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Excitations in dense Bose gases of tilted dipoles in coupled 2D-layers

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Abstract

In this bachelor thesis excitations in strongly interacting dipolar Bose gases, that are trapped in coupled 2D-layers, are investigated. Equations of motion are derived using a least-action principle equivalent to the Schrödinger equation. We solve the equations of motion to determine the density-density linear response matrix in a very general way for inhomogeneous multi-component systems. This result is a generalisation of the work of Clements et al. [Phys. Rev. B 53.18, 12253 (1996)] for multi-component systems. We discuss how the general formalism can be applied to homogeneous systems and how numerical evaluations can be performed for them. Based on the ground state results from Martin Hebenstreit [Bachelor thesis, JKU Linz, 2013], obtained with the hypernetted-chain Euler-Lagrange method, numerical evaluations of the density-density response matrix are performed for one- and bilayer systems, that have either a polarisation perpendicular to the layers or a tilted polarisation. We find systems with tilted dipoles, that are about to solidify in the direction orthogonal to the polarisation of the system.

Zusammenfassung

In dieser Bachelorarbeit werden stark wechselwirkende dipolare Bose-Systeme in gekoppelten 2D-Schichten untersucht. Bewegungsgleichungen werden unter Verwendung des Prinzips der kleinsten Wirkung äquivalent zur Schrödinger-Gleichung abgeleitet. Wir lösen die Bewegungsgleichungen um die Dichte-Dichte „linear response“-Matrix in einer sehr allgemeinen Form für inhomogene mehrkomponentige Systeme zu bestimmen. Dieses Ergebnis ist eine Verallgemeinerung der Arbeit von Clements et al. [Phys. Rev. B 53.18, 12253 (1996)] für mehrkomponentige Systeme. Wir diskutieren, wie der allgemeine Formalismus auf homogene Systeme angewandt und numerische Auswertungen durchgeführt werden können. Basierend auf den Grundzustands-Ergebnissen von Martin Hebenstreit [Bachelorarbeit, JKU Linz, 2013], die mithilfe der „hypernetted-chain Euler-Lagrange“-Methode ermittelt wurden, werden numerische Auswertungen der Dichte-Dichte ‘response’-Matrix für ein- und zweischichtige Systeme durchgeführt, die entweder eine Polarisation normal zu den Ebenen oder eine gekippte Polarisation aufweisen. Dabei finden wir Systeme mit gekippten Dipolen vor, die sich in der Richtung normal zur Polarisation beinahe verfestigen.

Acknowledgements

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Of course I am also very thankful for the good cooperation with *Martin Hebenstreit*, who provided me with the ground state data from his bachelor thesis, which he wrote in parallel to my thesis.

Last but not least, I also want to thank my *parents* for enabling me to study physics. All my life they encouraged and supported me to study, what I am interested in and for this I am more thankful than words could say.

Contents

1 Introduction

This bachelor thesis deals with excitations in dipolar boson systems consisting of multiple 2D-layers (see figure 1.1) at low temperatures, which is equivalent to multi-component Bose systems, if we allow no tunnelling or hopping between the layers. Experiments of this kind can nowadays be performed in laboratories, for example see [Aik+12], [Lah+07], [Lu+11], [Stu+12] and [Tak+12]. For more details about dipolar quantum gases see the review article [Bar+12].

In the first part of this work we derive a general formalism for excitations in inhomogeneous systems of multiple particle types and later carry out numerical evaluations, where each 2D-layer is treated as a different particle type. This approach has the advantage, that our system is homogeneous, which makes computations both easier and faster. An alternative would be a calculation for an inhomogeneous one-component 3D-system.

Two parallel aligned dipoles interact via the pair interaction potential

$$v(\boldsymbol{r}) = \frac{1}{4\pi}\left(\frac{\mu^2}{r^3} - 3\frac{(\boldsymbol{r}\cdot\boldsymbol{\mu})^2}{r^5}\right), \tag{1.1}$$

where $\boldsymbol{\mu}$ is a generalised dipole moment, such that for the magnetic case $\boldsymbol{\mu} = \sqrt{\mu_0}\boldsymbol{\mu}_{\mathrm{mag}}$ with the permeability of free space μ_0 and $\boldsymbol{r}$ is the vector connecting the two interacting dipoles. For dipole moments $\boldsymbol{\mu} = \mu\left(\sin(\vartheta)\hat{\boldsymbol{e}}_x + \cos(\vartheta)\hat{\boldsymbol{e}}_z\right)$ (see figure 1.1) the intra- and inter-layer pair potential along the x- and the y-axis is shown in figure 1.2.

Within this bachelor thesis the results of Clements, Krotscheck, and Tymczak [CKT96] were generalised for multi-component systems by performing the whole derivation again including each detail and applying the multi-component adaptations. Also the source code necessary for the numeric evaluations was implemented as a part of this work.

In the following chapter 2 we will derive equations of motion for our systems analogous to the work of Saarela, Apaja, and Halinen [SAH04] using a variational principle as it was suggested by Kerman and Koonin [KK76].

Afterwards we will solve the equations of motion in chapter 3 based on the work of [CKT96] and Clements et al. [Cle+93] to obtain an expression for the density-density response function. The main difference between the referenced investigations and the present thesis is the generalisation from single- to multi-component systems, which requires a new reasonable notation, as for example the response function is no longer a scalar, but a matrix.

Finally in chapter 4 we perform numerical evaluations of the density-density response matrix for bilayer Bose gases. We especially focus on anisotropic, but homogeneous bilayer systems, where the dipole moments of the particles are not perpendicular to the layers. The calculation of the response function requires knowledge of the ground state, which is provided from the hypernetted-chain Euler-Lagrange computations of Martin Hebenstreit [Heb13].

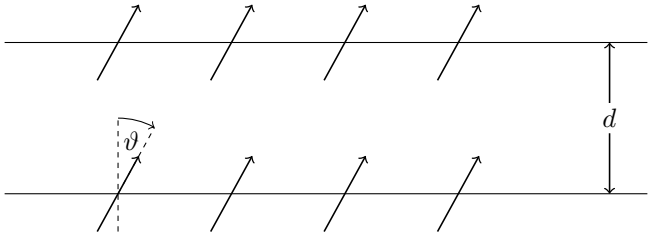


Figure 1.1: A sketch of the experimental setup, where the horizontal lines represent the 2D-layers parallel to the xy-plane with a distance of d. The small arrows illustrate the single bosons with the direction of their dipole moments $\boldsymbol{\mu} = \mu\,(\sin(\vartheta)\hat{\boldsymbol{e}}_x + \cos(\vartheta)\hat{\boldsymbol{e}}_z)$.

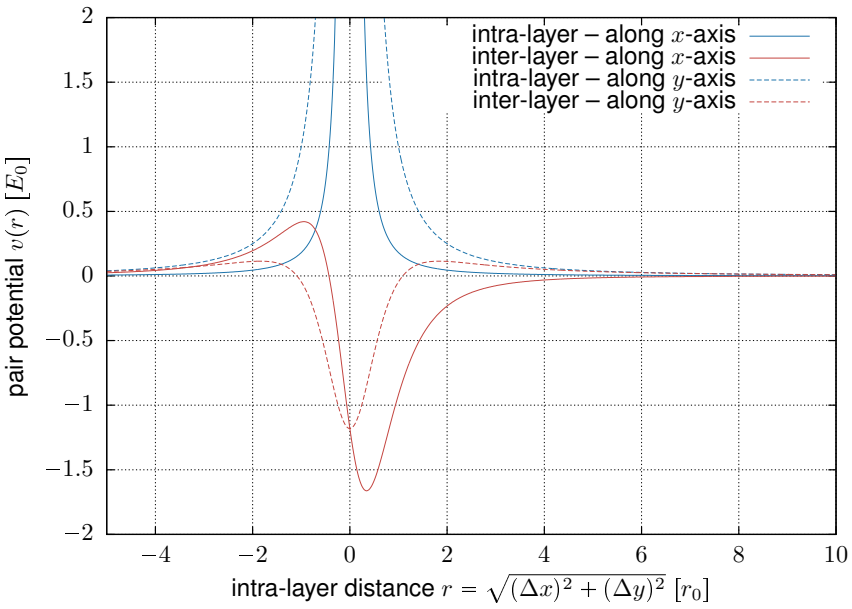


Figure 1.2: These are the pair interaction potentials in units of the characteristic energy E_0 for two dipoles in the same (blue) or in neighbouring layers (red) as a function of their distance r, when projected on the xy-plain in units of the characteristic length r_0. The solid lines show the potential for two dipoles in the xz-plain and the dashed lines for two dipoles in the yz-plain. Note that the dipoles are all aligned in parallel in the xz-plain, which breaks the line symmetry of the inter-layer interaction along the x-axis (see the red solid curve). The intra-layer interaction is always proportional to r^{-3}, which means that it is repulsive. In contrast the inter-layer interaction always has a minimum, around which dipoles attract each other between the layers. Note that in the direction, in which dipoles are tilted, the inter-layer interaction can also be repulsive (see again the red solid curve).

2 Deriving the equations of motion

In this chapter we derive equations of motion for our multi-component system, which contain density fluctuations and external perturbations, so that we can determine the linear response matrix between them in the following chapter.

2.1 Statement of the problem

The ground state of our system can be described using the time-independent Hamiltonian

$$\widehat{\mathcal{H}}_0(\boldsymbol{R}) := -\sum_{\alpha}\sum_{i}^{N_\alpha}\frac{\hbar^2}{2m_\alpha}\Delta_{\alpha,i} + V(\boldsymbol{R}). \tag{2.1}$$

With the small Greek letters α, β, γ, η, ϑ and κ certain particle types are labelled and N_α stands for the number of particles of type α. One has to imagine that the particles within a type α are numbered with $i \in \{1, \ldots, N_\alpha\}$ (although any two of them could be exchanged without any consequences) and so the vector $\boldsymbol{r}_{\alpha,i}$ indicates the position of a certain particle in our system. So the double sum in equation (2.1) is simply a sum over all particles. Whenever the vector $\boldsymbol{R}$ is used in this work, the coordinates of all particles are meant. $V(\boldsymbol{R})$ stands for an arbitrary potential depending on the coordinates of the particles.

As the problem, we deal with, is of course a time-dependent problem we start with defining a perturbed Hamiltonian [LL77, p. 133]

$$\widehat{\mathcal{H}}(\boldsymbol{R}, t) := \widehat{\mathcal{H}}_0(\boldsymbol{R}) + \delta\widehat{\mathcal{H}}(\boldsymbol{R}, t). \tag{2.2}$$

The explicit time-dependent perturbation of our system is defined as [CKT96]

$$\delta\widehat{\mathcal{H}}(\boldsymbol{R}, t) := \sum_{\alpha}\sum_{i=1}^{N_\alpha} U_{\mathrm{ext},\alpha}(\boldsymbol{r}_{\alpha,i}, t)\,. \tag{2.3}$$

The function $U_{\mathrm{ext},\alpha}(\boldsymbol{r}, t)$ is the external potential a particle of type α 'feels' at a position $\boldsymbol{r}$ and time t.

We proceed with an ansatz for the wave function $\psi(\boldsymbol{R}, t)$ of our system. To get an idea how this can be done, we take inspiration from the Jastrow-ansatz for the ground state theory [SAH04, p. 132] and define the complex-valued excitation operator [SAH04, p. 163]

$$\delta U(\boldsymbol{R}, t) := \sum_{\alpha}\sum_{i}\delta u_\alpha(\boldsymbol{r}_{\alpha,i}, t) + \frac{1}{2}\sum_{\alpha,\beta}{\sum_{i,j}}'\delta u_{\alpha\beta}(\boldsymbol{r}_{\alpha,i}, \boldsymbol{r}_{\beta,j}, t) + \ldots \tag{2.4}$$

as the fluctuations of the correlation functions. In equation (2.4) the prime at the second sum means that the addend for the case $\alpha = \beta$ and $i = j$ is left out. In contrast to the Jastrow-form of a homogeneous ground state we also need the fluctuations of the one-body correlations δu_α here, as in the theory of excitations there will most likely be a breaking of the translational invariance. [SAH04, p. 163] Of course also correlations of higher order – e. g. triplet correlations $\delta u_{\alpha\beta\gamma}$ – could be included in δU like it was done by Campbell and Krotscheck [CK10] for one-component homogeneous systems, but as the derivations presented in this work are tedious enough, we will just treat one-body and pair correlations.

We assume to know the normalised wave function $\psi_0(\boldsymbol{R})$, which is the result of the ground state calculation and make the ansatz [SAH04, p. 163]

$$\psi(\boldsymbol{R},t) := \frac{e^{-i\omega_0 t} e^{\frac{1}{2}\delta U(\boldsymbol{R},t)}}{\sqrt{\mathcal{N}(t)}} \psi_0(\boldsymbol{R}) \tag{2.5}$$

for the wave function of our excited system, where $E_0 = \hbar\omega_0$ is the ground state energy, such that the time-independent Schrödinger equation $\widehat{\mathcal{H}}_0\psi_0(\boldsymbol{R}) = E_0\psi_0(\boldsymbol{R})$ holds and $\mathcal{N}(t)$ ensures that $\psi(\boldsymbol{R},t)$ is again normalised, so one gets [SAH04, p. 163]

$$\mathcal{N}(t) = \left\langle \psi_0(\boldsymbol{R}) \right| e^{\mathfrak{Re}\,\delta U(\boldsymbol{R},t)} \left| \psi_0(\boldsymbol{R}) \right\rangle. \tag{2.6}$$

So up to now have defined our system and the actual target of all the following calculation is to solve the excitations δU caused by the external perturbation $\delta\widehat{\mathcal{H}}$. In the limit $\delta\widehat{\mathcal{H}} \to 0$ also δU vanishes and therefore the excited wave function ψ becomes identical to ψ_0.

2.2 The variational principle

The next step on our way to the equations of motion is to apply a variational principle as it is also described by Kerman and Koonin [KK76]. For that reason we define

$$L\left[\psi,\psi^*\right](t) := \left\langle \psi(\boldsymbol{R},t) \right| \widehat{\mathcal{H}}(\boldsymbol{R},t) - i\hbar\frac{\partial}{\partial t} \left| \psi(\boldsymbol{R},t) \right\rangle, \tag{2.7}$$

which is quite similar to the Lagrangian from classical mechanics, as we can define an action functional

$$S\left[\psi,\psi^*\right] := \int \mathrm{d}t\; L\left[\psi,\psi^*\right](t), \tag{2.8}$$

such that the many-body Schrödinger equation is equivalent to the least-action principle

$$\frac{\delta S\left[\psi,\psi^*\right]}{\delta\psi(\boldsymbol{R},t)} = 0. \tag{2.9}$$

Before we apply the least-action principle, we reformulate the Lagrangian for our specific problem as it was also done in [SAH04]. In the following the parameters are omitted to increase readability. First we carry out the time derivative of the trivial time dependence $e^{-i\omega_0 t}$ of ψ to obtain

$$L = \left\langle \psi_0 \right| \frac{e^{\frac{1}{2}\delta U^*}}{\sqrt{\mathcal{N}}} \left(\widehat{\mathcal{H}} - E_0 - i\hbar\frac{\partial}{\partial t} \right) \frac{e^{\frac{1}{2}\delta U}}{\sqrt{\mathcal{N}}} \left| \psi_0 \right\rangle. \tag{2.10}$$

Next we insert the Hamiltonian from definition (2.2) and make use of the ground state Schrödinger equation $E_0\psi_0 = \widehat{\mathcal{H}}_0\psi_0$, which enables us to write a commutator.

$$L = \left\langle \psi_0 \right| \frac{e^{\frac{1}{2}\delta U^*}}{\mathcal{N}} \left[\widehat{\mathcal{H}}_0, e^{\frac{1}{2}\delta U} \right] - i\hbar \frac{e^{\frac{1}{2}\delta U^*}}{\sqrt{\mathcal{N}}} \frac{\partial}{\partial t} \frac{e^{\frac{1}{2}\delta U^*}}{\sqrt{\mathcal{N}}} + \frac{e^{\mathfrak{Re}\,\delta U}}{\mathcal{N}} \delta\widehat{\mathcal{H}} \left| \psi_0 \right\rangle \tag{2.11}$$

After some further steps that can be found in more detail in [Saa08], we obtain the form

$$L = \left\langle \psi_0 \right| \frac{e^{\mathfrak{Re}\,\delta U}}{\mathcal{N}} \left(\sum_\beta \sum_j^{N_\beta} \frac{\hbar^2}{8m_\beta} \left|\nabla_{\beta,j}\delta U\right|^2 + \frac{\hbar}{2}\,\mathfrak{Im}\,\delta\dot{U} + \delta\widehat{\mathcal{H}} \right) \left| \psi_0 \right\rangle. \tag{2.12}$$

The presented procedure until now is basically identical to the approach of Saarela, Apaja, and Halinen [SAH04] for the one-component case, but to proceed we have to think about a suitable notation for multi-component systems. Hereafter quantities depending on n particle types $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)$ will occur like the n-body correlation function $\delta u_{\boldsymbol{\alpha}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n, t)$. We introduce a function $n_\beta(\boldsymbol{\alpha})$ that indicates the number of $\boldsymbol{\alpha}$-components that are equal to beta, e. g. for $\alpha \neq \beta$ and $\boldsymbol{\alpha} = (\alpha, \beta, \beta)$ one has $n_\alpha(\boldsymbol{\alpha}) = 1$ and $n_\beta(\boldsymbol{\alpha}) = 2$. Most functions depending on $\boldsymbol{\alpha}$ also have n coordinate-parameters $\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n$, which represent the positions of n *distinct* particles – $\boldsymbol{r}_j$ gives the coordinate of a particle with type α_j. As an abbreviation for the n position-parameters $\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n$ we will use $\boldsymbol{\sigma}_{\boldsymbol{\alpha}}$. It is also very common to have an integral over the coordinates of all particles except of those, whose positions are included in $\boldsymbol{\sigma}_{\boldsymbol{\alpha}}$. We write these integrals as $\int \mathrm{d}\tau_{\boldsymbol{\alpha}}$, so if one has a function $f(\boldsymbol{R})$ and an integral

$$I := \int \mathrm{d}\tau_{\boldsymbol{\alpha}}\, f(\boldsymbol{R}), \tag{2.13}$$

one also has $I = I(\boldsymbol{\sigma}_{\boldsymbol{\alpha}})$, so I only depends on the coordinates $\boldsymbol{\sigma}_{\boldsymbol{\alpha}}$.

Now we are ready to apply the least-action principle and so we require $\delta S / \delta\left(\delta u_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t)\right) \stackrel{!}{=} 0$, which means that the action is minimised with respect to a general n-correlation function $\delta u_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t)$. [SAH04] This approach is very elegant, as it leads us to the equation(s) of motion (for each possible $\boldsymbol{\alpha}$)

$$\int \mathrm{d}\tau_{\boldsymbol{\alpha}} \left\{ \sum_j \frac{\hbar^2}{4m_{\alpha_j}} \nabla_j \cdot \left(|\psi|^2 \nabla_j \delta U \right) + |\psi|^2 \left(\frac{i\hbar}{2} \delta \dot{U} - \delta \widehat{\mathcal{H}} - \left\langle \psi \middle| \frac{i\hbar}{2} \delta \dot{U} - \delta \widehat{\mathcal{H}} \middle| \psi \right\rangle \right) \right\} = 0 \tag{2.14}$$

and can be used for correlation functions of any order. The summation index j in (2.14) should run through the set of particles, whose positions would be labelled with $\boldsymbol{\sigma}_{\boldsymbol{\alpha}}$.

2.3 Continuity equations

Although equation (2.14) is already a valid form of our equations of motion, we need to bring it into a more tractable form.

First of all we define the useful abbreviation

$$\Pi_{\boldsymbol{\alpha}} := \prod_\beta \frac{N_\beta!}{(N_\beta - n_\beta(\boldsymbol{\alpha}))!} \tag{2.15}$$

and the familiar n-body density [SAH04, p. 165]

$$\rho_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) := \Pi_{\boldsymbol{\alpha}} \int \mathrm{d}\tau_{\boldsymbol{\alpha}}\, |\psi(\boldsymbol{R}, t)|^2 \tag{2.16}$$

analogue to the one-component case. If we use the ground state wave function ψ_0 instead of ψ we can also define the ground state density

$$\rho_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}) := \Pi_{\boldsymbol{\alpha}} \int \mathrm{d}\tau_{\boldsymbol{\alpha}}\, |\psi_0(\boldsymbol{R})|^2. \tag{2.17}$$

In fact we are interested in the fluctuations and so we make a linear expansion. [SAH04, p. 165]

$$\begin{aligned} \rho_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) &= \Pi_{\boldsymbol{\alpha}} \int \mathrm{d}\tau_{\boldsymbol{\alpha}}\, |\psi_0|^2 \frac{e^{\mathfrak{Re}\, \delta U}}{\langle \psi_0 |\, e^{\mathfrak{Re}\, \delta U} \,| \psi_0 \rangle} = \Pi_{\boldsymbol{\alpha}} \int \mathrm{d}\tau_{\boldsymbol{\alpha}}\, |\psi_0|^2 \frac{1 + \mathfrak{Re}\, \delta U}{1 + \langle \psi_0 |\, \mathfrak{Re}\, \delta U \,| \psi_0 \rangle} + \mathcal{O}\left(\delta U^2\right) \\ &= \Pi_{\boldsymbol{\alpha}} \int \mathrm{d}\tau_{\boldsymbol{\alpha}}\, |\psi_0|^2 \left(1 + \mathfrak{Re}\, \delta U\right) \left(1 - \langle \psi_0 |\, \mathfrak{Re}\, \delta U \,| \psi_0 \rangle\right) + \mathcal{O}\left(\delta U^2\right) \end{aligned} \tag{2.18}$$

This inspires the definition [SAH04, p. 165]

$$\delta\rho(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) := \Pi_{\boldsymbol{\alpha}} \int \mathrm{d}\tau_{\boldsymbol{\alpha}} \, |\psi_0|^2 \left(\delta U - \langle\psi_0| \, \delta U \, |\psi_0\rangle\right) \tag{2.19}$$

and so one has

$$\rho_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) = \rho_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}) + \mathfrak{Re}\, \delta\rho(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) + \mathcal{O}\left(\delta U^2\right). \tag{2.20}$$

Please note that we defined the density fluctuations $\delta\rho_{\boldsymbol{\alpha}}$ complex-valued only for convenience, since it fits perfectly into equation (2.14) – the real physical density fluctuations are $\mathfrak{Re}\, \delta\rho_{\boldsymbol{\alpha}}$.

Now we play a similar game for the n-body current density, which can be defined as [Saa08]

$$\boldsymbol{j}^{(\mathrm{ph})}_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) := \frac{\hbar}{2m_{\alpha_1} i} \Pi_{\boldsymbol{\alpha}} \int \mathrm{d}\tau_{\boldsymbol{\alpha}} \; \left(\psi^* \nabla_{\alpha_1} \psi - \psi \nabla_{\alpha_1} \psi^*\right). \tag{2.21}$$

As one can see the first component α_1 of $\boldsymbol{\alpha}$ plays a special role for the n-body current density. Analogous to $\delta\rho_{\boldsymbol{\alpha}}$ we can define [SAH04, p. 165]

$$\boldsymbol{j}_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) := \frac{\hbar}{2m_{\alpha_1} i} \Pi_{\boldsymbol{\alpha}} \int \mathrm{d}\tau_{\boldsymbol{\alpha}} \; |\psi_0(\boldsymbol{R})|^2 \nabla_{\alpha_1} \delta U(\boldsymbol{R}, t), \tag{2.22}$$

whose real part is the first order-expansion of the real physical current density.

$$\boldsymbol{j}^{(\mathrm{ph})}_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) = \mathfrak{Re}\, \boldsymbol{j}_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) + \mathcal{O}\left(\delta U^2\right) \tag{2.23}$$

A last necessary preparation is the definition [SAH04, p. 165]

$$D_{\boldsymbol{\alpha}}(\boldsymbol{\sigma}_{\boldsymbol{\alpha}}, t) := \frac{2}{i\hbar} \Pi_{\boldsymbol{\alpha}} \int \mathrm{d}\tau_{\boldsymbol{\alpha}} \, |\psi_0(\boldsymbol{R})|^2 \left(\delta\widehat{\mathcal{H}}(\boldsymbol{R}, t) - \left\langle \psi_0(\boldsymbol{R}') \middle| \, \delta\widehat{\mathcal{H}}(\boldsymbol{R}', t) \, \middle| \psi_0(\boldsymbol{R}') \right\rangle\right). \tag{2.24}$$

From now on we omit the parameters $\boldsymbol{\sigma}_{\boldsymbol{\alpha}}$ and t to increase again readability, as the components of $\boldsymbol{\alpha}$ and $\boldsymbol{\sigma}_{\boldsymbol{\alpha}}$ always go hand in hand and we use the naming of the coordinates $\boldsymbol{\sigma}_{\boldsymbol{\alpha}} = (\boldsymbol{r}_{\alpha_1}, \ldots, \boldsymbol{r}_{\alpha_n})$ implicitly, such that

$$\nabla_\alpha = \sum_i \frac{\partial}{\partial x_{\alpha,i}} \hat{\boldsymbol{e}}_i. \tag{2.25}$$

This enables us to rewrite equation (2.14) using the definitions (2.19), (2.22) and (2.24). [SAH04, p. 165]

$$\nabla_\alpha \cdot \boldsymbol{j}_\alpha + \delta\dot{\rho}_\alpha = D_\alpha \tag{2.26}$$

$$\nabla_\alpha \cdot \boldsymbol{j}_{\alpha\beta} + \nabla_\beta \cdot \boldsymbol{j}_{\beta\alpha} + \delta\dot{\rho}_{\alpha\beta} = D_{\alpha\beta} \tag{2.27}$$

One should note that equations (2.26) and (2.27) are continuity equations with driving terms D_α and $D_{\alpha\beta}$, into which all the $\delta\widehat{\mathcal{H}}$-dependence is collected. The first equation really turns into a continuity equation, if the external perturbation vanishes.

3 Solving the equations of motion

In this chapter we will calculate the density-density linear response function from the equations of motion derived in the previous chapter as the linear relationship between the density fluctuations $\mathfrak{Re}\,\delta\rho_\alpha$ and the perturbation $U_{\mathrm{ext},\alpha}$. The solution, that will be obtained, is also known as the CBF response function in literature because of its first derivation done by Jackson [Jac73] within the theory of correlated basis functions (CBF) [CKT96].

Before we proceed with our calculation we need again some definitions and therefore we start with defining the *n-body distribution function* [SAH04, p. 165]

$$g_{\boldsymbol{\alpha}} := \frac{\rho_{\boldsymbol{\alpha}}}{\prod\limits_j \rho_{\alpha_j}}, \tag{3.1}$$

which we need for the special cases $n = 2$ and $n = 3$.

$$g_{\alpha\beta} = \frac{\rho_{\alpha\beta}}{\rho_\alpha \rho_\beta} \qquad\qquad g_{\alpha\beta\gamma} = \frac{\rho_{\alpha\beta\gamma}}{\rho_\alpha \rho_\beta \rho_\gamma} \tag{3.2}$$

Another very simple definition we will use excessively is [SAH04, p. 170]

$$h_{\alpha\beta} := g_{\alpha\beta} - 1. \tag{3.3}$$

We also introduce the so called tilde-notation for an arbitrary function $f_{\boldsymbol{\alpha}}$ [CKT96]

$$\tilde{f}_{\boldsymbol{\alpha}} = \prod_j \sqrt{\rho_{\alpha_j}} f_{\boldsymbol{\alpha}}, \tag{3.4}$$

but with the two exceptions

$$\delta\tilde{\rho}_\alpha = \frac{\delta\rho_\alpha}{\sqrt{\rho_\alpha}} \qquad \text{and} \qquad \tilde{\boldsymbol{j}}_\alpha = \frac{\boldsymbol{j}_\alpha}{\sqrt{\rho_\alpha}}. \tag{3.5}$$

The last definition we give for now is the *static structure factor* [CKT96]

$$S_{\alpha\beta} := \delta_{\alpha\beta}\delta(\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta) + \tilde{h}_{\alpha\beta} \tag{3.6}$$

and also a syntactic convention to combine sums and integrals is introduced.

$$\sum\!\!\!\!\!\!\int_\alpha f_\alpha = \sum_\alpha \int \mathrm{d}^s r_\alpha \; f_\alpha \tag{3.7}$$

After we are done with our preparations we start writing down the terms of the equations of motion (2.26) and (2.27) explicitly using the definitions (2.19), (2.22) and (2.24). We start with the driving terms D_α and $D_{\alpha\beta}$.

$$D_\alpha = \frac{2\rho_\alpha}{i\hbar}\left(U_{\mathrm{ext},\alpha} + \sum\!\!\!\!\!\!\int_\beta \rho_\beta h_{\alpha\beta} U_{\mathrm{ext},\beta}\right) = \frac{2\sqrt{\rho_\alpha}}{i\hbar}\sum\!\!\!\!\!\!\int_\beta S_{\alpha\beta}\widetilde{U}_{\mathrm{ext},\beta} \tag{3.8}$$

$$D_{\alpha\beta} = \frac{2\rho_\alpha\rho_\beta}{i\hbar}\left(g_{\alpha\beta}\left(U_{\mathrm{ext},\alpha} + U_{\mathrm{ext},\beta}\right) + \sum\!\!\!\!\!\!\int_\gamma \rho_\gamma \left(g_{\alpha\beta\gamma} - g_{\alpha\beta}\right) U_{\mathrm{ext},\gamma}\right) \tag{3.9}$$

Soon it will become clear that representations using convolutions with $S_{\alpha\beta}$ are very advantageous, so we already did this for D_α. The current densities are

$$\boldsymbol{j}_\alpha = \frac{\hbar\rho_\alpha}{2m_\alpha i}\left(\nabla_\alpha \delta u_\alpha + \sum\!\!\!\!\!\!\int_\beta \rho_\beta g_{\alpha\beta}\nabla_\alpha \delta u_{\alpha\beta}\right) \tag{3.10}$$

$$\boldsymbol{j}_{\alpha\beta} = \frac{\hbar\rho_\alpha\rho_\beta}{2m_\alpha i}\left(g_{\alpha\beta}\nabla_\alpha\left(\delta u_\alpha + \delta u_{\alpha\beta}\right) + \sum\!\!\!\!\!\!\int_\gamma \rho_\gamma g_{\alpha\beta\gamma}\nabla_\alpha \delta u_{\alpha\gamma}\right) \tag{3.11}$$

and the one-body density

$$\delta\rho_\alpha = \rho_\alpha\delta u_\alpha + \sum\!\!\!\!\!\!\int_\beta \rho_\alpha\rho_\beta h_{\alpha\beta}\delta u_\beta + \sum\!\!\!\!\!\!\int_\beta \rho_\alpha\rho_\beta g_{\alpha\beta}\delta u_{\alpha\beta} + \frac{1}{2}\sum\!\!\!\!\!\!\int_\beta\sum\!\!\!\!\!\!\int_\gamma \rho_\alpha\rho_\beta\rho_\gamma(g_{\alpha\beta\gamma} - g_{\beta\gamma})\delta u_{\beta\gamma}. \tag{3.12}$$

We can also reformulate the one-body density slightly using the static structure factor, which will help us later.

$$\delta\tilde{\rho}_\alpha = \sum\!\!\!\!\!\!\int_\beta \left(S_{\alpha\beta}\delta\tilde{u}_\beta + \sqrt{\rho_\beta}g_{\alpha\beta}\delta\tilde{u}_{\alpha\beta} + \frac{1}{2}\sum\!\!\!\!\!\!\int_\gamma \sqrt{\rho_\alpha\rho_\beta\rho_\gamma}(g_{\alpha\beta\gamma} - g_{\beta\gamma})\delta\tilde{u}_{\beta\gamma}\right) \tag{3.13}$$

Of course one could also write down $\delta\rho_{\alpha\beta}$ explicitly, but this would give us a four-body density, which we really want to avoid by all means. A different approach is to express the time derivative in terms of the pair distribution function

$$\delta\dot{\rho}_{\alpha\beta} = g_{\alpha\beta}\left(\rho_\alpha\delta\dot{\rho}_\beta + \rho_\beta\delta\dot{\rho}_\alpha\right) + \rho_\alpha\rho_\beta\dot{g}_{\alpha\beta} + \mathcal{O}\left(\delta U^2\right), \tag{3.14}$$

which suggests to subtract the first equation of motion (with appropriate coefficients) from the second as it is also done in [CKT96], such that only the last addend of equation (3.14) remains. Before we carry out this explicitly, we introduce some approximations in the following sections.

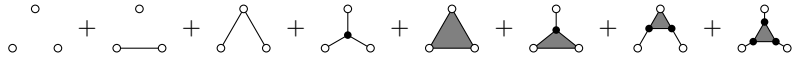
3.1 The convolution approximation

This section deals with the convolution approximation, that is well discussed in literature, [CKT96], [Fee69], [SAH04, p. 170], but before can get started, we need again some new notation.

At this time we introduce diagrams, which will help us to drastically simplify bookkeeping in our formulas. White circles denote external variables – in this case a variable is always connected to a particle type – and if they are not labelled, the diagram represents the sum of all distinct permutations of the external variables, which we usually call α, β and γ. A black circle indicates an internal variable, which comes with a sum over all particle types, an integral over the coordinate and a coefficient, that is the density corresponding to the particle type. A line that connects two circles α and β indicates the factor $h_{\alpha\beta}$ and a grey triangle connecting the circles α, β and γ stands for the triplet correlation function $X_{\alpha\beta\gamma}$. [CKT96] An example would be

$$= \sum\!\!\!\!\!\!\int_\eta \rho_\eta \sum\!\!\!\!\!\!\int_\vartheta \rho_\vartheta\left(h_{\alpha\eta}h_{\beta\vartheta}X_{\gamma\eta\vartheta} + h_{\alpha\eta}h_{\gamma\vartheta}X_{\beta\eta\vartheta} + h_{\beta\eta}h_{\gamma\vartheta}X_{\alpha\eta\vartheta}\right). \tag{3.15}$$

The diagrammatic notation is very useful to introduce the *convolution approximation* for the three-body distribution function

$g_{\alpha\beta\gamma} \approx$  . (3.16)

Clements, Krotscheck, and Tymczak [CKT96] point out, that this representation of $g_{\alpha\beta\gamma}$ is exact, if we know the exact triplet correlations $X_{\alpha\beta\gamma}$, but as they are not known and we will insert approximations taken from [Cle+93], we already call equation (3.16) the convolution approximation.

As we will need this expression quite often we define the part of $g_{\alpha\beta\gamma}$ that is non-nodal in α as [CKT96]

$$Y_{\alpha\beta\gamma} := \quad = h_{\alpha\beta}h_{\alpha\gamma} + \sum\!\!\!\!\!\!\int_\eta \sum\!\!\!\!\!\!\int_\vartheta \frac{S_{\beta\eta}S_{\gamma\vartheta}}{\sqrt{\rho_\alpha\rho_\beta\rho_\gamma}}\widetilde{X}_{\alpha\eta\vartheta}. \tag{3.17}$$

Lemma 1. *The convolution of the static structure factor $S_{\alpha\eta}$ and the non-nodal part $\widetilde{Y}_{\eta\beta\gamma}$ of $g_{\alpha\beta\gamma}$ can be expressed as*

$$\sum\!\!\!\!\!\!\int_\eta S_{\alpha\eta}\widetilde{Y}_{\eta\beta\gamma} = \sqrt{\rho_\alpha\rho_\beta\rho_\gamma}\left(\quad + \quad + \quad + \quad + \quad + \quad \right). \tag{3.18}$$

Proof.

$$\sum\!\!\!\!\!\!\int_\eta S_{\alpha\eta}\widetilde{Y}_{\eta\beta\gamma} = \sqrt{\rho_\alpha\rho_\beta\rho_\gamma}\left\{ Y_{\alpha\beta\gamma} + \sum\!\!\!\!\!\!\int_\eta \rho_\eta h_{\alpha\eta}\left(\quad + \quad + \quad + \quad + \quad \right)\right\} \tag{3.19}$$

$$= \sqrt{\rho_\alpha\rho_\beta\rho_\gamma}\left(\quad + \quad + \quad + \quad + \quad + \quad + \quad + \quad + \quad + \quad \right) \tag{3.20}$$

□

Lemma 2. *In the convolution approximation (given in equation (3.16)) on has*

$$g_{\alpha\beta\gamma} = \sum\!\!\!\!\!\!\int_\eta \frac{S_{\alpha\eta}\widetilde{Y}_{\eta\beta\gamma}}{\sqrt{\rho_\alpha\rho_\beta\rho_\gamma}} + \quad + \quad + \quad + \quad . \tag{3.21}$$

Proof. This is an immediate implication of lemma 1, if one adds the missing diagrams from (3.16) to (3.18) and solves for $g_{\alpha\beta\gamma}$. □

Now it becomes very easy to simplify $D_{\alpha\beta}$, if we first insert D_α and then use lemma 2. In the end we can again insert D_α for the convolution of $S_{\gamma\eta}$ and $\widetilde{U}_{\mathrm{ext},\gamma}$.

$$\begin{aligned} D_{\alpha\beta} &= g_{\alpha\beta}\left(\rho_\alpha D_\beta + \rho_\beta D_\alpha\right) + \rho_\alpha\rho_\beta \sum\!\!\!\!\!\!\int_\gamma \frac{2\rho_\gamma}{i\hbar}\left\{g_{\alpha\beta\gamma} - (1+h_{\alpha\beta})(1+h_{\alpha\gamma}+h_{\beta\gamma})\right\} U_{\mathrm{ext},\gamma} \\ &= g_{\alpha\beta}\left(\rho_\alpha D_\beta + \rho_\beta D_\alpha\right) + \rho_\alpha\rho_\beta \sum\!\!\!\!\!\!\int_\gamma \frac{2}{i\hbar}\sum\!\!\!\!\!\!\int_\eta \frac{S_{\gamma\eta}\widetilde{Y}_{\eta\alpha\beta}}{\sqrt{\rho_\alpha\rho_\beta}}\widetilde{U}_{\mathrm{ext},\gamma} \\ &= g_{\alpha\beta}\left(\rho_\alpha D_\beta + \rho_\beta D_\alpha\right) + \rho_\alpha\rho_\beta \sum\!\!\!\!\!\!\int_\gamma Y_{\gamma\alpha\beta}D_\gamma \end{aligned} \tag{3.22}$$

The next step is to eliminate the one-body correlation fluctuations δu_α in favour of $\delta\rho_\alpha$ from $\boldsymbol{j}_\alpha$ given in equation (3.10), which can again be done by exploiting the convolution approximation. We use lemma 2

to replace $g_{\alpha\beta\gamma}$ in equation (3.13) and then represent $\delta\tilde{\rho}_\alpha$ as a convolution with $S_{\alpha\beta}$.

$$\begin{aligned}\delta\tilde{\rho}_\alpha =& \sum\!\!\!\!\!\!\int_\beta \left(S_{\alpha\beta}\delta\tilde{u}_\beta + \sqrt{\rho_\beta} g_{\alpha\beta}\delta\tilde{u}_{\alpha\beta} + \sum\!\!\!\!\!\!\int_\gamma \sqrt{\rho_\alpha\rho_\beta\rho_\gamma}\,(h_{\alpha\beta} + h_{\alpha\beta}h_{\beta\gamma})\,\delta\tilde{u}_{\beta\gamma} + \frac{1}{2}\sum\!\!\!\!\!\!\int_\gamma \sum\!\!\!\!\!\!\int_\eta S_{\alpha\eta}\widetilde{Y}_{\eta\beta\gamma}\delta\tilde{u}_{\beta\gamma} \right) \\ =& \sum\!\!\!\!\!\!\int_\beta S_{\alpha\beta}\left(\delta\tilde{u}_\beta + \sum\!\!\!\!\!\!\int_\gamma \sqrt{\rho_\gamma} g_{\beta\gamma}\delta\tilde{u}_{\beta\gamma} + \frac{1}{2}\sum\!\!\!\!\!\!\int_\gamma \sum\!\!\!\!\!\!\int_\eta \widetilde{Y}_{\beta\gamma\eta}\delta\tilde{u}_{\gamma\eta} \right) \end{aligned} \tag{3.23}$$

Therefore we define [CKT96]

$$\delta\tilde{v}_\alpha := \delta\tilde{u}_\alpha + \sum\!\!\!\!\!\!\int_\beta \sqrt{\rho_\beta} g_{\alpha\beta}\delta\tilde{u}_{\alpha\beta} + \frac{1}{2}\sum\!\!\!\!\!\!\int_\beta \sum\!\!\!\!\!\!\int_\gamma \widetilde{Y}_{\alpha\beta\gamma}\delta\tilde{u}_{\beta\gamma}, \tag{3.24}$$

such that one gets

$$\delta\tilde{\rho}_\alpha = \sum\!\!\!\!\!\!\int_\beta S_{\alpha\beta}\delta\tilde{v}_\beta \tag{3.25}$$

for the one-body density. This convolution can be easily inverted using the Ornstein-Zernike equation, which states $S^{-1}_{\alpha\beta} = \delta_{\alpha\beta}\delta(\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta) - \widetilde{X}_{\alpha\beta}$, where $X_{\alpha\beta}$ is the *direct correlation function*. [CKT96] Indeed this explicit representation of $S^{-1}_{\alpha\beta}$ is often counterproductive, but we will need the direct correlation function, especially in the following section.

Now we replace δu_α from equation (3.10) using definition (3.24) and inserting $\delta\tilde{\rho}_\alpha$ from (3.25).

$$\boldsymbol{j}_\alpha = \frac{\hbar\rho_\alpha}{2m_\alpha i}\left(\nabla_\alpha \frac{1}{\sqrt{\rho_\alpha}} \sum\!\!\!\!\!\!\int_\beta S^{-1}_{\alpha\beta}\delta\tilde{\rho}_\beta - \sum\!\!\!\!\!\!\int_\beta \rho_\beta \delta u_{\alpha\beta}\nabla_\alpha g_{\alpha\beta} - \frac{1}{2}\sum\!\!\!\!\!\!\int_\beta \sum\!\!\!\!\!\!\int_\gamma \rho_\beta\rho_\gamma \delta u_{\beta\gamma}\nabla_\alpha Y_{\alpha\beta\gamma} \right) \tag{3.26}$$

3.2 The uniform limit approximation

An important approximation we introduce is the uniform limit approximation, discussed by Feenberg [Fee69], where the limit $g_{\alpha\beta} \to 1$ is analysed, which enables us to write the following. [CKT96]

$$\delta u_{\alpha\beta} \approx \delta X_{\alpha\beta} \tag{3.27}$$

$$g_{\alpha\beta}\nabla_\alpha \delta u_{\alpha\beta} \approx \nabla_\alpha \delta u_{\alpha\beta} \tag{3.28}$$

$$(g_{\alpha\beta\gamma} - g_{\alpha\beta}g_{\alpha\gamma})\nabla_\alpha \delta u_{\alpha\beta} \approx h_{\beta\gamma}\nabla_\alpha \delta u_{\alpha\gamma} \tag{3.29}$$

Soon we will subtract the one-body equation of motion from the two-body equation of motion as previously mentioned to avoid the four-body distribution function and so we prepare a term, that will appear in the course of that process, using the uniform limit approximation.

$$J_{\alpha\beta} := \nabla_\alpha \cdot (\boldsymbol{j}_{\alpha\beta} - g_{\alpha\beta}\rho_\beta \boldsymbol{j}_\alpha) \tag{3.30}$$

$$= \frac{\hbar}{2m_\alpha i}\nabla_\alpha \cdot \rho_\alpha\rho_\beta \left(g_{\alpha\beta}\nabla_\alpha \delta u_{\alpha\beta} + \sum\!\!\!\!\!\!\int_\gamma \rho_\gamma (g_{\alpha\beta\gamma} - g_{\alpha\beta}g_{\alpha\gamma})\nabla_\alpha \delta u_{\alpha\gamma} \right) \tag{3.31}$$

$$= \frac{\hbar\sqrt{\rho_\beta}}{2m_\beta i}\nabla_\alpha \cdot \rho_\alpha \nabla_\alpha \frac{1}{\sqrt{\rho_\alpha}} \sum\!\!\!\!\!\!\int_\gamma S_{\beta\gamma}\delta\widetilde{X}_{\alpha\gamma} \tag{3.32}$$

3.3 Reformulation of the second equation of motion

In the preceding sections we have introduced the necessary approximations and now it is time to finally reformulate our two-body equation of motion (2.27) using the insights gained up to now. First we subtract the one-body equation of motion (2.26) for both particle types α and β multiplied with $g_{\alpha\beta}$ and the appropriate density from (2.27), which leads us to [CKT96]

$$J_{\alpha\beta} + J_{\beta\alpha} + \left(\rho_\beta \boldsymbol{j}_\alpha \cdot \nabla_\alpha + \rho_\alpha \boldsymbol{j}_\beta \cdot \nabla_\alpha\right) g_{\alpha\beta} + \rho_\alpha \rho_\beta \dot{g}_{\alpha\beta} = \rho_\alpha \rho_\beta \coprod_\gamma Y_{\gamma\alpha\beta} D_\gamma. \tag{3.33}$$

The operators

$$\widehat{\partial}_\rho f := \coprod_\alpha \frac{\delta f}{\delta \rho_\alpha} \delta\dot{\rho}_\alpha \qquad \text{and} \qquad \widehat{\partial}_u f := \coprod_\alpha \coprod_\beta \frac{\delta f}{\delta u_{\alpha\beta}} \delta\dot{u}_{\alpha\beta} \tag{3.34}$$

can be used to express the time derivative of $g_{\alpha\beta}$, as the hypernetted-chain equations provide a relationship between $g_{\alpha\beta}$, $\delta\rho_\alpha$ and $\delta u_{\alpha\beta}$. [CKT96]

$$\dot{g}_{\alpha\beta} = \left(\widehat{\partial}_\rho + \widehat{\partial}_u\right) g_{\alpha\beta} \tag{3.35}$$

The Ornstein-Zernike equation can be used to derive [CKT96]

$$\widehat{\partial}_\rho g_{\alpha\beta} = \coprod_\gamma Y_{\gamma\alpha\beta} \delta\dot{\rho}_\beta \tag{3.36}$$

and also to rewrite the second part of the time derivative [CKT96]

$$\sqrt{\rho_\alpha \rho_\beta}\widehat{\partial}_u g_{\alpha\beta} = \widehat{\partial}_u \tilde{g}_{\alpha\beta} = \coprod_\gamma \coprod_\eta S_{\alpha\gamma} \left(\widehat{\partial}_u \delta\widetilde{X}_{\gamma\eta}\right) S_{\beta\eta}. \tag{3.37}$$

In the uniform limit approximation $\delta X_{\alpha\beta}$ is identical to $\delta u_{\alpha\beta}$, so the $\widehat{\partial}_u$-operator acting on $\delta X_{\alpha\beta}$ is identical to the common time derivative. Therefore the final form of our second equation of motion in coordinate space is given by

$$J_{\alpha\beta} + J_{\beta\alpha} + \left(\rho_\beta \boldsymbol{j}_\alpha \cdot \nabla_\alpha + \rho_\alpha \boldsymbol{j}_\beta \cdot \nabla_\beta\right) g_{\alpha\beta} + \sqrt{\rho_\alpha \rho_\beta} \coprod_\gamma \coprod_\eta S_{\alpha\gamma} \dot{\widetilde{X}}_{\gamma\eta} S_{\beta\eta} = \rho_\alpha \rho_\beta \coprod_\gamma Y_{\gamma\alpha\beta} \nabla_\gamma \cdot \boldsymbol{j}_\gamma. \tag{3.38}$$

3.4 The Feynman states

We define the operator [CKT96]

$$\widehat{\mathcal{H}}_\alpha := -\frac{\hbar^2}{2m_\alpha} \frac{1}{\sqrt{\rho_\alpha}} \nabla_\alpha \cdot \rho_\alpha \nabla_\alpha \frac{1}{\sqrt{\rho_\alpha}} \tag{3.39}$$

and use it to define the *Feynman states* $\psi_{\alpha,n}$ [Bij40], [Fey54] as the solutions of the generalised eigenvalue problem [CKT96]

$$\widehat{\mathcal{H}}_\alpha \psi_{\alpha,n} = \hbar\omega_n \coprod_\beta S_{\alpha\beta} \psi_{\beta,n} \tag{3.40}$$

with the orthonormalisation condition [CKT96]

$$\sum\!\!\!\!\!\!\int_{\alpha} \psi^*_{\alpha,m} \widehat{\mathcal{H}}_\alpha \psi_{\alpha,n} = \hbar\omega_m \delta_{mn}. \tag{3.41}$$

Next we define the states [CKT96]

$$\phi_{\alpha,n} := \frac{1}{\hbar\omega_n} \widehat{\mathcal{H}}_\alpha \psi_{\alpha,n} = \sum\!\!\!\!\!\!\int_{\beta} S_{\alpha\beta} \psi_{\beta,n}, \tag{3.42}$$

that are orthonormal to the Feynman states.

$$\sum\!\!\!\!\!\!\int_{\alpha} \psi^*_{\alpha,m} \phi_{\alpha,n} = \sum\!\!\!\!\!\!\int_{\alpha} \psi_{\alpha,m} \phi^*_{\alpha,n} = \delta_{mn} \tag{3.43}$$

As it will be an useful abbreviation later, we introduce [CKT96]

$$\zeta_{\alpha,n} := \frac{\phi_{\alpha,n} - \psi_{\alpha,n}}{\sqrt{\rho_\alpha}}. \tag{3.44}$$

Now we can use the states just defined to introduce the following expansions. [CKT96]

$$\delta\tilde{\rho}_\alpha = \sum_m r_m(t) \phi_{\alpha,m} \tag{3.45}$$

$$\delta\widetilde{X}_{\alpha\beta} = \sum_{m,n} X_{mn}(t) \psi_{\alpha,m} \psi_{\beta,n} \tag{3.46}$$

$$\widetilde{U}_{\mathrm{ext},\alpha} = \sum_m u_m(t) \psi_{\alpha,m} \tag{3.47}$$

We insert equations (3.45)–(3.47) into the equations of motion and project them onto the Feynman states. First this is done for the two addends of equation (2.26) where the procedure is straight forward and gives

$$\sum\!\!\!\!\!\!\int_{\alpha} \psi^*_{\alpha,m} \delta\dot{\tilde{\rho}}_\alpha = \sum\!\!\!\!\!\!\int_{\alpha} \psi^*_{\alpha,m} \sum_n \dot{r}_n(t) \phi_{\alpha,n} = \dot{r}_m(t) \tag{3.48}$$

$$\sum\!\!\!\!\!\!\int_{\alpha} \psi^*_{\alpha,m} \frac{D_\alpha}{\sqrt{\rho_\alpha}} = \sum\!\!\!\!\!\!\int_{\alpha} \psi^*_{\alpha,m} \frac{2}{i\hbar} \sum\!\!\!\!\!\!\int_{\beta} S_{\alpha\beta} \sum_n u_n(t) \psi_{n,\beta} = \frac{2}{i\hbar} \sum_n u_n(t) \sum\!\!\!\!\!\!\int_{\alpha} \psi^*_{\alpha,m} \phi_{\alpha,n} = \frac{2}{i\hbar} u_m(t). \tag{3.49}$$

The term with the current density from equation (2.26) requires some tedious algebra, but finally results in

$$\sum\!\!\!\!\!\!\int_{\alpha} \psi^*_{\alpha,m} \frac{\nabla_\alpha \cdot \boldsymbol{j}_\alpha}{\sqrt{\rho_\alpha}} = i\omega_m r_m(t) + \frac{i}{2\hbar} \sum_{p,q} X_{pq}(t)\, V_{pq,m} \tag{3.50}$$

with the definitions [CKT96]

$$V_{pq,n} := \sum\!\!\!\!\!\!\int_{\alpha} \frac{\hbar^2}{2m_\alpha} \frac{\psi^*_{\alpha,n}}{\sqrt{\rho_\alpha}} \nabla_\alpha \cdot \sqrt{\rho_\alpha} \boldsymbol{W}_{\alpha,pq} \tag{3.51}$$

$$\boldsymbol{W}_{\alpha,mn} := \phi_{\alpha,m} \nabla_\alpha \zeta_{\alpha,n} + \phi_{\alpha,n} \nabla_\alpha \zeta_{\alpha,m} + \sqrt{\rho_\alpha} \nabla_\alpha Z_{\alpha,mn} \tag{3.52}$$

$$Z_{\alpha,mn} := \frac{1}{\sqrt{\rho_\alpha}} \sum\!\!\!\!\!\!\int_{\beta} \sum\!\!\!\!\!\!\int_{\gamma} \phi_{\beta,m} \phi_{\gamma,n} \widetilde{X}_{\alpha\beta\gamma}. \tag{3.53}$$

A very similar approach is necessary to project the Feynman states on equation (3.38), which leads us to [CKT96]

$$i\hbar\dot{X}_{mn}(t) - \hbar(\omega_m + \omega_n)X_{mn}(t) = -i\hbar \sum\!\!\!\!\!\!\int_\alpha \tilde{\boldsymbol{j}}_\alpha \cdot \boldsymbol{W}^*_{\alpha,mn}. \tag{3.54}$$

Starting with equation (3.26) we can reformulate the right side of equation (3.54) as [CKT96]

$$\sum\!\!\!\!\!\!\int_\alpha \tilde{\boldsymbol{j}}_\alpha \cdot \boldsymbol{W}^*_{\alpha,mn} = \sum\!\!\!\!\!\!\int_\alpha \frac{\hbar}{2m_\alpha i}\left(\sqrt{\rho_\alpha}\nabla_\alpha \frac{1}{\sqrt{\alpha}}\sum_p r_p(t)\psi_{\alpha,p} - \frac{1}{2}\sum_{p,q} X_{pq}(t)\boldsymbol{W}_{\alpha,pq}\right)\cdot \boldsymbol{W}^*_{\alpha,mn}, \tag{3.55}$$

which finally lets us eliminate the one-body current and write our equations of motion in Feynman space. [CKT96]

$$i\hbar\dot{r}_m(t) - \hbar\omega_m r_m(t) - \frac{1}{2}\sum_{p,q} X_{pq}(t)V_{pq,m} = 2u_m(t) \tag{3.56}$$

$$i\hbar\dot{X}_{mn}(t) - \hbar(\omega_m + \omega_n)X_{mn}(t) - \sum_{p,q} X_{pq}(t)\sum\!\!\!\!\!\!\int_\alpha \frac{\hbar^2}{4m_\alpha}\boldsymbol{W}^*_{\alpha,mn}\cdot\boldsymbol{W}_{\alpha,pq} = \sum_p r_p(t)V^*_{mn,p} \tag{3.57}$$

3.5 The triplet correlations

Before heading towards the response function, we define the triplet correlations $X_{\alpha\beta\gamma}$ as a expansion into Feynman states similar to as it is done by Clements et al. [Cle+93], such that one has

$$\widetilde{X}_{\alpha\beta\gamma} := \sum_{m,n,o} \psi_{\alpha,m}\psi^*_{\beta,n}\psi^*_{\gamma,o}\frac{V_{mno}}{\hbar(\omega_m + \omega_n + \omega_o)} \tag{3.58}$$

$$\begin{aligned} V_{mno} := -\sum\!\!\!\!\!\!\int_\alpha \frac{\hbar^2}{2m_\alpha}\sqrt{\rho_\alpha}\Big(&\phi^*_{\alpha,m}\left(\nabla_\alpha\zeta_{\alpha,n}\right)\cdot\left(\nabla_\alpha\zeta_{\alpha,o}\right) + \phi_{\alpha,n}\left(\nabla_\alpha\zeta^*_{\alpha,m}\right)\cdot\left(\nabla_\alpha\zeta_{\alpha,o}\right) \\ &+ \phi_{\alpha,o}\left(\nabla_\alpha\zeta^*_{\alpha,m}\right)\cdot\left(\nabla_\alpha\zeta_{\alpha,n}\right)\Big). \end{aligned} \tag{3.59}$$

Using the triplet correlations we can then write down $V_{st,n}$ from equation (3.51) in terms of the Feynman states, which gives

$$V_{pq,n} = \sum\!\!\!\!\!\!\int_\alpha \frac{\hbar^2}{2m_\alpha}\frac{\psi^*_{\alpha,n}}{\sqrt{\rho_\alpha}}\nabla_\alpha\cdot\sqrt{\rho_\alpha}\left(\phi_{\alpha,p}\nabla_\alpha\zeta_{\alpha,q} + \phi_{\alpha,q}\nabla_\alpha\zeta_{\alpha,p}\right) + \frac{\omega_n V_{nst}}{\omega_n + \omega_p + \omega_q}. \tag{3.60}$$

3.6 Removing the time dependence

The next problem we have to solve is removing the time dependence and the time derivatives from equations (3.56) and (3.57). For this reason we introduce the following representations of the decomposition coefficients in frequency space. Note that we switch on the time dependence adiabatically. [SAH04, p. 167]

$$r_m(t) = \lim_{\varepsilon\to 0+} e^{\varepsilon t}\int\frac{\mathrm{d}\omega}{2\pi}\, e^{-i\omega t}r_m(\omega) \tag{3.61}$$

$$X_{mn}(t) = \lim_{\varepsilon\to 0+} e^{\varepsilon t}\int\frac{\mathrm{d}\omega}{2\pi}\, e^{-i\omega t}X_{mn}(\omega) \tag{3.62}$$

$$u_m(t) = \lim_{\varepsilon\to 0+} e^{\varepsilon t}\int\frac{\mathrm{d}\omega}{2\pi}\, e^{-i\omega t}u_m(\omega) \tag{3.63}$$

We use the frequency space representations (3.61)–(3.63) to insert into equation (3.57), which leads us to

$$\hbar\left(\omega-\omega_m-\omega_n+i\varepsilon\right)X_{mn}(\omega)-\sum_{p,q}X_{pq}(\omega)\sum\!\!\!\!\!\!\int_{\alpha}\frac{\hbar^2}{4m_\alpha}\boldsymbol{W}^*_{\alpha,mn}\cdot\boldsymbol{W}_{\alpha,pq}=\sum_o r_o(\omega)V^*_{mn,o}. \tag{3.64}$$

Defining [CKT96]

$$A_{mnpq}(\omega):=\hbar\left(\omega-\omega_m-\omega_n+i\varepsilon\right)\delta_{mp}\delta_{nq}-\sum\!\!\!\!\!\!\int_{\alpha}\frac{\hbar^2}{4m_\alpha}\boldsymbol{W}^*_{\alpha,mn}\cdot\boldsymbol{W}_{\alpha,pq} \tag{3.65}$$

we can formally solve for the decomposition coefficient [CKT96]

$$X_{mn}(\omega)=\sum_o r_o(\omega)\sum_{p,q}A^{-1}_{mnst}(\omega)V^*_{pq,o}. \tag{3.66}$$

One should think of $A_{mnst}(\omega)$ as a simple matrix with the indices (m,n) and (s,t), such that the first term in definition (3.65) is diagonal and the inverse matrix is defined as

$$\sum_{p',q'}A^{-1}_{mnp'q'}(\omega)A_{p'q'pq}(\omega)=\delta_{mp}\delta_{nq}. \tag{3.67}$$

Next we want to solve $r_m(\omega)$ from equation (3.56) and for that reason we insert the solution (3.66) for $X_{mn}(\omega)$, which gives us [CKT96]

$$\hbar\left(\omega-\omega_m+i\varepsilon\right)r_m(\omega)-\frac{1}{2}\sum_{p,q}V_{pq,m}\sum_o r_o(\omega)\sum_{p',q'}A^{-1}_{pqp'q'}(\omega)V^*_{p'q',o}=2u_m(\omega) \tag{3.68}$$

We can define the *self energy* [CKT96]

$$\Sigma_{mn}(\omega):=\frac{1}{2}\sum_{p,q,p',q'}V_{pq,m}A^{-1}_{pqp'q'}(\omega)V^*_{p'q',n}, \tag{3.69}$$

which lets us simplify equation (3.68).

$$\sum_n\Big\{\hbar\left(\omega-\omega_m+i\varepsilon\right)\delta_{mn}-\Sigma_{mn}(\omega)\Big\}r_n(\omega)=2u_m(\omega) \tag{3.70}$$

With the definition

$$G_{mn}(\omega):=\Big\{\hbar\left(\omega-\omega_m+i\varepsilon\right)\delta_{mn}-\Sigma_{mn}(\omega)\Big\}^{-1} \tag{3.71}$$

we can finally solve for the decomposition coefficients

$$r_m(\omega)=2\sum_n G_{mn}(\omega)u_n(\omega). \tag{3.72}$$

From $r_m(\omega)$ we can now obtain $\delta\rho_\alpha$, but remember that we defined $\delta\rho_\alpha$ as the complex-valued density fluctuations and the response function $\chi_{\alpha\beta}$ we are looking for describes the linear relationship between perturbations $U_{\mathrm{ext},\alpha}$ and the real physical density fluctuations $\mathfrak{Re}\,\delta\rho_\alpha$.

3.7 The density-density linear response function

It is time to give a formal definition of it, which reads

$$\underset{t\to\omega}{\mathrm{FT}}\left[\mathfrak{Re}\,\delta\tilde{\rho}_\alpha\right](\boldsymbol{r}_\alpha,\omega)=:\sum\!\!\!\!\!\!\int_{\beta}\chi_{\alpha\beta}(\boldsymbol{r}_\alpha,\boldsymbol{r}_\beta,\omega)\widetilde{U}_{\mathrm{ext},\beta}(\boldsymbol{r}_\beta,\omega). \tag{3.73}$$

Please note that $\delta\tilde{\rho}_\alpha$ in equation (3.73) is a function of frequency and not of time. Therefore we start with taking the real part of equation (3.45) and apply a Fourier transformation from time to frequency domain.

$$\underset{t\to\omega}{\mathrm{FT}}\left[\mathfrak{Re}\,\delta\tilde{\rho}_\alpha\right](\boldsymbol{r}_\alpha,\omega) = \frac{1}{2}\sum_m \int \mathrm{d}t\; e^{i\omega t}\left(r_m(t)\phi_{\alpha,m} + r_m^*(t)\phi_{\alpha,m}^*\right) \tag{3.74}$$

We proceed with inserting the frequency decompositions for $r_m(\omega)$ from equation (3.61), which leads us to

$$\underset{t\to\omega}{\mathrm{FT}}\left[\mathfrak{Re}\,\delta\tilde{\rho}_\alpha\right] = \frac{1}{2}\sum_m \int \mathrm{d}t\; e^{i\omega t}\int\frac{\mathrm{d}\omega'}{2\pi}\;\left(\phi_{\alpha,m}e^{-i\omega' t}r_m(\omega') + \phi_{\alpha,m}^* e^{i\omega' t}r_m^*(\omega')\right). \tag{3.75}$$

Now we can carry out the time integration, which gives us the Dirac deltas in the following equation.

$$\underset{t\to\omega}{\mathrm{FT}}\left[\mathfrak{Re}\,\delta\tilde{\rho}_\alpha\right] = \frac{1}{2}\sum_m \int \mathrm{d}\omega'\;\left(\phi_{\alpha,m}r_m(\omega')\delta(\omega-\omega') + \phi_{\alpha,m}^* r_m^*(\omega')\delta(\omega+\omega')\right) \tag{3.76}$$

After performing the ω'-integration we can insert the result obtained in the last section from equation (3.72).

$$\underset{t\to\omega}{\mathrm{FT}}\left[\mathfrak{Re}\,\delta\tilde{\rho}_\alpha\right] = \sum_m\left(\phi_{\alpha,m}\sum_n G_{mn}(\omega)u_n(\omega) + \phi_{\alpha,m}^*\sum_n G_{mn}^*(-\omega)u_n^*(-\omega)\right) \tag{3.77}$$

Changing the subscript index of u_n to o using the Kronecker delta from equation (3.43) we can write

$$\underset{t\to\omega}{\mathrm{FT}}\left[\mathfrak{Re}\,\delta\tilde{\rho}_\alpha\right] = \sum_{m,n,o}\sum\!\!\!\!\!\!\int_\beta\left(\phi_{\alpha,m}G_{mn}(\omega)u_o(\omega)\phi_{\beta,n}^*\psi_{\beta,o} + \phi_{\alpha,m}^*G_{mn}^*(-\omega)u_o^*(-\omega)\phi_{\beta,n}\psi_{\beta,o}^*\right), \tag{3.78}$$

where we can now insert $\widetilde{U}_{\mathrm{ext},\beta}(\boldsymbol{r}_\beta,\omega)$ from the decomposition (3.47).

$$\underset{t\to\omega}{\mathrm{FT}}\left[\mathfrak{Re}\,\delta\tilde{\rho}_\alpha\right] = \sum\!\!\!\!\!\!\int_\beta\sum_{m,n}\left(\phi_{\alpha,m}\phi_{\beta,n}^*G_{mn}(\omega)\widetilde{U}_{\mathrm{ext},\beta}(\boldsymbol{r}_\beta,\omega) + \phi_{\alpha,m}^*\phi_{\beta,n}G_{mn}^*(-\omega)\widetilde{U}_{\mathrm{ext},\beta}^*(\boldsymbol{r}_\beta,-\omega)\right) \tag{3.79}$$

For the last step we have to recall that $\widetilde{U}_{\mathrm{ext},\beta}(\boldsymbol{r}_\beta,t)$ is real, so we can use the well known Fourier relation $\widetilde{U}_{\mathrm{ext},\beta}(\boldsymbol{r}_\beta,\omega) = \widetilde{U}_{\mathrm{ext},\beta}^*(\boldsymbol{r}_\beta,-\omega)$.

$$\underset{t\to\omega}{\mathrm{FT}}\left[\mathfrak{Re}\,\delta\tilde{\rho}_\alpha\right] = \sum\!\!\!\!\!\!\int_\beta\sum_{m,n}\left(\phi_{\alpha,m}\phi_{\beta,n}^*G_{mn}(\omega) + \phi_{\alpha,m}^*\phi_{\beta,n}G_{mn}^*(-\omega)\right)\widetilde{U}_{\mathrm{ext},\beta}(\boldsymbol{r}_\beta,\omega) \tag{3.80}$$

This is finally the linear relationship between the perturbation and the density fluctuations, which enables us to write the density-density linear response function as

$$\chi_{\alpha\beta}(\boldsymbol{r}_\alpha,\boldsymbol{r}_\beta,\omega) = \sum_{m,n}\left(\phi_{\alpha,m}(\boldsymbol{r}_\alpha)\,\phi_{\beta,n}^*(\boldsymbol{r}_\beta)\,G_{mn}(\omega) + \phi_{\alpha,m}^*(\boldsymbol{r}_\alpha)\,\phi_{\beta,n}(\boldsymbol{r}_\beta)\,G_{mn}^*(-\omega)\right). \tag{3.81}$$

3.8 One additional approximation

For the numerical evaluations in the following chapter we make one last approximation by neglecting the off-diagonal term of [CKT96]

$$A_{mnpq} \approx \hbar\,(\omega-\omega_m-\omega_n+i\varepsilon)\,\delta_{mp}\delta_{nq}, \tag{3.82}$$

which gives us the following form of the self-energy. [CKT96]

$$\Sigma_{mn}(\omega) = \frac{1}{2}\sum_{p,q}\frac{V_{pq,m}V_{pq,n}^*}{\hbar\,(\omega-\omega_p-\omega_q+i\varepsilon)} \tag{3.83}$$

4 Applications

After establishing the necessary framework in the previous chapter it is now time to focus on numerical applications of the theory. In this chapter we deal with excitations in dipolar one- and two-layer boson systems at low temperatures, as they are sketched in figure 1.1.

These setups can be described as homogeneous systems, if we describe each layer as a single particle type and denote a position within a layer α using the 2D-vector $\boldsymbol{r}_\alpha$.

As we saw in the previous chapter we need to know the ground state values of the static structure factor to determine the Feynman states and dispersion relation for the computation of the response function. In this thesis we use the results gained by Martin Hebenstreit [Heb13], who used the hypernetted-chain Euler-Lagrange method to get $S_{\alpha\beta}(\boldsymbol{k})$, which is hermitian with respect to both particle types and $\boldsymbol{k}$ – so $S_{\alpha\beta}(\boldsymbol{k}) = S^*_{\beta\alpha}(\boldsymbol{k}) = S^*_{\alpha\beta}(-\boldsymbol{k})$ holds.

4.1 The homogeneous Feynman eigenvalue problem

If we deal with homogeneous systems, the operator from definition (3.39) simply turns to the one-body Hamiltonian

$$\widehat{\mathcal{H}}_\alpha = -\frac{\hbar^2}{2m_\alpha}\Delta_\alpha, \tag{4.1}$$

which allows us to write the general quantum number n from the Feynman states as the pair $(n, \boldsymbol{k})$ and make the plane wave ansatz

$$\psi_{\alpha,n}(\boldsymbol{r}_\alpha) \longrightarrow \psi_{\alpha,n,\boldsymbol{k}}(\boldsymbol{r}_\alpha) := e^{i\boldsymbol{k}\cdot\boldsymbol{r}_\alpha}\psi_{\alpha,n}(\boldsymbol{k}), \tag{4.2}$$

that we insert in equation (3.40) to obtain

$$\frac{\hbar^2k^2}{2m_\alpha}e^{i\boldsymbol{k}\cdot\boldsymbol{r}_\alpha}\psi_{\alpha,n}(\boldsymbol{k}) = \hbar\omega_n \sum_\beta \int S_{\alpha\beta}(\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta)e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}_\alpha-\boldsymbol{r}_\beta)}e^{i\boldsymbol{k}\cdot\boldsymbol{r}_\alpha}\psi_{\beta,n}(\boldsymbol{k}). \tag{4.3}$$

On the right side we introduce the Fourier transform of the static structure factor and therefore get the generalised Feynman eigenvalue problem in momentum space.

$$\frac{\hbar^2k^2}{2m_\alpha}\psi_{\alpha,n}(\boldsymbol{k}) = \hbar\omega_n(\boldsymbol{k})\sum_\beta S_{\alpha\beta}(\boldsymbol{k})\psi_{\beta,n}(\boldsymbol{k}) \tag{4.4}$$

As it makes the numerical evaluation easier and more efficient we define

$$\xi_{\alpha,n}(\boldsymbol{k}) := \frac{1}{\sqrt{m_\alpha}}\psi_{\alpha,n}(\boldsymbol{k}), \tag{4.5}$$

which leads us to the hermitian eigenvalue problem

$$\frac{\hbar k^2}{2\omega_n(\boldsymbol{k})}\xi_{\alpha,n}(\boldsymbol{k}) = \sum_\beta \sqrt{m_\alpha m_\beta}S_{\alpha\beta}(\boldsymbol{k})\xi_{\beta,n}(\boldsymbol{k}). \tag{4.6}$$

If we take the complex conjugate of both sides and use $S^*_{\alpha\beta}(\boldsymbol{k}) = S_{\alpha\beta}(-\boldsymbol{k})$, it is immediately clear that $\xi^*_{\alpha,n}(\boldsymbol{k}) = \xi_{\alpha,n}(-\boldsymbol{k})$ holds.

One should note that with introducing the pair of quantum numbers $(n, \boldsymbol{k}_n)$, also the transitions

$$\sum_n \longrightarrow \sum_n \int \mathrm{d}^s k_n \qquad \text{and} \qquad \delta_{mn} \longrightarrow \delta_{mn}\delta(\boldsymbol{k}_m - \boldsymbol{k}_n) \tag{4.7}$$

are necessary. Although we are only interested in 2D-systems, we keep writing our equations for the general s-dimensional case. An important Fourier identity we will also need is

$$\int \mathrm{d}^s r \; e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = (2\pi)^s \delta\big(\boldsymbol{k} - \boldsymbol{k}'\big) \,. \tag{4.8}$$

4.2 The normalisation

The eigenvalues and eigenvectors of equation (4.6) are calculated using LAPACK-routines and therefore are determined with the normalisation

$$\sum_\alpha \xi^{(\mathrm{LP})*}_{\alpha,m}(\boldsymbol{k})\, \xi^{(\mathrm{LP})}_{\alpha,n}(\boldsymbol{k}) = \delta_{mn}, \tag{4.9}$$

which is in conflict with the normalisation we required in equation (3.41). Therefore after computing $\psi_{\alpha,n}(\boldsymbol{k})$ from equation (4.5) we have to renormalise the Feynman states in the following way.

$$\psi_{\alpha,n}(\boldsymbol{k}) = \sqrt{\frac{2m_\alpha \omega_n(\boldsymbol{k})}{\hbar k^2}} (2\pi)^{-\frac{s}{2}} \xi^{(\mathrm{LP})}_{\alpha,n}(\boldsymbol{k}) \tag{4.10}$$

This implies, that $\psi_{\alpha,n}(\boldsymbol{k})$ diverges for $\boldsymbol{k} \to \boldsymbol{0}$, as the dispersion $\omega_n(\boldsymbol{k})$ is linear for small $\boldsymbol{k}$. We also define

$$\phi_{\alpha,n}(\boldsymbol{k}) := \sqrt{\frac{\hbar k^2}{2m_\alpha \omega_n(\boldsymbol{k})}} (2\pi)^{-\frac{s}{2}} \xi^{(\mathrm{LP})}_{\alpha,n}(\boldsymbol{k}) \tag{4.11}$$

$$\zeta_{\alpha,n}(\boldsymbol{k}) := \frac{\phi_{\alpha,n}(\boldsymbol{k}) - \psi_{\alpha,n}(\boldsymbol{k})}{\sqrt{\rho_\alpha}}, \tag{4.12}$$

which enables us to write $\phi_{\alpha,n,\boldsymbol{k}}(\boldsymbol{r}_\alpha) = \phi_{\alpha,n}(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_\alpha}$ and $\zeta_{\alpha,n,\boldsymbol{k}}(\boldsymbol{r}_\alpha) = \zeta_{\alpha,n}(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_\alpha}$.

4.3 Final preparations

Just before we can start our ultimate march towards the numerical results we have to bring our expressions into a convenient form for the numerical implementation. Therefore we start with defining the abbreviations

$$\Lambda_{\alpha,mno}(\boldsymbol{k}_m, \boldsymbol{k}_n, \boldsymbol{k}_o) := \phi^*_{\alpha,m}(\boldsymbol{k}_m)\, \zeta_{\alpha,n}(\boldsymbol{k}_n)\, \zeta_{\alpha,o}(\boldsymbol{k}_o)\, \boldsymbol{k}_n \cdot \boldsymbol{k}_o \tag{4.13}$$

$$\Xi_{\alpha,mno}(\boldsymbol{k}_m, \boldsymbol{k}_n, \boldsymbol{k}_o) := \phi_{\alpha,m}(\boldsymbol{k}_m)\, \zeta_{\alpha,n}(\boldsymbol{k}_n)\, \zeta^*_{\alpha,o}(\boldsymbol{k}_o)\, \boldsymbol{k}_n \cdot \boldsymbol{k}_o, \tag{4.14}$$

which enable us then to rewrite $V_{pq,n}$ of equation (3.60) as

$$\begin{aligned} V_{pq,n}(\boldsymbol{k}_p, \boldsymbol{k}_q, \boldsymbol{k}_n) = -\sum_\alpha \frac{\hbar^2}{2m_\alpha} (2\pi)^s \Big\{ \psi^*_{\alpha,n}(\boldsymbol{k}_n) \Big(\phi_{\alpha,p}(\boldsymbol{k}_p)\zeta_{\alpha,q}(\boldsymbol{k}_q)\boldsymbol{k}_q + \phi_{\alpha,q}(\boldsymbol{k}_q)\zeta_{\alpha,p}(\boldsymbol{k}_p)\boldsymbol{k}_p \Big) \cdot \boldsymbol{k}_n \\ - \frac{\omega_n(\boldsymbol{k}_n)\sqrt{\rho_\alpha}}{\omega_n(\boldsymbol{k}_n) + \omega_p(\boldsymbol{k}_p) + \omega_q(\boldsymbol{k}_q)} \Big(\Lambda_{\alpha,npq} - \Xi_{\alpha,pqn} - \Xi_{\alpha,qpn} \Big) \Big\} \delta(\boldsymbol{k}_n - (\boldsymbol{k}_p + \boldsymbol{k}_q)) \,. \end{aligned} \tag{4.15}$$

We factor out the Dirac deltas and define

$$\overline{V}_{pq,n}(\boldsymbol{k}_p, \boldsymbol{k}_n)\, \delta(\boldsymbol{k}_n - (\boldsymbol{k}_p + \boldsymbol{k}_q)) := V_{pq,n}(\boldsymbol{k}_p, \boldsymbol{k}_q, \boldsymbol{k}_n). \tag{4.16}$$

Due to the Dirac delta $\overline{V}_{pq,n}$ only depends on two of the three $\boldsymbol{k}$-vectors and here $\boldsymbol{k}_q = \boldsymbol{k}_n - \boldsymbol{k}_p$ is chosen. This notation lets us write the product of equation (3.83) as

$$V_{pq,m}(\boldsymbol{k}_p, \boldsymbol{k}_q, \boldsymbol{k}_m) V^*_{pq,n}(\boldsymbol{k}_p, \boldsymbol{k}_q, \boldsymbol{k}_n) = \delta(\boldsymbol{k}_m - (\boldsymbol{k}_p + \boldsymbol{k}_q))\, \delta(\boldsymbol{k}_m - \boldsymbol{k}_n)\, \overline{V}_{pq,m}(\boldsymbol{k}_p, \boldsymbol{k}_m) \overline{V}^*_{pq,n}(\boldsymbol{k}_p, \boldsymbol{k}_n), \tag{4.17}$$

which shows that the self energy is diagonal with respect to $\boldsymbol{k}_m$ and $\boldsymbol{k}_n$.

$$\Sigma_{mn}(\boldsymbol{k}_m, \boldsymbol{k}_n, \omega) = \frac{1}{2} \sum_{p,q} \int \mathrm{d}^s k_p \; \frac{\overline{V}_{pq,m}(\boldsymbol{k}_p, \boldsymbol{k}_m) \overline{V}^*_{pq,n}(\boldsymbol{k}_p, \boldsymbol{k}_m)}{\hbar(\omega - \omega_p(\boldsymbol{k}_p) - \omega_q(\boldsymbol{k}_m - \boldsymbol{k}_p) + i\varepsilon)} \delta(\boldsymbol{k}_m - \boldsymbol{k}_n) \tag{4.18}$$

Again we factor out the Dirac delta and define

$$\overline{\Sigma}_{mn}(\boldsymbol{k}, \omega)\, \delta\big(\boldsymbol{k} - \boldsymbol{k}'\big) := \Sigma_{mn}(\boldsymbol{k}, \boldsymbol{k}', \omega). \tag{4.19}$$

Based on the definition of G_{mn} in equation (3.71) we can write

$$G_{mn}(\boldsymbol{k}_m, \boldsymbol{k}_n, \omega) = \Big(\hbar(\omega - \omega_m(\boldsymbol{k}_m) + i\varepsilon)\delta_{mn} - \overline{\Sigma}_{mn}(\boldsymbol{k}_m, \omega)\Big)^{-1} \delta(\boldsymbol{k}_m - \boldsymbol{k}_n), \tag{4.20}$$

as $G_{mn}(\boldsymbol{k}_m, \boldsymbol{k}_n)$ is diagonal with respect to $\boldsymbol{k}_m$ and $\boldsymbol{k}_n$. Once more we define

$$\overline{G}_{mn}(\boldsymbol{k}, \omega)\, \delta\big(\boldsymbol{k} - \boldsymbol{k}'\big) := G_{mn}(\boldsymbol{k}, \boldsymbol{k}', \omega). \tag{4.21}$$

Now we are ready to write down $\chi_{\alpha\beta}$, which is a function of $\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta$ in the homogeneous case. We start from equation (3.81), substitute $\boldsymbol{k} \to -\boldsymbol{k}$ in the second addend and make use of $\phi^*_{\alpha,n}(\boldsymbol{k}) = \phi_{\alpha,n}(-\boldsymbol{k})$, which leads us to

$$\chi_{\alpha\beta}(\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta, \omega) = \sum_{m,n} \int \mathrm{d}^s k \; e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta)} \phi_{\alpha,m}(\boldsymbol{k}) \phi^*_{\beta,n}(\boldsymbol{k}) \left(\overline{G}_{mn}(\boldsymbol{k}, \omega) + \overline{G}^*_{mn}(-\boldsymbol{k}, -\omega)\right). \tag{4.22}$$

As we want to calculate the response function in momentum and frequency space, we simply omit the parts of the previous equation that form the inverse Fourier transformation from $\boldsymbol{k}$ to $\boldsymbol{r}$.

$$\chi_{\alpha\beta}(\boldsymbol{k}, \omega) = (2\pi)^s \sum_{m,n} \phi_{\alpha,m}(\boldsymbol{k}) \phi^*_{\beta,n}(\boldsymbol{k}) \left(\overline{G}_{mn}(\boldsymbol{k}, \omega) + \overline{G}^*_{mn}(-\boldsymbol{k}, -\omega)\right) \tag{4.23}$$

From this an immediate implication is the relation

$$\chi^*_{\alpha\beta}(-\boldsymbol{k}, -\omega) = \chi_{\alpha\beta}(\boldsymbol{k}, \omega). \tag{4.24}$$

4.4 Results

For presenting the numerical results we use the system of units also introduced in [Ast+07]. We express masses in units of the characteristic mass m_0 and as all our particles have the same mass we choose m_0 to be the particle mass. Further we express lengths in units of

$$r_0 := \frac{m_0 \mu^2}{4\pi\hbar^2} \tag{4.25}$$

and energies in units of

$$E_0 := \frac{\hbar^2}{m_0 r_0^2}, \tag{4.26}$$

where μ is the magnitude of the boson's generalised dipole moments. Note that in the specific magnetic case one has $\boldsymbol{\mu}_{\text{mag}} = \mu_0^{-\frac{1}{2}} \boldsymbol{\mu}$ with μ_0 as the permeability of free space and in the case of electric dipoles, one has $\boldsymbol{\mu}_{\text{el}} = \varepsilon_0^{\frac{1}{2}} \boldsymbol{\mu}$ with the permittivity of free space ε_0.

We evaluate the response matrix $\chi_{\alpha\beta}(\boldsymbol{k}, \omega)$ for three different system configurations (ϑ is the angle enclosed by the z-axis and $\boldsymbol{\mu}$, ρ the density of each layer and d the distance between the layers):

- one layer, $\vartheta = 0$, $\rho = 256\, r_0^{-2}$
- two layers, $\vartheta = 0$, $\rho = 256\, r_0^{-2}$, $d = 0.06\, r_0$
- two layers, $\vartheta = 0.175\, \pi$, $\rho = 256\, r_0^{-2}$, $d = 0.06\, r_0$

To determine the Feynman states from equation (4.6), we need the static structure factor, which is taken from the calculations of Martin Hebenstreit [Heb13] and illustrated in figure 4.1.

4.4.1 One layer with non-tilted dipoles

The negative imaginary part of the density-density response function $\chi(\boldsymbol{k}, \omega)$ for a system with one layer, $\rho = 256\, r_0^{-2}$, $\vartheta = 0$ and $d = 0.06\, r_0$ is shown in figure 4.2. This kind of system is also studied in [Maz+09] for several densities. The response function is connected to the dynamic structure factor of the system via the fluctuations-dissipation-theorem [SAH04, p. 146]

$$S(\boldsymbol{k}, \omega) = -\frac{1}{\pi} \operatorname{\mathfrak{Im}} \chi(\boldsymbol{k}, \omega). \tag{4.27}$$

One notices, that the collective mode in the CBF calculation becomes lowered in comparison to the Feynman-Bijl dispersion. It becomes also noticeable, that the CBF approximation is no single-pole approximation [SAH04, p. 169] like the Feynman approximation, as there are regions at higher ω than the collective mode, where the response function does not vanish. These regions correspond to excitations, which can decay into two Feynman excitations [SAH04, p. 176]. The ω-dependence for the fixed wave vector $\boldsymbol{k} = 6.33\sqrt{\rho}\, \hat{\boldsymbol{e}}_r$ (at the roton-minimum) is illustrated in figure 4.3. Here one can see the sharp peak of the imaginary part (the collective mode) and the diverging real part. In fact the width of the peak depends on the choice of ε in equations (4.18) and (4.20) and for the calculations performed in this entire work, we choose $\varepsilon = 0.059\, \hbar \rho m_0^{-1}$. This choice also determines the width of the collective mode in the colour map of figure 4.2. At $\omega \approx 50\, \hbar \rho m_0^{-1}$ one can see a minor peak in figure 4.3, which corresponds to states that can decay into two Feynman-maxons. Another interesting feature of the dispersion in figure 4.2 is the so called Pitaevskii-plateau [Pit59] for $k > 11\sqrt{\rho}$, above which excitations can decay into two Feynman-rotons.

4.4.2 Two layers with non-tilted dipoles

In the second example we have two layers with a $\rho = 256\, r_0^{-2}$, $d = 0.06\, r_0$ and $\vartheta = 0$. Now χ turns into a 2×2 matrix $\chi_{\alpha\beta}$. Figure 4.4 shows $-\operatorname{\mathfrak{Im}} \chi_{AA}(\boldsymbol{k}, \omega)$ – the negative imaginary part of the first diagonal element. Note that we use the capital Latin letters A and B to indicate the particle type, i. e. the layer. The most important feature of $\boldsymbol{\chi}(\boldsymbol{k}, \omega)$ is the collective mode, which can be seen also in the other matrix elements, but in the plot of a diagonal element it is most easily seen, so we do not show a colour map plot of an off-diagonal element. An important insight from this calculation is that the two Feynman-Bijl

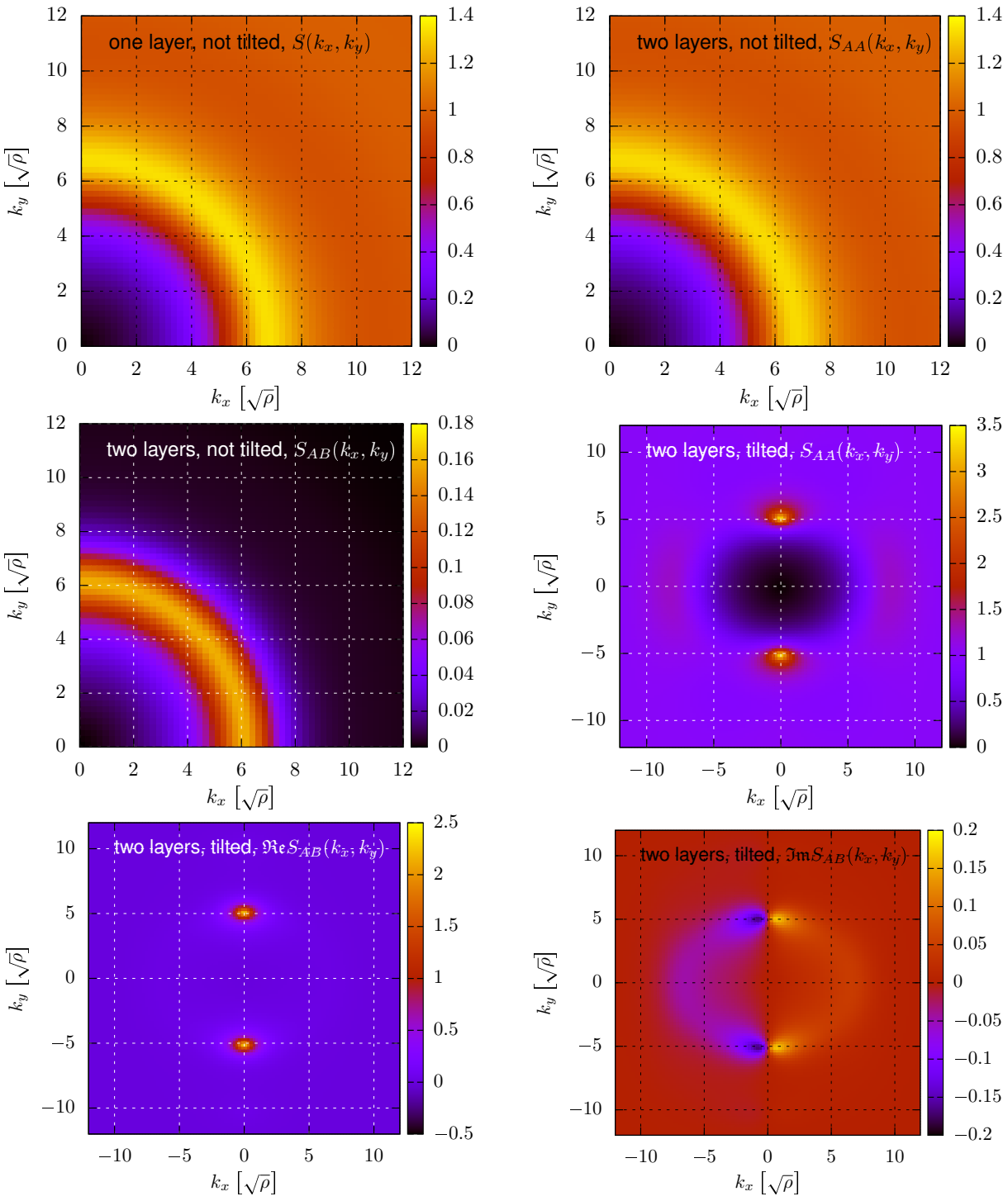


Figure 4.1: The static structure factor obtained by Martin Hebenstreit [Heb13] for the situations indicated by the label at the top of each plot: one layer and two layers not tilted; two layers tilted. In each case the density per layer is $\rho = 256\, r_0^{-2}$ and unless the real and imaginary part are given explicitly, the shown function is real. For the two layer cases the distance between the layers is $d = 0.06\, r_0$ and only one diagonal and one off-diagonal element is given. In the tilted case the angle between the z-axis and the dipole moments is $0.175\, \pi$.

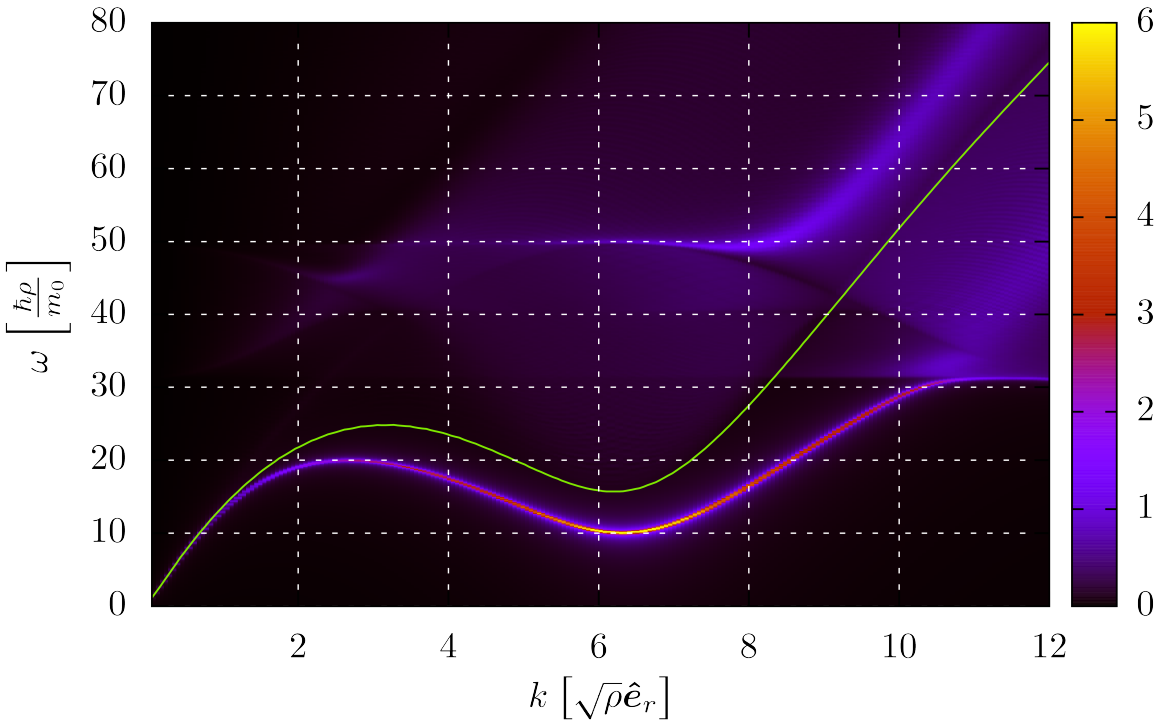


Figure 4.2: $-\,\mathfrak{Im}\,\chi(\boldsymbol{k},\omega)$ for a one-layer system with non-tilted dipoles at the density $\rho = 256\,r_0^{-2}$ as a colour map with $\varepsilon = 0.059\,\hbar\rho m_0^{-1}$ in equations (4.18) and (4.20). The solid green line shows the dispersion in Feynman-Bijl approximation. The values are transformed with the mapping $\chi \to \sqrt{\chi}$ to increase the contrast in the image.

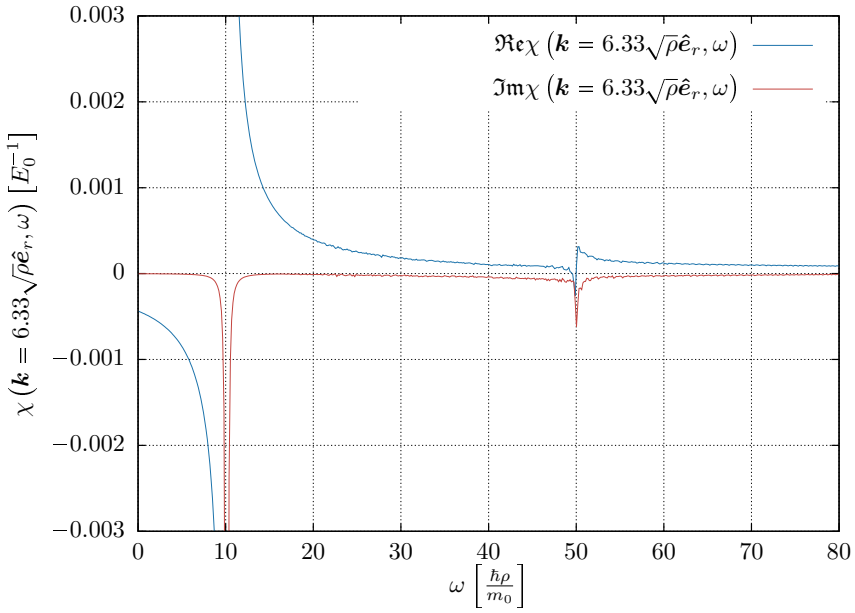


Figure 4.3: $\mathfrak{Re}\,\chi(\boldsymbol{k},\omega)$ and $\mathfrak{Im}\,\chi(\boldsymbol{k},\omega)$ for a one-layer system with non-tilted dipoles at the density $\rho = 256\,r_0^{-2}$ with $\boldsymbol{k} = 6.33\,\sqrt{\rho}\,\hat{\boldsymbol{e}}_r$, which is at the roton-minimum of the dispersion (see figure 4.2).

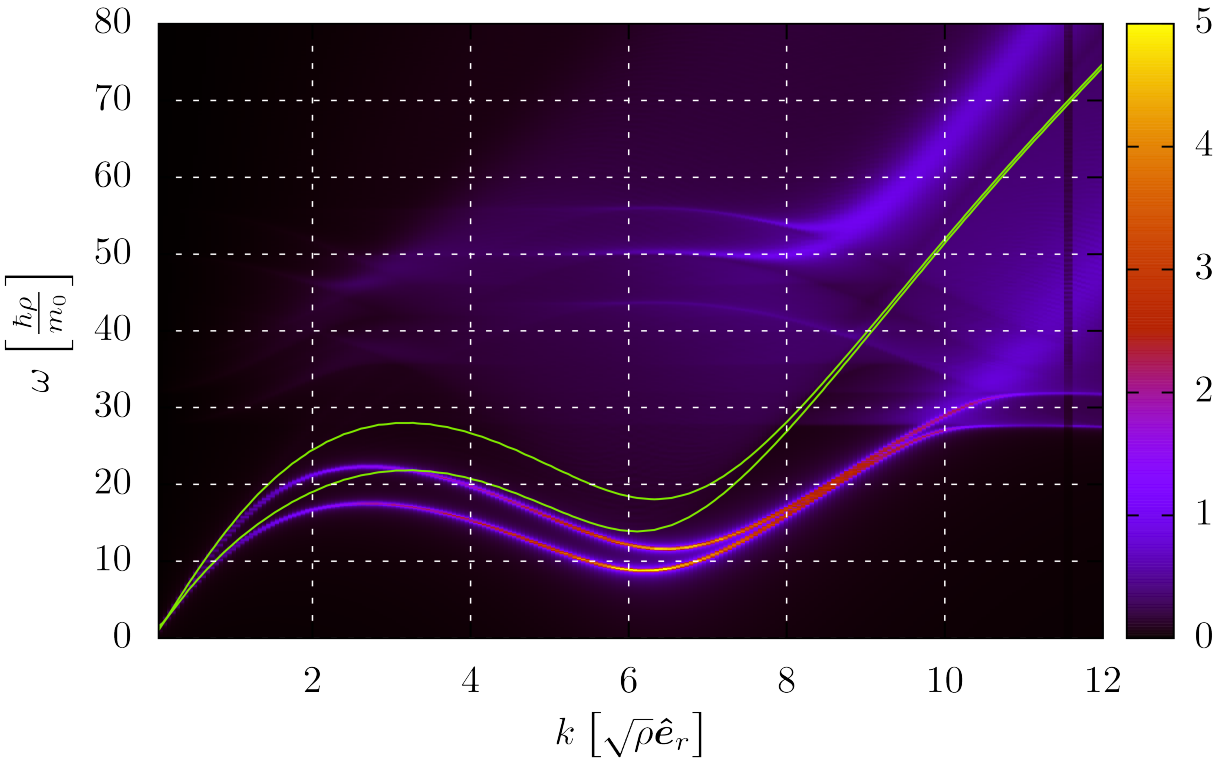


Figure 4.4: $-\,\mathfrak{Im}\,\chi_{AA}(\boldsymbol{k},\omega)$ for a two-layer system (distance of the layers is $d = 0.06\,r_0$) with non-tilted dipoles at the density $\rho = 256\,r_0^{-2}$ in each layer as a colour map with $\varepsilon = 0.059\,\hbar\rho m_0^{-1}$ in equations (4.18) and (4.20). The solid green lines show the dispersion in Feynman-Bijl approximation. The values are transformed with the mapping $\chi_{AA} \to \sqrt{\chi_{AA}}$ to increase the contrast in the image.

modes split up, as the layers are coupled. In figure 4.5 $\chi_{AA}(\boldsymbol{k},\omega)$ and $\chi_{AB}(\boldsymbol{k},\omega)$ are plotted for the fixed wave vector $\boldsymbol{k} = 6.33\sqrt{\rho}\,\hat{\boldsymbol{e}}_r$, where one can see that the location of the collective mode is the same in the diagonal and in the off-diagonal-term, but the poles have different signs in the off-diagonal part. In figure 4.4 one can see again the Pitaevskii-plateau, but this time it splits up into two levels, as the roton of the Feynman-Bijl-dispersion is also split up into two levels.

4.4.3 Two layers with tilted dipoles

The last system we analyse consists of two layers at $\rho = 256\,r_0^{-2}$, $d = 0.06\,r_0$ and $\vartheta = 0.175\,\pi$, which is a generalisation of the investigations of Macia et al. [Mac+12]. This time the system is anisotropic and so in figure 4.6 we give the $-\,\mathfrak{Im}\,\chi_{AA}(\boldsymbol{k},\omega)$ for $\boldsymbol{k} \uparrow\uparrow \hat{\boldsymbol{e}}_x$ and $\boldsymbol{k} \uparrow\uparrow \hat{\boldsymbol{e}}_y$. One can clearly see, that the interaction between the dipoles strongly depends on the direction in $\boldsymbol{k}$-space. The plot for the case $\boldsymbol{k} \uparrow\uparrow \hat{\boldsymbol{e}}_x$ shows a behaviour similar to the previous non-tilted cases, but with a higher roton-energy and a blurred dispersion in the maxon-region, as excitations are able to decay at such low frequencies. For the second direction $\boldsymbol{k} \uparrow\uparrow \hat{\boldsymbol{e}}_y$ the collective mode of the system has a second minimum, which can be interpreted as the system is about to solidify in y-direction, as the dispersion tends to become periodic. The lower roton energy becomes almost 0 at the wave vector, we call $\boldsymbol{k}_0$ for now. If the collective mode of a system really reaches $\omega = 0$ at $\boldsymbol{k}_0$, then time-independent waves proportional to $e^{i\boldsymbol{k}_0\cdot\boldsymbol{r}}$ could exist in this system. That a phase transition is about to happen, is also supposed by Martin Hebenstreit [Heb13]

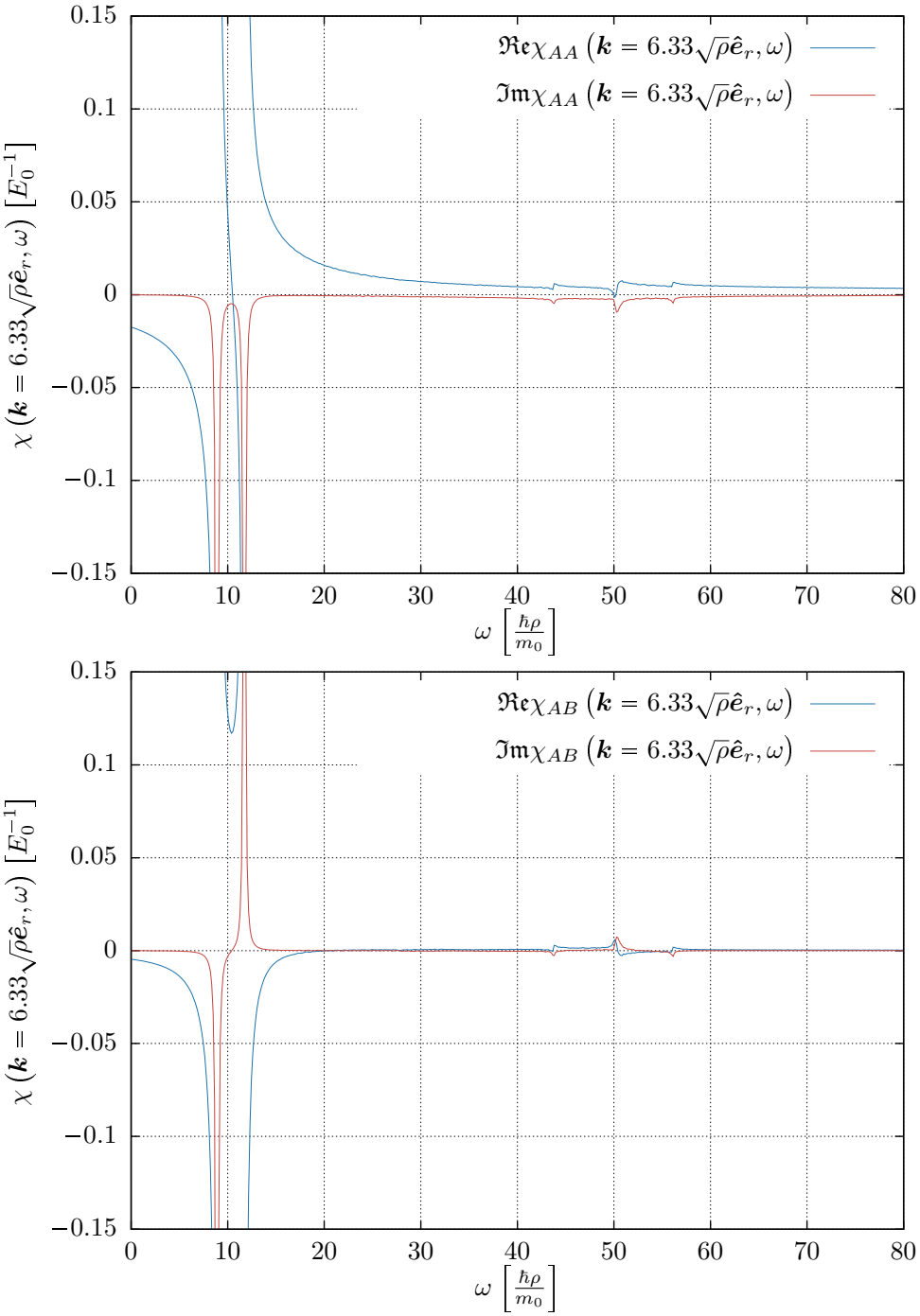


Figure 4.5: $\mathfrak{Re}\,\chi_{AA}(\boldsymbol{k},\omega)$ and $\mathfrak{Im}\,\chi_{AA}(\boldsymbol{k},\omega)$ in the upper plot and $\mathfrak{Re}\,\chi_{AB}(\boldsymbol{k},\omega)$ and $\mathfrak{Im}\,\chi_{AB}(\boldsymbol{k},\omega)$ in the lower plot for a two-layer system with non-tilted dipoles at the density $\rho = 256\,r_0^{-2}$ in each layer with $\boldsymbol{k} = 6.33\,\sqrt{\rho}\,\hat{\boldsymbol{e}}_r$, which is at the roton-minimum of the dispersion (see figure 4.2).

on the basis of the ground state data. In is also clearly to see, that in the region of the second minimum of the collective mode, the splitting up of the Feynman-Bijl dispersion also increases a second time.

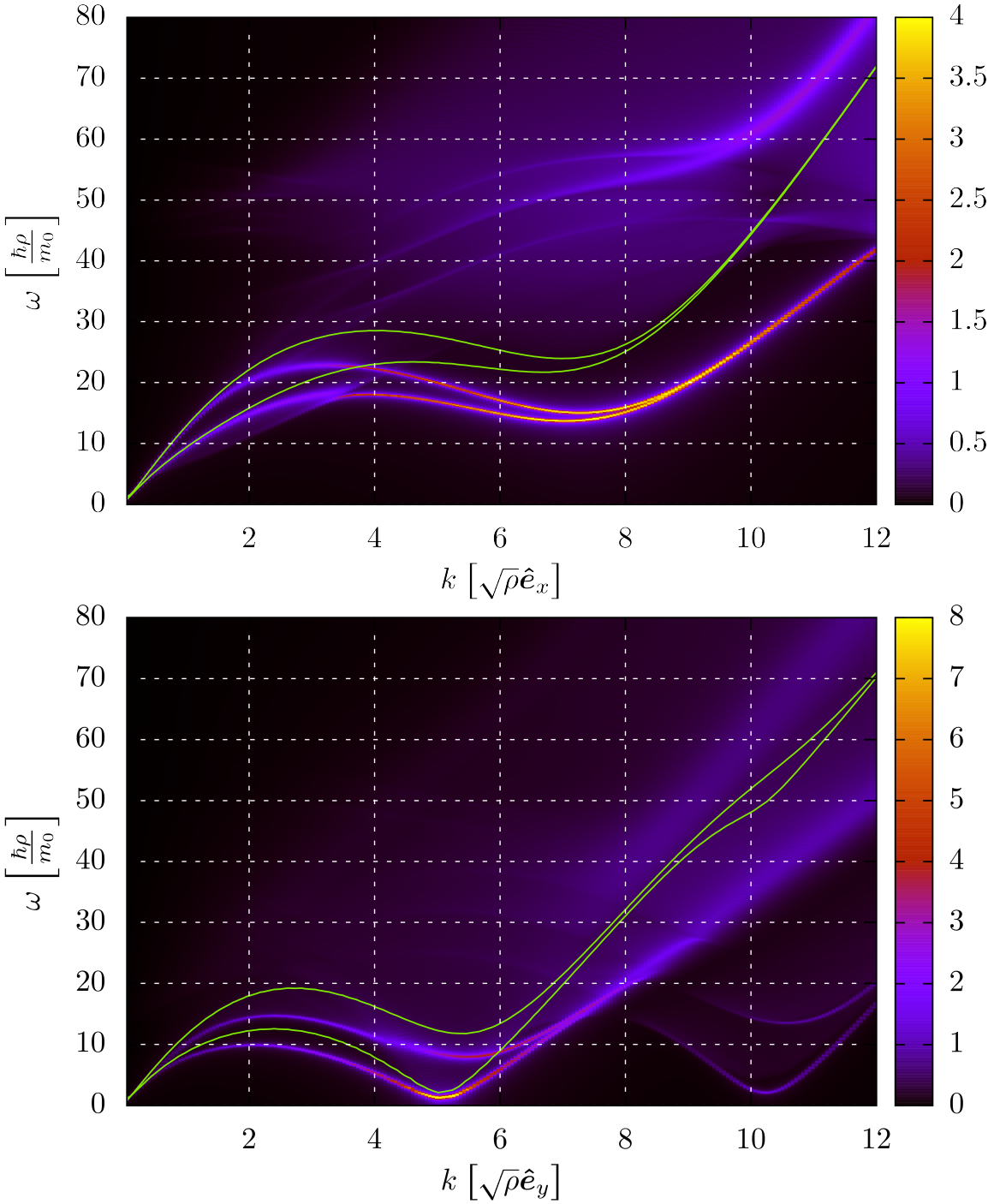


Figure 4.6: $-\,\mathfrak{Im}\,\chi_{AA}(k_x\hat{\boldsymbol{e}}_x,\omega)$ (upper plot) and $-\,\mathfrak{Im}\,\chi_{AA}(k_y\hat{\boldsymbol{e}}_y,\omega)$ (lower plot) for a two-layer system with tilted dipoles ($\vartheta = 0.175\,\pi$) at the density $\rho = 256\,r_0^{-2}$ in each layer as a colour map with $\varepsilon = 0.059\,\hbar\rho m_0^{-1}$ in equations (4.18) and (4.20). The solid green lines show the dispersions in Feynman-Bijl approximation. The values are transformed with the mapping $\chi_{AA} \to \sqrt{\chi_{AA}}$ to increase the contrast in the image.

5 Conclusion and Outlook

In this work we have dealt with the calculation of excitations in 2D-multilayer dipolar Bose gases. These kinds of systems are a very active experimental research topic, see for example [Aik+12], [Lah+07], [Lu+11], [Stu+12] and [Tak+12]. The approach of this work was to describe the multilayer systems as homogeneous 2D multi-component systems instead of inhomogeneous 3D single-component systems.

We have derived a general formalism to determine the density-density response matrix $\chi_{\alpha\beta}$ in inhomogeneous multi-component Bose systems. The starting point was an ansatz for the wave function, where we allowed fluctuations of the correlation functions from the Jastrow-form for the ground state theory. We defined an action functional, that was minimised with respect to the fluctuations of a general n-body-correlation function $\delta u_{\boldsymbol{\alpha}}$. With introducing the complex-valued n-particle density $\delta\rho_{\boldsymbol{\alpha}}$ and the complex-valued n-particle current density $\boldsymbol{j}_{\boldsymbol{\alpha}}$, we could write our equations of motion in the form of continuity equations with driving terms $D_{\boldsymbol{\alpha}}$.

To avoid the appearance of the four-body distribution function we subtracted the one-body equation of motion from the two-body equation of motion and we applied the convolution approximation and the uniform limit approximation. We introduced the Feynman states $\psi_{\alpha,n}$ and the states $\phi_{\alpha,n}$, which are orthonormal to the Feynman states. The equations of motion were projected onto the basis defined by the states $\psi_{\alpha,n}$ and $\phi_{\alpha,n}$, which led us to the density-density response matrix $\chi_{\alpha\beta}(\boldsymbol{r}_\alpha, \boldsymbol{r}_\beta, \omega)$.

In the case of homogeneous systems the momentum $\boldsymbol{k}$ is a good quantum number for the Feynman states $\psi_{\alpha,n,\boldsymbol{k}}$, which enabled us to numerically evaluate $\chi_{\alpha\beta}(\boldsymbol{k}, \omega)$ for a given static structure factor $S_{\alpha\beta}(\boldsymbol{k})$. We analysed three systems, where the first one consisted of a single layer of dipolar bosons with a polarisation perpendicular to the layer. The resulting dispersion showed the characteristics of a bosonic system: the maxon- and the roton-region and the Pitaevskii-plateau. For the second system we dealt with, which was a system of two layers with non-tilted dipoles, the response function became a matrix and we saw the collective mode splitting up. The third system we took a look at, was the same as the second system, but with tilted dipoles. Therefore the third system was an anisotropic system and we noticed that the system was about to solidify in the direction normal to both the z-axis and the tilting direction.

While we derived a formalism to treat inhomogeneous problems, there are still some difficulties left. The first and maybe biggest problem is to get ground state data for an inhomogeneous system. Another problem is that the Feynman eigenvalue problem becomes more difficult. If a specific system has some kind of symmetry, another ansatz than the plain-wave ansatz for the Feynman states could solve the problem, e. g. in [KZ01] spherical harmonics are used for ^{4}He droplets. A more detailed discussed of the spherical symmetry can be found in [CK95]. For problems without any symmetry finite element methods might be suitable.

Although inhomogeneous systems always come with increases complexity, they are especially interesting as the real world experiments on cold gases are hardly ever homogeneous. Usually harmonic trapping potentials are used and so in the centre of the gas the density would be larger than at the edge. On the other hand with the approach of this work, describing multi-layer systems as homogeneous 2D-multi-component systems, we also can not describe layers with a finite thickness, as it was done in [HZ13].

The static structure factor, that is taken from a ground state calculation to determine the Feynman states, could also be taken from a Monte Carlo ground state calculation. As such ground state data would be more accurate than data from the hypernetted-chain equations, also the results for the response

function can be expected to be more precise. The price one has to pay for the improvement of precision is that the ground state calculation becomes much more computationally expensive.

There are also tentative steps at using Monte Carlo methods for directly calculating the excitations of quantum systems, for example [Nav+13], where the results for the collective mode are already satisfactory. But these Monte Carlo approaches need further improvements to be able to treat the finite lifetime and decaying of excitations, as they were analysed within this work.

A way to improve the accuracy of the method presented in this work, is to add the fluctuations of triplet correlations to the excitation operator defined in equation (2.4). This was done in [CK10] for the homogeneous geometry and the numerical results agree much better with experimental data than without the fluctuations of the triplet correlations included. Indeed the derivation for inhomogeneous systems including fluctuations of the triplet correlations would be a tedious task.

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