{\psi}_{<,\mathrm{ph}}(x) = \sum_{\mathbf{k}<|\mathbf{k}_1|} A_{\mathbf{k}} \left[\hat{\alpha}_{\mathbf{k}} \cdot e^{-i\omega_+ t} u_{\mathbf{k},+}(\mathbf{x}) + \hat{\alpha}^\dagger_{\mathbf{k}} e^{i\omega_+ t} v^*_{\mathbf{k},+}(\mathbf{x}) \right] \tag{144}$$

$$+ \sum_{\mathbf{k}<|\mathbf{k}_1|} B_{\mathbf{k}} \left[\hat{\beta}_{\mathbf{k}}(t) e^{i\frac{\pi}{4}} \tilde{u}_{\mathbf{k},+}(\mathbf{x}) + \hat{\gamma}_{\mathbf{k}}(t) e^{i\frac{\pi}{4}} \tilde{v}^*_{-\mathbf{k},-}(\mathbf{x}) \right],$$

$$\hat{\psi}^\dagger_<(\mathbf{x},t) := \hat{\psi}^\dagger_{<,\mathrm{at}}(x) + \hat{\psi}^\dagger_{<,\mathrm{ph}}(x) = \sum_{\mathbf{k}<|\mathbf{k}_1|} A_{\mathbf{k}} \left[\hat{\alpha}^\dagger_{\mathbf{k}} e^{i\omega_+ t} u^*_{\mathbf{k},+}(\mathbf{x}) + \hat{\alpha}_{\mathbf{k}} e^{-i\omega_+ t} \tilde{v}_{\mathbf{k},+}(\mathbf{x}) \right] \tag{145}$$

$$+ \sum_{\mathbf{k}<|\mathbf{k}_1|} B_{-\mathbf{k}} \left[\hat{\beta}_{\mathbf{k}}(t) e^{-i\frac{\pi}{4}} \tilde{u}^*_{-\mathbf{k},+}(\mathbf{x}) + \hat{\gamma}_{\mathbf{k}}(t) e^{-i\frac{\pi}{4}} \tilde{v}_{\mathbf{k},-}(\mathbf{x}) \right].$$

Here, $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ are constants which are determined by the commutation relations and the equations of motion. Furthermore, $\hat{\beta}_{\mathbf{k}}$ and $\hat{\gamma}_{\mathbf{k}}$ are the operators for the complex modes. These operators satisfy $\hat{\beta}_{\mathbf{k}} = \hat{\beta}^\dagger_{-\mathbf{k}}$ and $\hat{\gamma}_{\mathbf{k}} = \hat{\gamma}^\dagger_{-\mathbf{k}}$. Furthermore, we impose

$$[\hat{\beta}_{\mathbf{k}}(t), \hat{\gamma}_{-\mathbf{p}}(t)] = -i\delta_{\mathbf{kp}}, \tag{146}$$

and all other commutation relations vanish. To obtain the explicit time dependence of the new operators, we should first determine the part of the Hamiltonian with the complex operators. By using (144) and (145), we define

$$\begin{bmatrix} \hat{\psi}_{<,\mathrm{ph},\mathbf{k}} \\ \hat{\psi}^\dagger_{<,\mathrm{ph},-\mathbf{k}} \end{bmatrix} := M \begin{bmatrix} \hat{\beta}_{\mathbf{k}}(t) \\ \hat{\gamma}_{\mathbf{k}}(t) \end{bmatrix}, \tag{147}$$

where

$$M := \begin{bmatrix} e^{+i\frac{\pi}{4}} \tilde{u}_{\mathbf{k},+} & e^{+i\frac{\pi}{4}} \tilde{v}^*_{\mathbf{k},-} \\ e^{-i\frac{\pi}{4}} \tilde{u}^*_{\mathbf{k},+} & e^{-i\frac{\pi}{4}} \tilde{v}_{\mathbf{k},-} \end{bmatrix}. \tag{148}$$

Here $\tilde{u}_{\mathbf{k},+}$ and $\tilde{v}_{\mathbf{k},-}$ are defined in (139) and (140). In momentum space the complex part of the Hamiltonian is given by

$$\hat{H} = \frac{1}{2} \sum_{\mathbf{k}<|\mathbf{k}_1|} \begin{bmatrix} \hat{\psi}_{<,\mathrm{ph},\mathbf{k}} \\ \hat{\psi}^\dagger_{<,\mathrm{ph},-\mathbf{k}} \end{bmatrix}^\dagger H \begin{bmatrix} \hat{\psi}_{<,\mathrm{ph},\mathbf{k}} \\ \hat{\psi}^\dagger_{<,\mathrm{ph},-\mathbf{k}} \end{bmatrix}, \tag{149}$$

where

$$H = \begin{bmatrix} \mathbf{k}^2 + \Delta + T & T \\ T & \mathbf{k}^2 + \Delta + T \end{bmatrix}, \tag{150}$$

and

$$T = \frac{g^2}{(\hbar\omega_-)^2 - c^2\mathbf{k}^2 + i\eta}. \tag{151}$$

Note that we do not use the Hamiltonian with the frequency-dependent T. Instead, we use a Hamiltonian where the $\hbar\omega$ in T is replaced by the quasiparticle dispersions $\hbar\omega_-$. To obtain the part of the Hamiltonian with the new operators $\hat{\beta}_{\mathbf{k}}(t)$ and $\hat{\gamma}_{\mathbf{k}}(t)$, we have to calculate

$$M^\dagger H M = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix}, \tag{152}$$

where

$$
\begin{aligned}
D_{11} &= 2(\mathbf{k}^2 + \Delta + T)|\tilde{u}_{\mathbf{k},+}|^2 - iT\{(\tilde{u}^*_{\mathbf{k},+})^2 - (\tilde{u}_{\mathbf{k},+})^2\}, \\
D_{12} &= (\mathbf{k}^2 + \Delta + T)\{\tilde{u}^*_{\mathbf{k},+}\tilde{v}^*_{\mathbf{k},-} + \tilde{u}_{\mathbf{k},+}\tilde{v}_{\mathbf{k},-}\} - iT\{\tilde{u}^*_{\mathbf{k},+}\tilde{v}_{\mathbf{k},-} - \tilde{u}_{\mathbf{k},+}\tilde{v}^*_{\mathbf{k},-}\}, \\
D_{21} &= D_{12}, \\
D_{22} &= 2(\mathbf{k}^2 + \Delta + T)|\tilde{v}_{\mathbf{k},-}|^2 + iT\{(\tilde{v}^*_{\mathbf{k},-})^2 - (\tilde{v}_{\mathbf{k},-})^2\}.
\end{aligned}
\tag{153}
$$

By using the fact that $\det[G^{-1}(\mathbf{k}, \omega_-)] = 0$, where $G^{-1}(\mathbf{k}, \omega)$ is defined in (92), we obtain that $\hbar\omega_-$ satisfies

$$(\mathbf{k}^2 + \Delta)^2 - (\hbar\omega_-)^2 + 2(\mathbf{k}^2 + \Delta)T = 0. \tag{154}$$

Therefore,

$$
\begin{aligned}
D_{11} &= \frac{(\mathbf{k}^2 + \Delta + T)[(\mathbf{k}^2 + \Delta)^2 - (\hbar\omega_-)^2] + T[(\mathbf{k}^2 + \Delta)^2 + (\hbar\omega_-)^2]}{2(\mathbf{k}^2 + \Delta)|\hbar\omega_-|} \\
&= \frac{-T[\mathbf{k}^2 + \Delta + T] + T[\mathbf{k}^2 + \Delta + T]}{|\hbar\omega_-|} = 0, \\
D_{22} &= \frac{(\mathbf{k}^2 + \Delta + T)[(\mathbf{k}^2 + \Delta)^2 - (\hbar\omega_-)^2] + T[(\mathbf{k}^2 + \Delta)^2 + (\hbar\omega_-)^2]}{2(\mathbf{k}^2 + \Delta)|\hbar\omega_-|} = D_{11} = 0,
\end{aligned}
\tag{155}
$$

and

$$
\begin{aligned}
D_{12} &= \frac{(\mathbf{k}^2 + \Delta + T)[(\mathbf{k}^2 + \Delta)^2 + (\hbar\omega_-)^2] + T[(\mathbf{k}^2 + \Delta)^2 - (\hbar\omega_-)^2]}{2(\mathbf{k}^2 + \Delta)|\hbar\omega_-|} \\
&= \frac{(\mathbf{k}^2 + \Delta + T)^2 - T^2}{|\hbar\omega_-|} = \frac{(\hbar\omega_-)^2}{|\hbar\omega_-|} = -|\hbar\omega_-|.
\end{aligned}
\tag{156}
$$

Here, we used (139) and (140) and the fact that $(\hbar\omega_-)^* = -\hbar\omega_-$. By combining these results, the Hamiltonian in momentum space reads

$$
\begin{aligned}
\hat{H} &= \frac{1}{2}\sum_{\mathbf{k} < |\mathbf{k}_1|} \left\{ \begin{bmatrix} \hat{\beta}_{\mathbf{k}}(t) \\ \hat{\gamma}_{\mathbf{k}}(t) \end{bmatrix}^\dagger \begin{bmatrix} 0 & -|\hbar\omega_-| \\ -|\hbar\omega_-| & 0 \end{bmatrix} \begin{bmatrix} \hat{\beta}_{\mathbf{k}}(t) \\ \hat{\gamma}_{\mathbf{k}}(t) \end{bmatrix} \right\} \\
&= -\frac{1}{2}\sum_{\mathbf{k} < |\mathbf{k}_1|} \left\{ |\hbar\omega_-|(\hat{\beta}^\dagger_{\mathbf{k}}(t)\hat{\gamma}_{\mathbf{k}}(t) + \hat{\gamma}^\dagger_{\mathbf{k}}(t)\hat{\beta}_{\mathbf{k}}(t)) \right\} \\
&= -\frac{1}{2}\sum_{\mathbf{k} < |\mathbf{k}_1|} \left\{ |\hbar\omega_-|(\hat{\beta}_{-\mathbf{k}}(t)\hat{\gamma}_{\mathbf{k}}(t) + \hat{\gamma}_{-\mathbf{k}}(t)\hat{\beta}_{\mathbf{k}}(t)) \right\}.
\end{aligned}
\tag{157}
$$

Notice that this part of the Hamiltonian is hermitian. With this expression for the complex part of the Hamiltonian, we can determine the time dependence of the complex operators by using the Heisenberg equations of motion given in (116). Therefore, we calculate

$$
\begin{aligned}
[\hat{H}, \hat{\beta}_{\mathbf{k}}] &= \hbar\omega_-\hat{\beta}_{\mathbf{k}}, \\
[\hat{H}, \hat{\gamma}_{\mathbf{k}}] &= -\hbar\omega_-\hat{\gamma}_{\mathbf{k}}.
\end{aligned}
\tag{158}
$$

The Heisenberg equations of motion are given by

$$
\begin{aligned}
\frac{d}{dt}\hat{\beta}_{\mathbf{k}}(t) &= |\omega_-|\hat{\beta}_{\mathbf{k}}(t), \\
\frac{d}{dt}\hat{\gamma}_{\mathbf{k}}(t) &= -|\omega_-|\hat{\gamma}_{\mathbf{k}}(t),
\end{aligned}
\tag{159}
$$

The solution is

$$\hat{\beta}_{\mathbf{k}}(t) = e^{|\omega_-|t}\hat{\beta}_{\mathbf{k}}, \tag{160}$$
$$\hat{\gamma}_{\mathbf{k}}(t) = e^{-|\omega_-|t}\hat{\gamma}_{\mathbf{k}},$$

where

$$[\hat{\beta}_{\mathbf{k}}, \hat{\gamma}_{-\mathbf{p}}] = -i\delta_{\mathbf{kp}}. \tag{161}$$

Furthermore, we can write

$$\hat{H} = \frac{1}{2}\sum_{\mathbf{k}<|\mathbf{k}_1|}\left\{-|\hbar\omega_-|\left(\hat{\beta}_{-\mathbf{k}}\hat{\gamma}_{\mathbf{k}} + \hat{\gamma}_{-\mathbf{k}}\hat{\beta}_{\mathbf{k}}\right)\right\}. \tag{162}$$

This representation is consistent with the fact that the $\hat{H}$ is time independent. However, at this point the meaning of the complex mode operator $\hat{\beta}_{\mathbf{k}}$ and $\hat{\gamma}_{\mathbf{k}}$ is not clear. To get a better understanding of these operators, we introduce bosonic operators $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^\dagger$ as follows,

$$\hat{\beta}_{\mathbf{k}} = \frac{1}{\sqrt{2}}\left(\hat{b}_{\mathbf{k}} + \hat{b}_{-\mathbf{k}}^\dagger\right), \tag{163}$$
$$\hat{\gamma}_{\mathbf{k}} = \frac{i}{\sqrt{2}}\left(\hat{b}_{\mathbf{k}} - \hat{b}_{-\mathbf{k}}^\dagger\right). \tag{164}$$

Note that these definitions are in agreement with $\hat{\beta}_{\mathbf{k}} = \hat{\beta}_{-\mathbf{k}}^\dagger$ and $\hat{\gamma}_{\mathbf{k}} = \hat{\gamma}_{-\mathbf{k}}^\dagger$. By rewriting,

$$\hat{b}_{\mathbf{k}} = \frac{1}{\sqrt{2}}\left(\hat{\beta}_{\mathbf{k}} - i\hat{\gamma}_{\mathbf{k}}\right), \tag{165}$$
$$\hat{b}_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{2}}\left(\hat{\beta}_{-\mathbf{k}} + i\hat{\gamma}_{-\mathbf{k}}\right). \tag{166}$$

By using the fact that $\hat{\beta}_{\mathbf{k}}$ and $\hat{\gamma}_{\mathbf{k}}$ satisfy the commutation relations defined in (161), we obtain

$$[\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{p}}^\dagger] = \delta_{\mathbf{kp}}, \tag{167}$$

and the other commutation relations vanish. Thus $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^\dagger$ are indeed bosonic operators. Now we can also rewrite the complex part of the Hamiltonian, given in (162), in terms of these bosonic operators. By using (163) and (164), we obtain

$$\hat{H} = \frac{1}{2}\sum_{\mathbf{k}<|\mathbf{k}_1|}\left\{\hbar\omega_{-,-}\hat{b}_{\mathbf{k}}\hat{b}_{-\mathbf{k}} + \hbar\omega_{+,-}\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{-\mathbf{k}}^\dagger\right\}, \tag{168}$$

as our expression for the Hamiltonian in terms of the bosonic operators $\hat{b}_{\mathbf{k}}$ and $\hat{b}_{\mathbf{k}}^\dagger$. Here $\hbar\omega_{\sigma',-}$ are defined in (93). Furthermore in terms of the complex mode operators, the field operators are given by

$$\hat{\psi}_<(\mathbf{x},t) = \sum_{\mathbf{k}<|\mathbf{k}_1|}A_{\mathbf{k}}\left[\hat{\alpha}_{\mathbf{k}}\cdot e^{-i\omega_+t}u_{\mathbf{k},+}(\mathbf{x}) + \hat{\alpha}_{\mathbf{k}}^\dagger e^{i\omega_+t}v_{\mathbf{k},+}^*(\mathbf{x})\right] \tag{169}$$

$$+ \sum_{\mathbf{k}<|\mathbf{k}_1|}B_{\mathbf{k}}\left[\hat{\beta}_{\mathbf{k}}e^{i\frac{\pi}{4}+|\omega_-|t}\tilde{u}_{\mathbf{k},+}(\mathbf{x}) + \hat{\gamma}_{\mathbf{k}}e^{i\frac{\pi}{4}-|\omega_-|t}\tilde{v}_{-\mathbf{k},-}^*(\mathbf{x})\right],$$

$$\hat{\psi}_<^\dagger(\mathbf{x},t) = \sum_{\mathbf{k}<|\mathbf{k}_1|}A_{\mathbf{k}}\left[\hat{\alpha}_{\mathbf{k}}^\dagger\cdot e^{i\omega_+t}u_{\mathbf{k},+}^*(\mathbf{x}) + \hat{\alpha}_{\mathbf{k}}e^{-i\omega_+t}v_{\mathbf{k},+}(\mathbf{x})\right] \tag{170}$$

$$+ \sum_{\mathbf{k}<|\mathbf{k}_1|}B_{-\mathbf{k}}\left[\hat{\beta}_{\mathbf{k}}e^{-i\frac{\pi}{4}+|\omega_-|t}\tilde{u}_{-\mathbf{k},+}^*(\mathbf{x}) + \hat{\gamma}_{\mathbf{k}}e^{-i\frac{\pi}{4}-|\omega_-|t}\tilde{v}_{\mathbf{k},-}(\mathbf{x})\right].$$

33

And the expression for the phonon field in the operator formalism

$$\hat{\phi}_<(\mathbf{x},t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}<|\mathbf{k}_1|} C_{\mathbf{k}} \left[\hat{\alpha}_{\mathbf{k}} \cdot e^{i(\mathbf{k}\cdot x - \omega_+ t)} + \hat{\alpha}_{\mathbf{k}}^\dagger \cdot e^{-i(\mathbf{k}\cdot x - \omega_+ t)} \right] \tag{171}$$

$$+ \frac{1}{\sqrt{V}} \sum_{\mathbf{k}<|\mathbf{k}_1|} D_{\mathbf{k}} \left[\hat{\beta}_{\mathbf{k}} e^{|\omega_-|t + i\mathbf{k}\cdot\mathbf{x}} + \hat{\gamma}_{\mathbf{k}} e^{-|\omega_-|t + i\mathbf{k}\cdot\mathbf{x}} \right].$$

Note that $\hat{\phi}_<(\mathbf{x},t)$ is indeed real, because $\hat{\beta}_{\mathbf{k}}^\dagger = \hat{\beta}_{-\mathbf{k}}$, $\hat{\gamma}_{\mathbf{k}}^\dagger = \hat{\gamma}_{-\mathbf{k}}$ and we assume that $D_{\mathbf{k}}^* = D_{-\mathbf{k}}$.

5.2.3 Normalization constants

For the full solution of this problem, we have to determine the constants $E_{\mathbf{k},\sigma}$, $F_{\mathbf{k},\sigma}$, $A_{\mathbf{k}}$, $B_{\mathbf{k}}$, $C_{\mathbf{k}}$ and $D_{\mathbf{k}}$. To find the constants we use that $\hat{\psi}(\mathbf{x},t)$ should satisfy the canonical commutation relation

$$[\hat{\psi}(\mathbf{x}_1,t), \hat{\pi}_\psi(\mathbf{x}_2,t)] = [\hat{\psi}(\mathbf{x}_1,t), i\hbar\hat{\psi}^\dagger(\mathbf{x}_2,t)] = i\hbar\delta(\mathbf{x}_1 - \mathbf{x}_2). \tag{172}$$

Here in the second step (84) is used to calculate $\hat{\pi}_\psi(\mathbf{x}_2,t)$. Also $\hat{\phi}(\mathbf{x},t)$ should satisfy the canonical commutation relation. Again by using (84) this commutation relation can be written as

$$[\hat{\phi}(\mathbf{x}_1,t), \hat{\pi}_\phi(\mathbf{x}_2,t)] = [\hat{\phi}(\mathbf{x}_1,t), 2i\hbar^2\partial_\tau\hat{\phi}(\mathbf{x}_2,t)] = i\hbar\delta(\mathbf{x}_1 - \mathbf{x}_2). \tag{173}$$

Because the low-momentum and the high-momentum parts commute, we can only satisfy these commutation relations if

$$[\hat{\psi}_<(\mathbf{x}_1,t), \hat{\psi}_<^\dagger(\mathbf{x}_2,t)] = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}<|\mathbf{k}_1|} e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}, \tag{174}$$

$$[\hat{\psi}_>(\mathbf{x}_1,t), \hat{\psi}_>^\dagger(\mathbf{x}_2,t)] = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}>|\mathbf{k}_1|} e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}, \tag{175}$$

$$[\hat{\phi}_<(\mathbf{x}_1,t), 2\hbar\partial_\tau\hat{\phi}_<(\mathbf{x}_2,t)] = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}<|\mathbf{k}_1|} e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}, \tag{176}$$

$$[\hat{\phi}_>(\mathbf{x}_1,t), 2\hbar\partial_\tau\hat{\phi}_>(\mathbf{x}_2,t)] = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}>|\mathbf{k}_1|} e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}. \tag{177}$$

Furthermore, the field operators should satisfy the equations of motion. The equations of motion are given by

$$0 = \left\{ \hbar\frac{\partial}{\partial\tau} - \nabla^2 + \Delta \right\} \hat{\psi}(\mathbf{x},t) + g\sqrt{2}\hat{\phi}(\mathbf{x},t), \tag{178}$$

$$0 = 2\left\{ -\hbar^2\frac{\partial^2}{\partial\tau^2} - c^2\nabla^2 \right\} \hat{\phi}(\mathbf{x},t) + g\sqrt{2}\left\{ \hat{\psi}(\mathbf{x},t) + \hat{\psi}^\dagger(\mathbf{x},t) \right\}. \tag{179}$$

Thus the low-momentum and high-momentum part completely decouples, and therefore we can can consider both part separately. For the high-momentum part (175) implies

$$E_{\mathbf{k},+} = \sqrt{Z_{\mathbf{k}}}, \tag{180}$$

$$E_{\mathbf{k},-} = \sqrt{1 - Z_{\mathbf{k}}}. \tag{181}$$

for some constant $Z_{\mathbf{k}}$. Furthermore by using (177)

$$4\hbar\omega_+ F_{\mathbf{k},+}^2 + 4\hbar\omega_- F_{\mathbf{k},-}^2 = 1. \tag{182}$$

By substituting the mode expansions in the first equation of motion we obtain

$$g\sqrt{2}F_{\mathbf{k},+} = -\sqrt{Z_{\mathbf{k}}}\frac{(\mathbf{k}^2+\Delta)^2-\hbar\omega_+^2}{\sqrt{4(\mathbf{k}^2+\Delta)\hbar\omega_+}}, \tag{183}$$

$$g\sqrt{2}F_{\mathbf{k},-} = -\sqrt{1-Z_{\mathbf{k}}}\frac{(\mathbf{k}^2+\Delta)^2-\hbar\omega_-^2}{\sqrt{4(\mathbf{k}^2+\Delta)\hbar\omega_-}}, \tag{184}$$

and the constraints due to the second equation of motion

$$2F_{\mathbf{k},+}(\hbar\omega_+^2-c^2\mathbf{k}^2) = \sqrt{Z_{\mathbf{k}}}\frac{(\mathbf{k}^2+\Delta)g\sqrt{2}}{\sqrt{(\mathbf{k}^2+\Delta)\hbar\omega_+}}, \tag{185}$$

$$2F_{\mathbf{k},-}(\hbar\omega_-^2-c^2\mathbf{k}^2) = \sqrt{1-Z_{\mathbf{k}}}\frac{(\mathbf{k}^2+\Delta)g\sqrt{2}}{\sqrt{(\mathbf{k}^2+\Delta)\hbar\omega_-}}. \tag{186}$$

Due to the fact that $\hbar\omega_\sigma$ should satisfy

$$(\mathbf{k}^2+\Delta)^2-\hbar\omega_\sigma^2+\frac{2g^2(\mathbf{k}^2+\Delta)}{\hbar\omega_\sigma^2-c^2\mathbf{k}^2}=0, \tag{187}$$

the constraints coming from the second equation of motion are the same as the constraints of the first equation of motion. By combining these constraints with (182) and using the analytic expression of $\hbar\omega_{+,\sigma}$ given in (93), we obtain

$$Z_{\mathbf{k}} = \frac{(\mathbf{k}^2+\Delta)^2-\hbar\omega_-^2}{\hbar\omega_+^2-\hbar\omega_-^2}. \tag{188}$$

From the analytic expressions of $\hbar\omega_\sigma$ it follows that $0 < Z_{\mathbf{k}} < 1$ for non-zero coupling. Hence

$$E_{\mathbf{k},+} = \sqrt{\frac{(\mathbf{k}^2+\Delta)^2-\hbar\omega_-^2}{\hbar\omega_+^2-\hbar\omega_-^2}}, \tag{189}$$

$$E_{\mathbf{k},-} = \sqrt{\frac{\hbar\omega_+^2-(\mathbf{k}^2+\Delta)^2}{\hbar\omega_+^2-\hbar\omega_-^2}}. \tag{190}$$

Furthermore,

$$F_{\mathbf{k},+} = -\frac{1}{g\sqrt{2}}\sqrt{\frac{(\mathbf{k}^2+\Delta)^2-\hbar\omega_-^2}{\hbar\omega_+^2-\hbar\omega_-^2}}\frac{(\mathbf{k}^2+\Delta)^2-\hbar\omega_+^2}{\sqrt{4(\mathbf{k}^2+\Delta)\hbar\omega_+}}, \tag{191}$$

$$F_{\mathbf{k},-} = -\frac{1}{g\sqrt{2}}\sqrt{\frac{\hbar\omega_+^2-(\mathbf{k}^2+\Delta)^2}{\hbar\omega_+^2-\hbar\omega_-^2}}\frac{(\mathbf{k}^2+\Delta)^2-\hbar\omega_-^2}{\sqrt{4(\mathbf{k}^2+\Delta)\hbar\omega_-}}. \tag{192}$$

Now we consider the low-momentum part and determine the constants $A_{\mathbf{k}}$, $B_{\mathbf{k}}$, $C_{\mathbf{k}}$ and $D_{\mathbf{k}}$. First (174) and (176) imply

$$A_{\mathbf{k}}^2+B_{\mathbf{k}}^2 = 1, \tag{193}$$
$$4\hbar\omega_+C_{\mathbf{k}}^2+4|\hbar\omega_-|D_{\mathbf{k}}D_{-\mathbf{k}} = 1.$$

Hence,

$$A_{\mathbf{k}} = \sqrt{Y_{\mathbf{k}}}, \tag{194}$$
$$B_{\mathbf{k}} = \sqrt{1-Y_{\mathbf{k}}},$$

where $Y_{\mathbf{k}}$ is some constant. Furthermore, the field operators should satisfy the equations of motion defined in (178) and (179). By substituting the mode expansion into these equations, we obtain

$$g\sqrt{2}C_{\mathbf{k}} = -\sqrt{Y_{\mathbf{k}}}\frac{(\mathbf{k}^2+\Delta)^2-\hbar\omega_+^2}{\sqrt{4(\mathbf{k}^2+\Delta)\hbar\omega_+}}, \tag{195}$$

$$g\sqrt{2}D_{\mathbf{k}} = -\sqrt{1-Y_{\mathbf{k}}}\frac{(\mathbf{k}^2+\Delta)^2-\hbar\omega_-^2}{\sqrt{4(\mathbf{k}^2+\Delta)|\hbar\omega_-|}}, \tag{196}$$

as a constraint coming from the first equation of motion and due to the second equation of motion

$$2C_{\mathbf{k}}(\hbar\omega_+^2 - c^2\mathbf{k}^2) = \sqrt{Y_{\mathbf{k}}} \frac{(\mathbf{k}^2 + \Delta)g\sqrt{2}}{\sqrt{(\mathbf{k}^2 + \Delta)\hbar\omega_+}}, \tag{197}$$

$$2D_{\mathbf{k}}(\hbar\omega_-^2 - c^2\mathbf{k}^2) = \sqrt{1 - Y_{\mathbf{k}}} \frac{(\mathbf{k}^2 + \Delta)g\sqrt{2}}{\sqrt{(\mathbf{k}^2 + \Delta)|\hbar\omega_-|}}. \tag{198}$$

By using all these equation we obtain that $D_{\mathbf{k}} = D_{-\mathbf{k}}$ and therefore by defining

$$D_{\mathbf{k}} = E_{\mathbf{k}} \frac{\sqrt{\hbar\omega_-}}{\sqrt{|\hbar\omega_-|}}, \tag{199}$$

we have the same equations as when all dispersions were real. Therefore,

$$A_{\mathbf{k}} = \sqrt{\frac{(\mathbf{k}^2 + \Delta)^2 - \hbar\omega_-^2}{\hbar\omega_+^2 - \hbar\omega_-^2}} = E_{\mathbf{k},+}, \tag{200}$$

$$B_{\mathbf{k}} = \sqrt{\frac{\hbar\omega_+^2 - (\mathbf{k}^2 + \Delta)^2}{\hbar\omega_+^2 - \hbar\omega_-^2}} = E_{\mathbf{k},-}, \tag{201}$$

$$C_{\mathbf{k}} = -\frac{1}{g\sqrt{2}} \sqrt{\frac{(\mathbf{k}^2 + \Delta)^2 - \hbar\omega_-^2}{\hbar\omega_+^2 - \hbar\omega_-^2}} \frac{(\mathbf{k}^2 + \Delta)^2 - \hbar\omega_+^2}{\sqrt{4(\mathbf{k}^2 + \Delta)\hbar\omega_+}} = F_{\mathbf{k},+}, \tag{202}$$

$$D_{\mathbf{k}} = -\frac{1}{g\sqrt{2}} \sqrt{\frac{\hbar\omega_+^2 - (\mathbf{k}^2 + \Delta)^2}{\hbar\omega_+^2 - \hbar\omega_-^2}} \frac{(\mathbf{k}^2 + \Delta)^2 - \hbar\omega_-^2}{\sqrt{4(\mathbf{k}^2 + \Delta)|\hbar\omega_-|}}. \tag{203}$$

So the complete expression for the field operators is given by

$$\hat{\phi}(\mathbf{x}, t) = \hat{\phi}_<(\mathbf{x}, t) + \hat{\phi}_>(\mathbf{x}, t) \tag{204}$$

$$= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}<|\mathbf{k}_1|} C_{\mathbf{k}} \left[\hat{\alpha}_{\mathbf{k}} \cdot e^{i(\mathbf{k}\cdot x - \omega_+ t)} + \hat{\alpha}_{\mathbf{k}}^\dagger \cdot e^{-i(\mathbf{k}\cdot x - \omega_+ t)} \right]$$

$$+ \frac{1}{\sqrt{V}} \sum_{\mathbf{k}<|\mathbf{k}_1|} D_{\mathbf{k}} \left[\hat{\beta}_{\mathbf{k}} e^{|\omega_-|t + i\mathbf{k}\cdot\mathbf{x}} + \hat{\gamma}_{\mathbf{k}} e^{-|\omega_-|t + i\mathbf{k}\cdot\mathbf{x}} \right]$$

$$+ \frac{1}{\sqrt{V}} \sum_{\mathbf{k}>|\mathbf{k}_1|, \sigma\in\{+,-\}} F_{\mathbf{k},\sigma} \left[d_{\mathbf{k},\sigma} e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_\sigma t)} + d_{\mathbf{k},\sigma}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{x} - \omega_\sigma t)} \right],$$

where the constants are defined in (192), (202) and (203). Furthermore,

$$\hat{\psi}(\mathbf{x}, t) = \hat{\psi}_<(\mathbf{x}, t) + \hat{\psi}_>(\mathbf{x}, t) \tag{205}$$

$$= \sum_{\mathbf{k}<|\mathbf{k}_1|} A_{\mathbf{k}} \left[\hat{\alpha}_{\mathbf{k}} \cdot e^{-i\omega_+ t} u_{\mathbf{k},+}(\mathbf{x}) + \hat{\alpha}_{\mathbf{k}}^\dagger e^{i\omega_+ t} v_{\mathbf{k},+}^*(\mathbf{x}) \right]$$

$$+ \sum_{\mathbf{k}<|\mathbf{k}_1|} B_{\mathbf{k}} \left[\hat{\beta}_{\mathbf{k}} e^{i\frac{\pi}{4} + |\omega_-|t} \tilde{u}_{\mathbf{k},+}(\mathbf{x}) + \hat{\gamma}_{\mathbf{k}} e^{i\frac{\pi}{4} - |\omega_-|t} \tilde{v}_{-\mathbf{k},-}^*(\mathbf{x}) \right]$$

$$+ \sum_{\mathbf{k}>|\mathbf{k}_1|, \sigma\in\{+,-\}} E_{\mathbf{k},\sigma} \left[\hat{d}_{\mathbf{k},\sigma} e^{-i\omega_\sigma t} u_{\mathbf{k},\sigma}(\mathbf{x}) + \hat{d}_{\mathbf{k},\sigma}^\dagger e^{i\omega_\sigma t} v_{\mathbf{k},\sigma}^*(\mathbf{x}) \right],$$

$$\hat{\psi}^\dagger(\mathbf{x}, t) = \hat{\psi}_<^\dagger(\mathbf{x}, t) + \hat{\psi}_>^\dagger(\mathbf{x}, t) \tag{206}$$

$$= \sum_{\mathbf{k}<|\mathbf{k}_1|} A_{\mathbf{k}} \left[\hat{\alpha}_{\mathbf{k}}^\dagger \cdot e^{i\omega_+ t} u_{\mathbf{k},+}^*(\mathbf{x}) + \hat{\alpha}_{\mathbf{k}} e^{-i\omega_+ t} v_{\mathbf{k},+}(\mathbf{x}) \right]$$

$$+ \sum_{\mathbf{k}<|\mathbf{k}_1|} B_{-\mathbf{k}} \left[\hat{\beta}_{\mathbf{k}} e^{-i\frac{\pi}{4} + |\omega_-|t} \tilde{u}_{-\mathbf{k},+}^*(\mathbf{x}) + \hat{\gamma}_{\mathbf{k}} e^{-i\frac{\pi}{4} - |\omega_-|t} \tilde{v}_{\mathbf{k},-}(\mathbf{x}) \right]$$

$$+ \sum_{\mathbf{k}>|\mathbf{k}_1|, \sigma\in\{+,-\}} E_{\mathbf{k},\sigma} \left[\hat{d}_{\mathbf{k},\sigma} e^{-i\omega_\sigma t} v_{\mathbf{k},\sigma}(\mathbf{x}) + \hat{d}_{\mathbf{k},\sigma}^\dagger e^{i\omega_\sigma t} u_{\mathbf{k},\sigma}^*(\mathbf{x}) \right],$$

36

where the constants are defined in (200) and (201). With these expressions for the constants, we have

$$[\hat{\phi}(\mathbf{x}_1, t), \hat{\psi}(\mathbf{x}_2, t)] = [\hat{\phi}(\mathbf{x}_1, t), \hat{\psi}^\dagger(\mathbf{x}_2, t)] = 0. \tag{207}$$

This result is expected, because creation or annihilation of a atom is uncorrelated to the creation or annihilation of a phonon. Now we take the limit of $g \to 0$. First note that in this limit $|\mathbf{k}_1| \to 0$. Thus $\hat{\psi}_<(\mathbf{x}, t) = \hat{\psi}^\dagger_<(\mathbf{x}, t) = \hat{\phi}_<(\mathbf{x}, t) = 0$ as $g \to 0$. Furthermore by using (93) we have

$$\hbar\omega_+ = \mathbf{k}^2 + \Delta \quad \text{and} \quad \hbar\omega_- = c|\mathbf{k}| \qquad \text{if } (\mathbf{k}^2 + \Delta)^2 > c^2\mathbf{k}^2, \tag{208}$$

$$\hbar\omega_+ = c|\mathbf{k}| \qquad \text{and} \quad \hbar\omega_- = \mathbf{k}^2 + \Delta \qquad \text{if } (\mathbf{k}^2 + \Delta)^2 < c^2\mathbf{k}^2. \tag{209}$$

Hence

$$Z_{\mathbf{k}} = 1 \qquad \text{if } (\mathbf{k}^2 + \Delta)^2 > c^2\mathbf{k}^2, \tag{210}$$

$$Z_{\mathbf{k}} = 0 \qquad \text{if } (\mathbf{k}^2 + \Delta)^2 < c^2\mathbf{k}^2, \tag{211}$$

and

$$u_{\mathbf{k},+} = 1 \quad \text{and} \quad v_{\mathbf{k},+} = 0 \qquad \text{if } (\mathbf{k}^2 + \Delta)^2 > c^2\mathbf{k}^2, \tag{212}$$

$$u_{\mathbf{k},-} = 1 \quad \text{and} \quad v_{\mathbf{k},-} = 0 \qquad \text{if } (\mathbf{k}^2 + \Delta)^2 < c^2\mathbf{k}^2, \tag{213}$$

in the limit of $g \to 0$. Hence,

$$\hat{\psi}(\mathbf{x}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}} e^{i(\mathbf{k} \cdot \mathbf{x} - (\mathbf{k}^2 + \Delta)t)}, \tag{214}$$

$$\hat{\psi}^\dagger(\mathbf{x}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} e^{-i(\mathbf{k} \cdot \mathbf{x} - (\mathbf{k}^2 + \Delta)t)}, \tag{215}$$

in the limit of zero coupling. Here,

$$\hat{c}_{\mathbf{k}} = \begin{cases} d_{\mathbf{k},+} = a_{\mathbf{k},+} & \text{if } (\mathbf{k}^2 + \Delta)^2 > c^2\mathbf{k}^2. \\ d_{\mathbf{k},-} = a_{\mathbf{k},-} & \text{if } (\mathbf{k}^2 + \Delta)^2 < c^2\mathbf{k}^2. \end{cases} \tag{216}$$

This is the result of an homogeneous quantum gas. Furthermore, in the limit of $g \to 0$

$$B_{\mathbf{k},+} = 0 \qquad \text{and} \quad B_{\mathbf{k},-} = -\frac{1}{2\sqrt{c|\mathbf{k}|}} \qquad \text{if } (\mathbf{k}^2 + \Delta)^2 > c^2\mathbf{k}^2, \tag{217}$$

$$B_{\mathbf{k},+} = \frac{1}{2\sqrt{c|\mathbf{k}|}} \quad \text{and} \quad B_{\mathbf{k},-} = 0 \qquad \text{if } (\mathbf{k}^2 + \Delta)^2 < c^2\mathbf{k}^2. \tag{218}$$

Thus in the limit of zero coupling

$$\hat{\phi}(\mathbf{x}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{2\sqrt{c|\mathbf{k}|}} \left\{ \hat{p}_{\mathbf{k}} e^{i(\mathbf{k} \cdot \mathbf{x} - c|\mathbf{k}|t)} + \hat{p}^\dagger_{\mathbf{k}} e^{-i(\mathbf{k} \cdot \mathbf{x} - c|\mathbf{k}|t)} \right\}, \tag{219}$$

where

$$\hat{p}_{\mathbf{k}} = \begin{cases} -d_{\mathbf{k},-} = -a_{\mathbf{k},-} & \text{if } (\mathbf{k}^2 + \Delta)^2 > c^2\mathbf{k}^2. \\ d_{\mathbf{k},+} = a_{\mathbf{k},+} & \text{if } (\mathbf{k}^2 + \Delta)^2 < c^2\mathbf{k}^2. \end{cases} \tag{220}$$

Note that the minus sign in front of $d_{\mathbf{k},-}$ is unimportant as for physical quantities one always calculates products of an even number operators. So the sum of the number of $\hat{\phi}(\mathbf{x}, t)$ is even and therefore the minus sign disappears in physical quantities. Hence, in the limit of $g \to 0$ we get the expected results.

5.3 Physical quantities

Now that we have the full expressions for the field operators, we can perform some calculations to obtain physical quantities.

5.3.1 The spectral-weight function

To calculate some physical quantities we have to determine the spectral-weight function, which is defined in (82). But first we have to determine the retarded Green's function. In the operator formalism, the retarded Green's function is defined as

$$G^{\text{ret}}(\mathbf{x}_1, t_1, \mathbf{x}_2, t_2) = i\Theta(t_1 - t_2)\langle[\hat{\psi}(\mathbf{x}_1, t_1), \hat{\psi}^\dagger(\mathbf{x}_2, t_2)]\rangle. \tag{221}$$

By using the (205) and (206), we can write

$$
\begin{aligned}
G^{\text{ret}}(\mathbf{x}_1, t_1, 0, 0) &= i\Theta(t_1)\sum_{\mathbf{p}} A_{\mathbf{p}}^2 \{|u_{\mathbf{p},+}|^2 e^{-i\omega_+ t_1} - |v_{\mathbf{p},+}|^2 e^{i\omega_+ t_1}\} e^{i\mathbf{p}\cdot\mathbf{x}_1} \\
&+ i\Theta(t_1)\sum_{\mathbf{p}>|\mathbf{k}_1|} B_{\mathbf{p}}^2 \{|u_{\mathbf{p},-}|^2 e^{-i\omega_- t_1} - |v_{\mathbf{p},-}|^2 e^{i\omega_- t_1}\} e^{i\mathbf{p}\cdot\mathbf{x}_1} \\
&+ \Theta(t_1)\sum_{\mathbf{p}<|\mathbf{k}_1|} B_{\mathbf{p}}^2 \{\tilde{u}_{\mathbf{p},+}\tilde{v}_{-\mathbf{p},-} e^{|\omega_-|t_1} - \tilde{u}_{\mathbf{p},+}^* \tilde{v}_{-\mathbf{p},-}^* e^{-|\omega_-|t_1}\} e^{i\mathbf{p}\cdot\mathbf{x}_1},
\end{aligned}
\tag{222}
$$

where without loss of generality we set $t_2 = x_2 = 0$. In this expression for the retarded Green's function, there is a part with exponential growth. Because the Fourier transform of a function is only well-defined if a function is absolute integrable, we have a problem to calculate the retarded Green's function in momentum space. However, to compare with the spectral function obtained
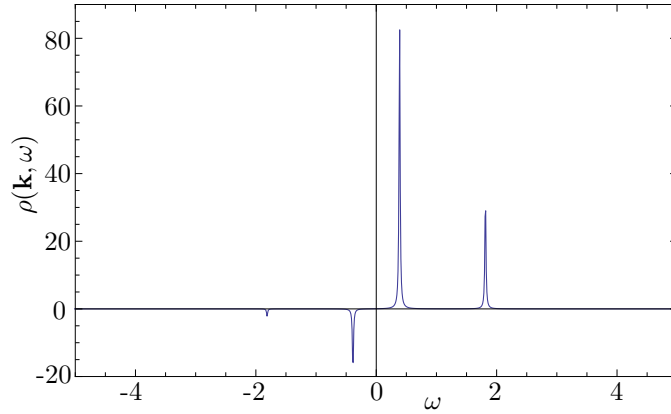

Figure 12: The atomic spectral function of the atom-phonon model for $\mathbf{k}^2 = 0.3$, $c = 5$, $g = 1$, $\epsilon = 10^{-2}$ and $\Delta = 1$. The four peaks corresponds to the four dispersions $\hbar\omega_{\sigma',\sigma}$.

from (92), we define

$$\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} \frac{d\mathbf{x}_1}{V} \tilde{u}_{\mathbf{p},+}\tilde{v}_{-\mathbf{p},-} e^{|\omega_-|t_1} e^{i\mathbf{p}\cdot\mathbf{x}_1} e^{-i\mathbf{k}\cdot\mathbf{x}_1} e^{i\omega t_1 - \epsilon t_1} := -\frac{\tilde{u}_{\mathbf{k},+}\tilde{v}_{-\mathbf{k},-}}{|\omega_-| + i\omega - \epsilon} \tag{223}$$

Hence,

$$
\begin{aligned}
G^{\text{ret}}(\mathbf{k}, \omega^+) &= \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} \frac{d\mathbf{x}_1}{V} G^{\text{ret}}(\mathbf{x}_1, t_1, 0, 0) e^{-i\mathbf{k}\cdot\mathbf{x}_1} e^{i\omega t_1 - \epsilon t_1} \\
&= -iA_{\mathbf{k}}^2 \left\{|u_{\mathbf{k},+}|^2 \frac{1}{i(\omega - \omega_+) - \epsilon} - |v_{\mathbf{k},+}|^2 \frac{1}{i(\omega + \omega_+) - \epsilon}\right\} \\
&- i\Theta(|\mathbf{k}| - |\mathbf{k}_1|)B_{\mathbf{k}}^2 \left\{|u_{\mathbf{k},-}|^2 \frac{1}{i(\omega - \omega_-) - \epsilon} - |v_{\mathbf{k},-}|^2 \frac{1}{i(\omega + \omega_-) - \epsilon}\right\} \\
&- \Theta(|\mathbf{k}_1| - |\mathbf{k}|)B_{\mathbf{k}}^2 \left\{\tilde{u}_{\mathbf{k},+}\tilde{v}_{-\mathbf{k},-} \frac{1}{|\omega_-| + i\omega - \epsilon} - \tilde{u}_{\mathbf{k},+}^* \tilde{v}_{-\mathbf{k},-}^* \frac{1}{-|\omega_-| + i\omega - \epsilon}\right\}.
\end{aligned}
\tag{224}
$$

38

Note that in the limit of $\epsilon \to 0$ the last term is real. So the complex dispersions do not contribute to the spectral function. Furthermore, by using

$$\lim_{\epsilon \downarrow 0} \frac{\epsilon}{x^2 + \epsilon^2} = \pi \delta(x), \tag{225}$$

the spectral function can be written as

$$
\begin{aligned}
\rho(\mathbf{k}, \omega) &= A_{\mathbf{k}}^2 \{|u_{\mathbf{k},+}|^2 \delta(\omega - \omega_+) - |v_{\mathbf{k},+}|^2 \delta(\omega + \omega_+)\} \\
&+ B_{\mathbf{k}}^2 \{|u_{\mathbf{k},-}|^2 \delta(\omega - \omega_-) - |v_{\mathbf{k},-}|^2 \delta(\omega + \omega_-)\} \Theta(|\mathbf{k}| - |\mathbf{k}_1|).
\end{aligned} \tag{226}
$$

Because $\omega_\sigma > 0$, it is clear from this result that the spectral function is larger than zero for positive frequencies and smaller than zero for negative frequencies. Also,

$$
\begin{aligned}
\int d\omega \rho(\mathbf{k}, \omega) &= A_{\mathbf{k}}^2 \{|u_{\mathbf{k},+}|^2 - |v_{\mathbf{k},+}|^2\} + B_{\mathbf{k}}^2 \{|u_{\mathbf{k},-}|^2 - |v_{\mathbf{k},-}|^2\} \\
&= A_{\mathbf{k}}^2 + B_{\mathbf{k}}^2 = 1,
\end{aligned} \tag{227}
$$

if $|\mathbf{k}| > |\mathbf{k}_1|$. Thus in this region the frequency sum rule for atoms is satisfied. However, if $|\mathbf{k}| < |\mathbf{k}_1|$

$$\int d\omega \rho(\mathbf{k}, \omega) = A_{\mathbf{k}}^2 \neq 1. \tag{228}$$

Thus for small momentum, the frequency sum rule is not satisfied. Instead of using the field operators, we can also use (92) to obtain the spectral function. First write

$$G_{11}(\mathbf{k}, \omega^+) = \frac{q + ir\epsilon}{s + it\epsilon}, \tag{229}$$

where

$$
\begin{aligned}
q &= g^2 + (\mathbf{k}^2 + \Delta + \hbar\omega)((\hbar\omega)^2 - c^2\mathbf{k}^2), \tag{230} \\
r &= 2\hbar\omega(\mathbf{k}^2 + \Delta + \hbar\omega) + (\hbar\omega)^2 - c^2\mathbf{k}^2, \tag{231} \\
s &= 2g^2(\mathbf{k}^2 + \Delta) + [(\hbar\omega)^2 - c^2k^2][(\mathbf{k}^2 + \Delta)^2 - (\hbar\omega)^2], \tag{232} \\
t &= 2\hbar\omega[c^2\mathbf{k}^2 + (\mathbf{k}^2 + \Delta)^2 - 2(\hbar\omega)^2]. \tag{233}
\end{aligned}
$$

Note that we are interested in $G_{11}(\mathbf{k}, \omega^+)$, since this corresponds to the normal average. By using
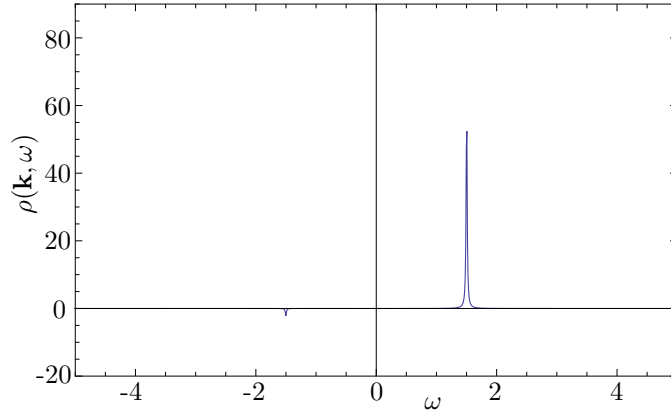

Figure 13: The atomic spectral function of the atom-phonon model for $\mathbf{k}^2 = 0.15$, $c = 5$, $g = 1$, $\epsilon = 10^{-2}$ and $\Delta = 1$. The two peaks corresponds to the two real dispersions $\hbar\omega_{\sigma',+}$.

(225) the imaginary part of $G_{11}(\mathbf{k}, \omega^+)$ can be rewritten as

$$
\begin{aligned}
\frac{1}{\pi} \text{Im}[G_{11}(\mathbf{k}, \omega^+)] &= \frac{r \cdot s}{t^2} \delta(s/t) - \frac{q}{t} \delta(s/t) \tag{234} \\
&= -\frac{q}{t} \delta(s/t).
\end{aligned}
$$

39

Here we use that the density is obtained by integrating the spectral function multiplied with the Bose function and therefore the term with $s \cdot \delta(s/t)$ can be neglected. Furthermore, by using

$$\delta(g(x)) = \sum_i \frac{\delta(x - x_i)}{|g'(x_i)|}, \tag{235}$$

where the summation is over all real roots of g, we have that

$$\frac{1}{\hbar\pi} \text{Im}[G_{11}(\mathbf{k}, \omega^+)] = \sum_{\sigma \in \{+,-\}} \{C_{1,\sigma}\delta(\omega - \omega_\sigma) - C_{2,\sigma}\delta(\omega + \omega_\sigma)\}, \tag{236}$$

with

$$C_{1,\sigma} = \frac{g^2 + (\mathbf{k}^2 + \Delta + \hbar\omega)((\hbar\omega)^2 - c^2\mathbf{k}^2)}{2\hbar\omega(c^2\mathbf{k}^2 + (\mathbf{k}^2 + \Delta)^2 - 2(\hbar\omega)^2)}\Big|_{\hbar\omega = \hbar\omega_{+,\sigma}}, \tag{237}$$

$$C_{2,\sigma} = \frac{g^2 + (\mathbf{k}^2 + \Delta + \hbar\omega)((\hbar\omega)^2 - c^2\mathbf{k}^2)}{2\hbar\omega(c^2\mathbf{k}^2 + (\mathbf{k}^2 + \Delta)^2 - 2(\hbar\omega)^2)}\Big|_{\hbar\omega = \hbar\omega_{-,\sigma}}, \tag{238}$$

if $|\mathbf{k}| > |\mathbf{k}_1|$, and otherwise

$$\frac{1}{\hbar\pi} \text{Im}[G_{11}(\mathbf{k}, \omega^+)] = \{C_{1,+}\delta(\omega - \omega_+) - C_{2,+}\delta(\omega + \omega_+)\}. \tag{239}$$

Because

$$A_{\mathbf{k}}^2 |u_{\mathbf{k},+}|^2 = C_{1,+}, \tag{240}$$
$$A_{\mathbf{k}}^2 |v_{\mathbf{k},+}|^2 = C_{2,+}, \tag{241}$$
$$B_{\mathbf{k}}^2 |u_{\mathbf{k},-}|^2 = C_{1,-}, \tag{242}$$
$$B_{\mathbf{k}}^2 |v_{\mathbf{k},-}|^2 = C_{2,-}, \tag{243}$$

we have that the spectral function for the atoms obtained from the operator formalism is the same as the spectral function obtained from the Green's function in (92). Numerical plots of the spectral function in the high-momentum and low-momentum region, are given in respectively Figure 12 and Figure 13. Furthermore for the phonon field

$$\rho(\mathbf{k}, \omega) = B_{\mathbf{k},+}^2\{\delta(\omega - \omega_+) - \delta(\omega + \omega_+)\} + B_{\mathbf{k},-}^2\{\delta(\omega - \omega_-) - \delta(\omega + \omega_-)\}\Theta(|\mathbf{k}| - |\mathbf{k}_1|) \tag{244}$$

which can be verified by using the calculation of the spectral function for the atoms for $u_{\mathbf{k},\sigma} = v_{\mathbf{k},\sigma} = 1$. Hence, we find for the phonon field,

$$\int d\omega \rho(\mathbf{k}, \omega) = 0. \tag{245}$$

By using (172) and (173), the analogy of the frequency sum rule of the atoms is given by

$$\int d\omega \rho(\mathbf{k}, \omega)\omega = 1. \tag{246}$$

This rule is only satisfied if all dispersions are real. In analogy with the previous case, where the atoms are integrated out, we can also use the action from (125) to calculate the spectral function for the phonons. By doing this, we can verify our expressions for $B_{\mathbf{k},\sigma}$ as the spectral functions should be the same in both formalisms. First write

$$G_{\text{ph}}(\mathbf{k}, \omega^+) = \frac{\alpha + i\beta\epsilon}{\gamma + i\zeta\epsilon}, \tag{247}$$

where

$$\alpha = (\hbar\omega)^2 - (\mathbf{k}^2 + \Delta)^2, \tag{248}$$
$$\beta = 2\hbar\omega, \tag{249}$$
$$\gamma = 2[2g^2(\mathbf{k}^2 + \Delta) + (c^2k^2 - (\hbar\omega)^2)((\hbar\omega)^2 - (\mathbf{k}^2 + \Delta)^2)], \tag{250}$$
$$\zeta = 4\hbar\omega[c^2\mathbf{k}^2 + (\mathbf{k}^2 + \Delta)^2 - 2(\hbar\omega)^2]. \tag{251}$$

Hence

$$\frac{1}{\pi}\text{Im}[G_{\text{ph}}(\mathbf{k},\omega^+)] = -\frac{\alpha}{\zeta}\delta\left(\frac{\gamma}{\zeta}\right) \tag{252}$$

$$= \sum_{\sigma\in\{+,-\}} -\frac{\alpha}{\zeta}\Big|_{\hbar\omega_\sigma}\{\delta(\omega-\omega_\sigma)-\delta(\omega+\omega_\sigma)\}.$$

Here we used (235). Because

$$-\frac{\alpha}{\zeta}\Big|_{\hbar\omega_\sigma} = B^2_{\mathbf{k},\sigma}, \tag{253}$$

we have that the spectral function obtained from the field-theoretical approach is the same as the one obtained from the operator formalism. However, we still do not satisfy the frequency sum rule if there are imaginary dispersions. To obtain a spectral function that satisfies this sum rule, we should find a generalized Fourier transform of the exponentially growing function. But since we have the explicit expression for the atomic and the phonon field operators, which satisfy the commutation relations and the equations of motion, we can switch to the operator formalism to calculate physical quantities.

5.3.2 Correlations

Because we have the explicit expression for the atomic and the phonon field, and written the complex mode operators in terms of bosonic operators, we can calculate some correlations. To calculate these expectation values we need an orthonormal set. Therefore, consider the set $\{|\mathbf{N},\tilde{\mathbf{N}}\rangle\} = \{|\mathbf{N}\rangle\otimes|\tilde{\mathbf{N}}\rangle\} = \{|....,N_{\mathbf{k}},....\rangle\otimes|....,\tilde{N}_{\mathbf{n}},....\rangle\}$. Here, $|\mathbf{N},\tilde{\mathbf{N}}\rangle$ corresponds to a state with N excitations with energy $\hbar\omega_+$ and $\tilde{N}$ excitations with energy $\hbar\omega_-$. Here the single-particle occupation numbers $N_{\mathbf{k}}$ and $\tilde{N}_{\mathbf{n}}$ are such that $\sum_{\mathbf{n}}\tilde{N}_{\mathbf{n}} = \tilde{N}$ and $\sum_{\mathbf{k}}N_{\mathbf{k}} = N$. By relaxing these constraints, this set becomes an orthonormal basis for the Hilbert space of all symmetric many-body states. This space is known as Fock space. We define the annihilation operators $\hat{\alpha}_{\mathbf{m}}$, $\hat{b}_{\mathbf{m}}$, $\hat{d}_{\mathbf{n},+}$ and $\hat{d}_{\mathbf{n},-}$ acting on a Fock state $|\mathbf{N},\tilde{\mathbf{N}}\rangle$ by

$$\hat{\alpha}_{\mathbf{m}}|\mathbf{N},\tilde{\mathbf{N}}\rangle = \sqrt{N_{\mathbf{m}}}\left(|....,N_{\mathbf{m}}-1,....\rangle\otimes|\tilde{\mathbf{N}}\rangle\right), \tag{254}$$

$$\hat{d}_{\mathbf{n},+}|\mathbf{N},\tilde{\mathbf{N}}\rangle = \sqrt{N_{\mathbf{n}}}\left(|....,N_{\mathbf{n}}-1,....\rangle\otimes|\tilde{\mathbf{N}}\rangle\right), \tag{255}$$

$$\hat{b}_{\mathbf{m}}|\mathbf{N},\tilde{\mathbf{N}}\rangle = \sqrt{\tilde{N}_{\mathbf{m}}}\left(|\mathbf{N}\rangle\otimes|....,\tilde{N}_{\mathbf{m}}-1,....\rangle\right), \tag{256}$$

$$\hat{d}_{\mathbf{n},-}|\mathbf{N},\tilde{\mathbf{N}}\rangle = \sqrt{\tilde{N}_{\mathbf{n}}}\left(|\mathbf{N}\rangle\otimes|....,\tilde{N}_{\mathbf{n}}-1,....\rangle\right). \tag{257}$$

where $|\mathbf{m}| < |\mathbf{k}_1|$ and $|\mathbf{n}| > |\mathbf{k}_1|$. Because $\hat{\alpha}_{\mathbf{k}}$, $\hat{b}_{\mathbf{k}}$ and $\hat{d}_{\mathbf{k},\sigma}$ are bosonic operators this implies

$$\hat{\alpha}^\dagger_{\mathbf{m}}\left(|....,N_{\mathbf{m}},....\rangle\otimes|\tilde{\mathbf{N}}\rangle\right) = \sqrt{1+N_{\mathbf{m}}}\left(|....,N_{\mathbf{m}}+1,....\rangle\otimes|\tilde{\mathbf{N}}\rangle\right), \tag{258}$$

$$\hat{d}^\dagger_{\mathbf{n},+}\left(|....,N_{\mathbf{n}},....\rangle\otimes|\tilde{\mathbf{N}}\rangle\right) = \sqrt{1+N_{\mathbf{n}}}\left(|....,N_{\mathbf{n}}+1,....\rangle\otimes|\tilde{\mathbf{N}}\rangle\right), \tag{259}$$

$$\hat{b}^\dagger_{\mathbf{m}}\left(|\mathbf{N}\rangle\otimes|....,\tilde{N}_{\mathbf{m}},....\rangle\right) = \sqrt{1+\tilde{N}_{\mathbf{m}}}\left(|\mathbf{N}\rangle\otimes|....,\tilde{N}_{\mathbf{m}}+1,....\rangle\right), \tag{260}$$

$$\hat{d}^\dagger_{\mathbf{n},-}\left(|\mathbf{N}\rangle\otimes|....,\tilde{N}_{\mathbf{n}},....\rangle\right) = \sqrt{1+\tilde{N}_{\mathbf{n}}}\left(|\mathbf{N}\rangle\otimes|....,\tilde{N}_{\mathbf{n}}+1,....\rangle\right). \tag{261}$$

Furthermore the vacuum state $|0\rangle$ is defined by

$$|0\rangle := |0\rangle_\alpha\otimes|0\rangle_b. \tag{262}$$

Observe that the vacuum state with zero particles $|0\rangle$ is the tensor product of the vacuum of the bosonic operators $\hat{\alpha}_{\mathbf{m}}$ and $\hat{b}_{\mathbf{m}}$. Note that the operators $\hat{b}_{\mathbf{m}}$ and $\hat{d}_{\mathbf{n},-}$ have the same vacuum. The

only difference between both is that $\hat{b}_{\mathbf{m}}^{\dagger}$ creates excitations with low-momentum and $\hat{d}_{\mathbf{n},-}^{\dagger}$ creates excitations with high-momentum. The same arguments also hold for the bosonic operators $\hat{d}_{\mathbf{n},+}^{\dagger}$ and $\hat{\alpha}_{\mathbf{m}}^{\dagger}$. Hence,

$$
\begin{aligned}
\hat{\alpha}_{\mathbf{m}}|0\rangle &= 0, \\
\hat{b}_{\mathbf{m}}|0\rangle &= 0, \\
\hat{d}_{\mathbf{n},-}|0\rangle &= 0, \\
\hat{d}_{\mathbf{n},+}|0\rangle &= 0
\end{aligned}
\tag{263}
$$

for all $\mathbf{m} < |\mathbf{k}_1|$ and $\mathbf{n} > |\mathbf{k}_1|$. From (258),(259),(260) and (261), it follows that any state $|\mathbf{N},\tilde{\mathbf{N}}\rangle$ in Fock space can be expressed as product of bosonic creation operators

$$
\begin{aligned}
|\mathbf{N},\tilde{\mathbf{N}}\rangle &= \prod_{\mathbf{k},\mathbf{p},\mathbf{m},\mathbf{n}} \frac{1}{\sqrt{N_{\mathbf{k}}!}\sqrt{N_{\mathbf{p}}!}\sqrt{\tilde{N}_{\mathbf{n}}!}\sqrt{\tilde{N}_{\mathbf{m}}!}} (\hat{\alpha}_{\mathbf{k}}^{\dagger})^{N_{\mathbf{k}}}(\hat{d}_{\mathbf{p},+}^{\dagger})^{N_{\mathbf{p}}}(\hat{b}_{\mathbf{n}}^{\dagger})^{\tilde{N}_{\mathbf{n}}}(\hat{d}_{\mathbf{m},-}^{\dagger})^{\tilde{N}_{\mathbf{m}}}|0\rangle \\
&:= \prod_{\mathbf{k},\mathbf{p},\mathbf{m},\mathbf{n}} \frac{(\hat{\alpha}_{\mathbf{k}}^{\dagger})^{N_{\mathbf{k}}}(\hat{d}_{\mathbf{p},+}^{\dagger})^{N_{\mathbf{p}}}|0\rangle_{\alpha} \otimes (\hat{b}_{\mathbf{n}}^{\dagger})^{\tilde{N}_{\mathbf{n}}}(\hat{d}_{\mathbf{m},-}^{\dagger})^{\tilde{N}_{\mathbf{m}}}|0\rangle_{b}}{\sqrt{N_{\mathbf{k}}!}\sqrt{N_{\mathbf{p}}!}\sqrt{\tilde{N}_{\mathbf{n}}!}\sqrt{\tilde{N}_{\mathbf{m}}!}}.
\end{aligned}
\tag{264}
$$

Note that the order of the creation operators is unimportant since we have bosonic creation operators. Furthermore we have the constraints

$$
\sum_{\mathbf{m}<|\mathbf{k}_1|}\tilde{N}_{\mathbf{m}} + \sum_{\mathbf{n}>|\mathbf{k}_1|}\tilde{N}_{\mathbf{n}} = \tilde{N},
\tag{265}
$$

$$
\sum_{\mathbf{l}<|\mathbf{k}_1|}N_{\mathbf{l}} + \sum_{\mathbf{p}>|\mathbf{k}_1|}N_{\mathbf{p}} = N.
\tag{266}
$$

Furthermore, the inner product between two states is given by

$$
\begin{aligned}
\langle \mathbf{N},\tilde{\mathbf{N}}|\mathbf{N}',\tilde{\mathbf{N}}'\rangle &= \prod_{\mathbf{k},\mathbf{k}',\mathbf{p},\mathbf{p}'} \frac{{}_{\alpha}\langle 0|(\hat{\alpha}_{\mathbf{k}})^{N_{\mathbf{k}}}(\hat{d}_{\mathbf{p},+})^{\tilde{N}_{\mathbf{p}'}}(\hat{d}_{\mathbf{p},+}^{\dagger})^{N_{\mathbf{p}}}(\hat{\alpha}_{\mathbf{k}'}^{\dagger})^{N_{\mathbf{k}'}}|0\rangle_{\alpha}}{\sqrt{N_{\mathbf{k}}!}\sqrt{N_{\mathbf{p}}!}\sqrt{N_{\mathbf{p}'}!}\sqrt{N_{\mathbf{k}'}!}} \\
&\times \prod_{\mathbf{n},\mathbf{m},\mathbf{n}',\mathbf{m}'} \frac{{}_{b}\langle 0|(\hat{b}_{\mathbf{n}})^{\tilde{N}_{\mathbf{n}}}(\hat{d}_{\mathbf{m},-})^{\tilde{N}_{\mathbf{m}}}(\hat{d}_{\mathbf{m},-}^{\dagger})^{\tilde{N}_{\mathbf{m}'}}(\hat{b}_{\mathbf{n}'}^{\dagger})^{\tilde{N}_{\mathbf{n}'}}|0\rangle_{b}}{\sqrt{\tilde{N}_{\mathbf{m}}!}\sqrt{\tilde{N}_{\mathbf{n}'}!}\sqrt{\tilde{N}_{\mathbf{n}}!}\sqrt{\tilde{N}_{\mathbf{m}'}!}}.
\end{aligned}
\tag{267}
$$

Hence,

$$
\langle \mathbf{N},\tilde{\mathbf{N}}|\mathbf{N}',\tilde{\mathbf{N}}'\rangle = \delta_{\mathbf{N},\mathbf{N}'}\delta_{\tilde{\mathbf{N}},\tilde{\mathbf{N}}'},
\tag{268}
$$

where we used (258) and (259). Thus our basis is indeed orthonormal and therefore it is clear that

$$
\langle \hat{\psi}(\mathbf{x},t)\rangle = \langle \hat{\psi}^{\dagger}(\mathbf{x},t)\rangle = \langle \hat{\phi}(\mathbf{x},t)\rangle = 0,
\tag{269}
$$

by using the explicit expressions of the phonon and atomic field operators given in (169), (170), (171). We also used the expressions of the complex operators in terms of the bosonic operators given in (163) and (164). This result can also be understood classically as the expectation value of the field operators is such that the potential has an extremum. Furthermore, classically we should expect that the particles remain in this metastable equilibrium. However, due to quantum fluctuations we get a non-zero probability of finding a particle at a different position. To illustrate this, let us determine some correlation functions. Therefore, we first need to calculate the expectation

value of products of two complex operators

$$\langle \hat{\beta}_{\mathbf{m}} \hat{\beta}_{\mathbf{m}'} \rangle \quad := \quad \frac{1}{2} \langle \mathbf{N}, \tilde{\mathbf{N}} | \left(\hat{b}_{\mathbf{m}} + \hat{b}^\dagger_{-\mathbf{m}} \right) \left(\hat{b}_{\mathbf{m}'} + \hat{b}^\dagger_{-\mathbf{m}'} \right) | \mathbf{N}, \tilde{\mathbf{N}} \rangle \tag{270}$$

$$= \quad \frac{1}{2} \langle \mathbf{N}, \tilde{\mathbf{N}} | \left(\hat{b}_{\mathbf{m}} \hat{b}^\dagger_{-\mathbf{m}'} + \hat{b}^\dagger_{-\mathbf{m}} \hat{b}_{\mathbf{m}'} \right) | \mathbf{N}, \tilde{\mathbf{N}} \rangle$$

$$= \quad \frac{1}{2} \delta_{\mathbf{m}, -\mathbf{m}'} \left(1 + \tilde{N}_{\mathbf{m}} + \tilde{N}_{-\mathbf{m}} \right),$$

$$\langle \hat{\gamma}_{\mathbf{m}} \hat{\gamma}_{\mathbf{m}'} \rangle \quad := \quad -\frac{1}{2} \langle \mathbf{N}, \tilde{\mathbf{N}} | \left(\hat{b}_{\mathbf{m}} - \hat{b}^\dagger_{-\mathbf{m}} \right) \left(\hat{b}_{\mathbf{m}'} - \hat{b}^\dagger_{-\mathbf{m}'} \right) | \mathbf{N}, \tilde{\mathbf{N}} \rangle = \langle \hat{\beta}_{\mathbf{m}} \hat{\beta}_{\mathbf{m}'} \rangle, \tag{271}$$

$$\langle \hat{\beta}_{\mathbf{m}} \hat{\gamma}_{\mathbf{m}'} \rangle \quad := \quad \frac{i}{2} \langle \mathbf{N}, \tilde{\mathbf{N}} | \left(\hat{b}_{\mathbf{m}} + \hat{b}^\dagger_{-\mathbf{m}} \right) \left(\hat{b}_{\mathbf{m}'} - \hat{b}^\dagger_{-\mathbf{m}'} \right) | \mathbf{N}, \tilde{\mathbf{N}} \rangle \tag{272}$$

$$= \quad -\frac{i}{2} \langle \mathbf{N}, \tilde{\mathbf{N}} | \left(\hat{b}_{\mathbf{m}} \hat{b}^\dagger_{-\mathbf{m}'} - \hat{b}^\dagger_{-\mathbf{m}} \hat{b}_{\mathbf{m}'} \right) | \mathbf{N}, \tilde{\mathbf{N}} \rangle$$

$$= \quad -\frac{i}{2} \delta_{\mathbf{m}, -\mathbf{m}'} \left(1 + \tilde{N}_{\mathbf{m}} - \tilde{N}_{-\mathbf{m}} \right),$$

$$\langle \hat{\gamma}_{\mathbf{m}} \hat{\beta}_{\mathbf{m}'} \rangle \quad := \quad \frac{i}{2} \langle \mathbf{N}, \tilde{\mathbf{N}} | \left(\hat{b}_{\mathbf{m}} - \hat{b}^\dagger_{-\mathbf{m}} \right) \left(\hat{b}_{\mathbf{m}'} + \hat{b}^\dagger_{-\mathbf{m}'} \right) | \mathbf{N}, \tilde{\mathbf{N}} \rangle = -\langle \hat{\beta}_{\mathbf{m}} \hat{\gamma}_{\mathbf{m}'} \rangle, \tag{273}$$

where $\tilde{N}_{\mathbf{m}}$ is the occupation number of excitations with energy $\hbar\omega_-$. Furthermore, for the bosonic operators $\hat{\alpha}_{\mathbf{k}}$ and $\hat{\alpha}^\dagger_{\mathbf{k}}$

$$\langle \hat{\alpha}_{\mathbf{m}} \hat{\alpha}^\dagger_{\mathbf{m}'} \rangle \quad = \quad (1 + N_{\mathbf{m}}) \, \delta_{\mathbf{m}, \mathbf{m}'}, \tag{274}$$

$$\langle \hat{\alpha}^\dagger_{\mathbf{m}} \hat{\alpha}_{\mathbf{m}'} \rangle \quad = \quad N_{\mathbf{m}} \delta_{\mathbf{m}, \mathbf{m}'}, \tag{275}$$

$$\langle \hat{\alpha}_{\mathbf{m}} \hat{\alpha}_{\mathbf{m}'} \rangle \quad = \quad \langle \hat{\alpha}^\dagger_{\mathbf{m}} \hat{\alpha}^\dagger_{\mathbf{m}'} \rangle = 0. \tag{276}$$

Here $N_{\mathbf{m}}$ is the occupation number of excitations with energy $\hbar\omega_+$. Note that there are similar expressions for the expectation values of products the bosonic operators $\hat{d}_{\mathbf{k},\sigma}$. By using the expressions of these expectation values, we can determine all kinds of correlation functions. First, we calculate

$$\langle \hat{\psi}(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{y}, t) \rangle \quad = \quad \sum_{\mathbf{k}} \left[A_{\mathbf{k}}^2 \{ (1 + N_{\mathbf{k}}) u_{\mathbf{k},+}(\mathbf{x}) u^*_{\mathbf{k},+}(\mathbf{y}) + N_{\mathbf{k}} v^*_{\mathbf{k},+}(\mathbf{x}) v_{\mathbf{k},+}(\mathbf{y}) \} \right] \tag{277}$$

$$+ \quad \frac{1}{2} \sum_{\mathbf{k} < |\mathbf{k}_1|} \left[B_{\mathbf{k}}^2 \left(1 + \tilde{N}_{\mathbf{k}} \right) \left\{ \cosh(2|\omega_-|t) \frac{(\mathbf{k}^2 + \Delta)^2 - (\hbar\omega_-)^2}{2(\mathbf{k}^2 + \Delta)|\hbar\omega_-|} + 1 \right\} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right]$$

$$+ \quad \frac{1}{2} \sum_{\mathbf{k} < |\mathbf{k}_1|} \left[B_{\mathbf{k}}^2 \tilde{N}_{-\mathbf{k}} \left\{ \cosh(2|\omega_-|t) \frac{(\mathbf{k}^2 + \Delta)^2 - (\hbar\omega_-)^2}{2(\mathbf{k}^2 + \Delta)|\hbar\omega_-|} - 1 \right\} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right]$$

$$+ \quad \sum_{\mathbf{k} > |\mathbf{k}_1|} \left[B_{\mathbf{k}}^2 \{ (1 + \tilde{N}_{\mathbf{k}}) u_{\mathbf{k},-}(\mathbf{x}) u^*_{\mathbf{k},-}(\mathbf{y}) + \tilde{N}_{\mathbf{k}} v^*_{\mathbf{k},-}(\mathbf{x}) v_{\mathbf{k},-}(\mathbf{y}) \} \right],$$

where we also used the explicit expressions for $\tilde{u}_{\mathbf{k},\sigma}(\mathbf{x})$ and $\tilde{v}_{\mathbf{k},\sigma}(\mathbf{x})$ given in (139) and (140). This expression gives the probability for finding a single atom at time t and position $\mathbf{x}$ that was added at position $\mathbf{y}$ at the same time t. For completeness, we will also give the expression for the other correlation functions

$$\langle \hat{\psi}(\mathbf{x}, t) \hat{\psi}(\mathbf{y}, t) \rangle \quad = \quad \sum_{\mathbf{k}} \left[A_{\mathbf{k}}^2 \{ (1 + N_{\mathbf{k}}) u_{\mathbf{k},+}(\mathbf{x}) v^*_{\mathbf{k},+}(\mathbf{y}) + N_{\mathbf{k}} v^*_{\mathbf{k},+}(\mathbf{x}) u_{\mathbf{k},+}(\mathbf{y}) \} \right] \tag{278}$$

$$+ \quad \frac{i}{2} \sum_{\mathbf{k} < |\mathbf{k}_1|} \left[B_{\mathbf{k}}^2 M_{\mathbf{k}} \left\{ e^{2|\omega_-|t} \tilde{u}_{\mathbf{k},+} \tilde{u}_{-\mathbf{k},+} + e^{-2|\omega_-|t} \tilde{v}^*_{-\mathbf{k},-} \tilde{v}^*_{\mathbf{k},-} \right\} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right]$$

$$+ \quad \sum_{\mathbf{k} > |\mathbf{k}_1|} \left[B_{\mathbf{k}}^2 \{ (1 + \tilde{N}_{\mathbf{k}}) u_{\mathbf{k},-}(\mathbf{x}) v^*_{\mathbf{k},-}(\mathbf{y}) + \tilde{N}_{\mathbf{k}} v^*_{\mathbf{k},-}(\mathbf{x}) u_{\mathbf{k},-}(\mathbf{y}) \} \right].$$

Note that the expression for $\langle \hat{\psi}^\dagger(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{y}, t)\rangle$ can be obtained by taking the complex conjugate of $\langle \hat{\psi}(\mathbf{x}, t)\hat{\psi}(\mathbf{y}, t)\rangle$ and interchanging $\mathbf{x}$ and $\mathbf{y}$. Also

$$\langle \hat{\phi}(\mathbf{x}, t)\hat{\phi}(\mathbf{y}, t)\rangle = \sum_{\mathbf{k}} \left[C_{\mathbf{k}}^2(1 + N_{\mathbf{k}} + N_{-\mathbf{k}})\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right] \tag{279}$$

$$+ \sum_{\mathbf{k}<|\mathbf{k}_1|} \left[D_{\mathbf{k}}^2 \cosh(2|\omega_-|t)M_{\mathbf{k}}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right] + \sum_{\mathbf{k}>|\mathbf{k}_1|} \left[F_{\mathbf{k},-}^2 M_{\mathbf{k}}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right],$$

and finally,

$$\langle \hat{\psi}(\mathbf{x}, t)\hat{\phi}(\mathbf{y}, t)\rangle = \sum_{\mathbf{k}} \left[A_{\mathbf{k}}C_{\mathbf{k}}\{(1 + N_{\mathbf{k}})u_{\mathbf{k},+} + N_{-\mathbf{k}}v_{-\mathbf{k},+}^*\}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right] \tag{280}$$

$$+ \frac{1}{2}\sum_{\mathbf{k}<|\mathbf{k}_1|} e^{i\frac{\pi}{4}} \left[B_{\mathbf{k}}D_{\mathbf{k}}M_{\mathbf{k}}\left\{ e^{2|\omega_-|t}\tilde{u}_{\mathbf{k},+} + e^{-2|\omega_-|t}\tilde{v}_{-\mathbf{k},-}^* \right\}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right]$$

$$+ \frac{1}{2}\sum_{\mathbf{k}<|\mathbf{k}_1|} \left[B_{\mathbf{k}}D_{\mathbf{k}}\left(1 + \tilde{N}_{\mathbf{k}} - \tilde{N}_{-\mathbf{k}}\right)\frac{|\hbar\omega_-|}{\sqrt{4(\mathbf{k}^2 + \Delta)|\hbar\omega_-|}}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right]$$

$$+ \frac{1}{2}\sum_{\mathbf{k}>|\mathbf{k}_1|} \left[B_{\mathbf{k}}F_{\mathbf{k},-}\{(1 + \tilde{N}_{\mathbf{k}})u_{\mathbf{k},-} + \tilde{N}_{-\mathbf{k}}v_{-\mathbf{k},-}^*\}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{V} \right],$$

where

$$M_{\mathbf{k}} := \left(1 + \tilde{N}_{\mathbf{k}} + \tilde{N}_{-\mathbf{k}}\right). \tag{281}$$

All these correlation functions show the same behaviour. Namely, if time increases the correlation functions exponentially increase. Furthermore, the expectation value of the number of particles, which for respectively atoms and phonons is defined as

$$\langle \hat{N}_{\text{at}}\rangle(t) = \int d\mathbf{x}\langle \hat{\psi}^\dagger(\mathbf{x}, t)\hat{\psi}(\mathbf{x}, t)\rangle, \tag{282}$$

$$\langle \hat{N}_{\text{ph}}\rangle(t) = \int d\mathbf{x}\langle \hat{\phi}(\mathbf{x}, t)\hat{\phi}(\mathbf{x}, t)\rangle, \tag{283}$$

also increases exponentially in time. The growth of the number of phonons is a consequence of the instability for the phonons discussed in section 5.1. Furthermore due to the linear coupling between the atomic and the phonon field, also the number of atoms grows in time. This model can also be compared with a laser. In a laser the number of photons grows in time due to stimulated emission. Therefore, our coupled atom-phonon model can schematically be compared with a laser, where the role of the photons is played by the phonon. However, in our model also the number of atoms increases, while in a laser, the number of atoms should remain constant. To obtain a more realistic model for a laser, we should change the coupling term in our model. For example we should have a term

$$g\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\psi^*(\mathbf{x}, \tau)\psi(\mathbf{x}, \tau)\phi(\mathbf{x}, \tau). \tag{284}$$

Then instead of the linear coupling where an atom is annihilated and a phonon created and visa versa, we have the processes that describes emission. Namely, this coupling term describes the process where an atom is annihilated and a phonon and an atom are created. The reversed process is of course also described by these terms. By incorporating this coupling term, we would have a more realistic model of a laser.

6 Conclusions and discussion

In this thesis we considered a gas of ultracold bosons at unitarity. First we discussed a many-body theory that correctly describes the two-atom physics near a Feshbach resonance. In addition, this effective theory is used to make a prediction of the energy per particle in the unitarity limit. By using a mean-field theory, we end up with a divergence of the chemical potential and therefore also the energy per particle is infinite. Besides this experimental relevant solution of an atomic condensate, we also found that this mean-field theory incorporates the actual groundstate which consists of a condensate of molecules.

In the mean-field calculations we neglected the depletion of the condensate. However, for reliable results, we should also include these fluctuations. In this thesis we started to incorporate these fluctuations in the theory. However, by using the Bogoliubov approximation we end up with an ill-behaved spectral function. Namely, for some momenta the spectral function is negative for $\omega > 0$ and positive for $\omega < 0$. Furthermore, this spectral function does not satisfy the sum rule. The latter is caused by the poles of in the spectral function in the upper complex plane.

To get a better understanding of these complex dispersions, we also considered another model where poles with positive imaginary part exist. We showed that these complex dispersions always occur with a linearly coupled harmonic oscillator, and therefore we studied a model consisting of linearly coupled atoms and phonons. In the operator formalism both fields, which describe the atoms and phonons, are quantized. To get full expressions for the atomic and phonon field operators, which satisfy the canonical commutation relations and the equations of motion, we have to incorporate all dispersions. The fact that we satisfy the commutation relations and nonetheless violate the sum rule, is caused by the fact that we cannot simply Fourier transform exponentially growing functions. In this model the imaginary parts are related to the instability of the model, and therefore we also obtain that correlations and the number of particles are not constant in time.

In the near future, we will continue on incorporating depletion into our theory. For fermions it is already known how to incorporate the fluctuations [8]. Hopefully, by doing similar calculations for bosons, we can in the future obtain a more physical result for the energy per particle in the unitarity limit.

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References

[1] J. Carlson and S. Reddy. Asymmetric two-component fermion systems in strong coupling. *Physical Review Letters*, 95(6), 2005.

[2] S. Cowell, H. Heiselberg, I. Mazets, J. Morales, V. Pandharipande, and C. Pethick. Cold bose gases with large scattering lengths. *Physical Review Letters*, 88(21), 2002.

[3] R. A. Duine and H. T. C. Stoof. Atom-molecule coherence in Bose gases. *Physics Reports-Review section of Physics Letters*, 396(3):115–195, 2004.

[4] S. Inouye, M. Andrews, J. Stenger, H. Miesner, D. Stamper-Kurn, and W. Ketterle. Observation of Feshbach resonances in a Bose-Einstein condensate. *Nature*, 392(6672):151–154, 1998.

[5] T. D. Lee, K. Huang, and C. N. Yang. Eigenvalues and Eigenfunctions of a Bose System of Hard Spheres and Its Low-Temperature Properties. *Physical Review*, 106(6):1135–1145, 1957.

[6] M. Mine, M. Okumura, T. Sunaga, and Y. Yamanaka. Quantum Field Theoretical Description of Unstable Behavior of Trapped Bose-Einstein Condensates with Complex Eigenvalues of Bogoliubov-de Gennes Equations. *arXiv:cond-mat/0609052v2*, 2006.

[7] S. Pollack, D. Dries, M. Junker, Y. P. Chen, T. Corcovilos, and R. Hulet. Extreme tunability of interactions in a 7Li Bose-Einstein condensate. *Physical Review Letters*, 102(9), 2009.

[8] M. W. J. Romans and H. T. C. Stoof. Bogoliubov theory of Feshbach molecules in the BEC-BCS crossover. *Physical Review A*, 74(5), 2006.

[9] J. J. Sakurai. *Modern Quantum Mechanics*. Addison Wesley, 1994.

[10] H. T. C. Stoof, K. B. Gubbels, and D. B. M. Dickerscheid. *Ultracold Quantum Fields*. Springer, 2009.

[11] E. Tiesinga, B. Verhaar, and H. Stoof. Threshold and Resonance Phenomena in Ultracold Ground-State Collisions. *Physical Review A*, 47(5, Part b):4114–4122, 1993.

[12] M. Veldhoen. Cold Bose Gases near a Feshbach Resonance. *MSc thesis, ITF Utrecht*, 2010.

[13] R. Wild, P. Makotyn, J. Pino, E. Cornell, and D. Jin. Contact Measurements on Atomic BEC. *arXiv:1112.0362v1*, 2011.