Sum-Rule Approach for Collective Excitations of Ultracold Quantum Gases

Bachelor Thesis by

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Contents

1 Introduction

One of the most general theories available to describe statistical systems out of but close to thermodynamic equilibrium is the Kubo formalism. This theory covers a variety of physical problems that can be treated in the context of linear response theory. Some of them are, for instance, discussed in the original paper by Kubo [1]. A major advantage of the Kubo formalism lies in the fact that the non-equilibrium system can be characterized solely via calculations in thermal equilibrium.

The fundamental concept of linear response theory is to construct a linear input-output relationship, or more precise a relation between an external effect and a corresponding reaction of the system. A primal result of the Kubo formalism is that the reaction of the system can be expressed as a convolution between the external modulation and a so called response function. Therefore, by definition, response functions do not depend on the external modulation, but rather correspond to material properties of the system itself. Physical quantities, defined through response functions, are often referred to as susceptibility or impedance as e.g. in electromagnetism.

Although in the Kubo formalism all calculations of response functions are performed at thermal equilibrium, analytic solutions may not exist or require tremendous effort. To account for these circumstances, a frequently used method to investigate response functions are sum rules. The latter provide a method to express the moments of the response function via nested commutators which may provide more accessible results. The moments can then be used to characterize or approximatively reconstruct the function. Sum rules have, for instance, been utilized to explore giant resonances in nuclei [2, 3] where the corresponding modes have been observed experimentally [4].

In this work we turn our focus to the vivid field of ultracold quantum gases that provide a promising playground for both theoretical and experimental physics. One of the observable phenomena in trapped ultracold quantum gases are collective motions of the gas, which can be excited via a modulation of the trap frequency [5] or via Feshbach resonance [6, 7]. Since the very beginning of the experimental realization of Bose-Einstein condensates in 1995 [8, 9] the physical properties of the system have been explored by the measurements of these collective oscillations [10, 11] and have been found to be in good agreement with the theoretical predictions [12]. Subsequently measurements of oscillation frequencies with high precision have been achieved [13]. Consequently, time dependent phenomena like collective excitations as well as the time-of-flight expansion of a condensate are subjects of thorough experimental and theoretical studies.

The main goal of this work is to derive a method to estimate the lowest excitation energy in ultracold quantum gases at zero temperature using sum rules. This method has been presented by Stringari [14], but no detailed derivation has been found available in the present literature. Therefore, a comprehensive derivation of the sum-rule approach is performed. First of all in Section 2 the foundation of the Kubo formalism is presented and

general application-oriented expressions like the sum rules are derived in a general context. In Section 3 we proceed with the relation of the Kubo formalism to correlation functions. These considerations lead to a profound result which is well known as the fluctuation dissipation theorem and can be easily proven in the context of the Kubo formalism. The mathematical expressions derived in this section will also enable us to construct estimates which are relevant for elementary excitations. In Section 4 the derived expressions will be applied to a generic case of elementary excitations in ultracold quantum gases at zero temperature.

A main result of this thesis is that, by applying the sum-rule approach, rather general expressions are derived for the estimation of specific elementary excitation energies. The obtained expressions consist only of the particular ground-state energies of the system, which are the kinetic, the trapping and the interaction energy. At once these expressions hold for any dimension and any underlying quantum statistics and are directly applicable for an important class of potentials. However, the respective ground-state energies have to be calculated separately for every specific many-body quantum system. This is exemplarily done by numerical calculations for an interacting Bose gas and a dipolar Fermi gas.

Additionally virial identities for the involved ground-state energies are discussed. These identities allow to reduce the effort required to calculate the ground-state energies. They further enable us to analytically discuss different physical limits. Finally, in Section 5 the quality of the results obtained and the general limits of the method are discussed.

2 Linear Response Theory

This section is devoted to a comprehensive discussion of the fundaments of the Kubo formalism. Furthermore, the method of sum rules will be discussed. We will mostly focus on the derivation of identities which are relevant for the development of further methods in the following sections.

2.1 System of Interest

We consider a system governed by a Hamiltonian H_0 which is not time dependent. If we regard a statistical system at finite temperature, all eigenstates $|\psi_i\rangle$ of H_0 have a certain probability p_i to be occupied. In general, this is described through the density matrix

$$\rho := \sum_i p_i |\psi_i\rangle \langle \psi_i| . \tag{2.1}$$

The expectation value of an operator G can then be written as

$$\langle G \rangle = \mathrm{Tr}\, \rho G , \tag{2.2}$$

where $\mathrm{Tr}\, G$ denotes the trace of an operator G. The system rests in thermal equilibrium until a time t_0, where a time dependent perturbation is switched on. The fact that prior to time t_0 the system is in equilibrium plays a crucial role for our theory.

We require that the time dependence of the perturbation Hamiltonian can be split into the product of a c-number $f(t)$ and a time independent operator B. Thus the perturbed Hamiltonian takes the form

$$H_t = H_0 - Bf(t) . \tag{2.3}$$

Thereby the subscript $\cdot_t$ denotes the explicit time dependence of an operator. Apparently the Hamiltonian H_t has the structure of many systems realized in experiments where a quantity of the system is modulated with time. The form $Bf(t)$ is often said to represent an operator B that *couples* to an external *field* $f(t)$.

2.2 Basics of Quantum Mechanical Formulation

We temporarily introduce the superscripts $\cdot^{\mathcal{S}}$, $\cdot^{\mathcal{H}}$ and $\cdot^{\mathcal{I}}$ for operators in the Schrödinger, Heisenberg and Interaction picture. The full Hamiltonian (2.3) then reads

$$H_t^{\mathcal{S}} = H_0^{\mathcal{S}} - B^{\mathcal{S}} f(t) . \tag{2.4}$$

First we briefly review the Heisenberg picture. The main requirement for different representations of quantum mechanics is that expectation values of operators must remain

picture independent. We know that the time evolution of a pure state in the Schrödinger picture is given by

$$|\psi(t)\rangle = U(t, t_0) |\psi\rangle \,, \tag{2.5}$$

where $U(t, t_0)$ is a unitary operator that fulfills the Schrödinger equation. The ket $|\psi\rangle := |\psi(t_0)\rangle$ denotes the static solution of the Schrödinger equation at time t_0. In the Heisenberg picture the observables rather than the states carry the time dependence

$$\langle\psi(t)|G^{\mathcal{S}}|\psi(t)\rangle = \langle\psi|U^\dagger(t, t_0)G^{\mathcal{S}}U(t, t_0)|\psi\rangle = \langle\psi|G^{\mathcal{H}}(t)|\psi\rangle \,. \tag{2.6}$$

As the expectation value should be independent of the picture, one finds that an observable $G_t^{\mathcal{H}}(t)$ must fulfill the *Heisenberg equation*

$$\frac{\mathrm{d}G_t^{\mathcal{H}}}{\mathrm{d}t}(t) = \frac{\mathrm{i}}{\hbar}[H_t^{\mathcal{S}}, G_t^{\mathcal{H}}(t)] + \frac{\partial G_t^{\mathcal{H}}}{\partial t}(t)\,. \tag{2.7}$$

Since $H_t(t)$ commutes with itself, we have the general result

$$\frac{\mathrm{d}H_t^{\mathcal{H}}}{\mathrm{d}t}(t) = \frac{\partial H_t^{\mathcal{H}}}{\partial t}(t)\,. \tag{2.8}$$

For operators that are not explicitly time dependent the Heisenberg equation reads

$$\frac{\mathrm{d}G^{\mathcal{H}}}{\mathrm{d}t}(t) = \frac{\mathrm{i}}{\hbar}[H_t^{\mathcal{S}}, G^{\mathcal{H}}(t)]\,. \tag{2.9}$$

If we look at the expectation value of a many-particle system, we notice that the density matrix (2.1) in the Schrödinger picture carries the time dependence as the states evolve with time. This time dependence is defined by the *Von Neumann equation*

$$\frac{\mathrm{d}\rho^{\mathcal{S}}}{\mathrm{d}t}(t) = -\frac{\mathrm{i}}{\hbar}[H_t^{\mathcal{S}}(t), \rho^{\mathcal{S}}(t)]\,. \tag{2.10}$$

As in the Heisenberg picture the states do not depend on time, the density matrix $\rho^{\mathcal{H}}$ also does not depend on time. Instead the operator $G^{\mathcal{H}}(t)$ includes the full unitary transformation $U(t, t_0)$.

In order to deal with the difficulties of time dependent systems, we introduce a further representation of quantum mechanics. For systems with a time independent Hamiltonian $H_0^{\mathcal{S}}$ the time evolution of states is simply given by

$$U(t, t_0) = U_0(t - t_0) := \mathrm{e}^{-\mathrm{i}H_0(t - t_0)/\hbar}\,. \tag{2.11}$$

To include this result in the theory of time dependent systems we define the operator $U_1(t, t_0)$ that fulfills the equation

$$U(t, t_0) =: U_0(t - t_0) \, U_1(t, t_0)\,. \tag{2.12}$$

Now we can distribute the time evolution to both the states and the observables via

$$G^{\mathcal{I}}(t) = U_0^\dagger(t - t_0)G^{\mathcal{S}}U_0(t - t_0)\,, \tag{2.13}$$

$$|\psi^{\mathcal{I}}(t)\rangle = U_1(t, t_0) |\psi\rangle \,. \tag{2.14}$$

We refer to this representation as the *Interaction picture*. In general every split-up of the full Hamiltonian $H_t = H_0 + H_{1t}$ defines such a separate Interaction picture. As we have already defined $U_0(t - t_0)$ to be based on $H_0^{\mathcal{S}}$, we have

$$H_{1t}^{\mathcal{S}} = -B^{\mathcal{S}} f(t) . \tag{2.15}$$

Observables $G(t)$ have to fulfill the modified Heisenberg equation of motion

$$
\begin{aligned}
\frac{\mathrm{d}G_t^{\mathcal{I}}}{\mathrm{d}t}(t) &= \frac{\mathrm{i}}{\hbar}[H_0^{\mathcal{S}}, G_t^{\mathcal{I}}(t)] + \frac{\partial G_t^{\mathcal{I}}}{\partial t}(t) \\
&= \frac{\mathrm{i}}{\hbar} U_0^{\dagger}(t - t_0)[H_0^{\mathcal{S}}, G_t^{\mathcal{S}}]U_0(t - t_0) + U_0^{\dagger}(t - t_0)\frac{\partial G_t^{\mathcal{S}}}{\partial t}U_0(t - t_0) \\
&= \frac{\mathrm{i}}{\hbar}[H_0^{\mathcal{S}}, G_t^{\mathcal{S}}]^{\mathcal{I}}(t) + \left(\frac{\partial G_t^{\mathcal{S}}}{\partial t}\right)^{\mathcal{I}}(t)
\end{aligned}
\tag{2.16}
$$

and respectively the simplified equation

$$\frac{\mathrm{d}G^{\mathcal{I}}}{\mathrm{d}t}(t) = \frac{\mathrm{i}}{\hbar}[H_0^{\mathcal{S}}, G^{\mathcal{S}}]^{\mathcal{I}}(t) \tag{2.17}$$

for observables that are not explicitly time dependent.

Aside from solving the equilibrium system the problem has now been squeezed to the calculation of the operator $U_1(t, t_0)$. From the requirement that $U(t, t_0)$ has to fulfill the Schrödinger equation, one easily finds that $U_1(t, t_0)$ also has to fulfill the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}U_1(t, t_0) = H_{1t}^{\mathcal{I}}(t)U_1(t, t_0) , \tag{2.18}$$

which has the formal solution

$$U_1(t, t_0) = \mathcal{T}\exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} H_1^{\mathcal{I}}(t')\,\mathrm{d}t'\right] , \tag{2.19}$$

where $\mathcal{T}$ denotes the time ordering superoperator [15].

2.3 Response Functions

In this section we develop a theory for a first-order approximation of equation (2.19) also referred to as *Kubo formalism*. The derivations mostly follow the approaches of the textbooks [15, 16] which are mainly based on the original work of Kubo [1].

2.3.1 Derivation

As previously discussed, the introduction of the Interaction picture squeezes the difficulties of systems with explicit time dependence to the calculation of the time evolution operator

$U_1(t, t_0)$. We found that this operator has the formal solution (2.19). The expansion in powers of H_{1t} yields

$$U_1(t, t_0) = \mathrm{Id} - \frac{\mathrm{i}}{\hbar} \int_{t_0}^{t} H_{1t}^{\mathcal{I}}(t') \, \mathrm{d}t' + \mathcal{O}\big(H_{1t}^{\mathcal{I}2}\big). \tag{2.20}$$

As from now on we will only consider first-order approximations, most of the equal signs imply this approximation, hence we write

$$U_1(t, t_0) = \mathrm{Id} - \frac{\mathrm{i}}{\hbar} \int_{t_0}^{t} H_1^{\mathcal{I}}(t') \, \mathrm{d}t'. \tag{2.21}$$

As already stated before, it plays a crucial role that the system is in thermal equilibrium prior to the time t_0. To implement the features of the system in equilibrium, we define the equilibrium average

$$\langle G(t) \rangle_{\mathrm{eq}} := \mathrm{Tr} \, \rho^{\mathcal{H}} G^{\mathcal{I}}(t). \tag{2.22}$$

Here only the time evolution $U_0(t - t_0)$ is involved which is explicitly given by equation (2.11). To distinguish the equilibrium average from averages at any time t, we denote the latter by $\langle G(t) \rangle_{\mathrm{ne}} \equiv \langle G(t) \rangle$.

We now turn to the effects of the perturbation namely the effects on an arbitrary operator A. To observe how the expectation value of A changes in time, we define the deviation from equilibrium via

$$\delta \langle A(t) \rangle := \langle A(t) \rangle_{\mathrm{ne}} - \langle A(t) \rangle_{\mathrm{eq}}. \tag{2.23}$$

To calculate this quantity, we explicitly write out the non-equilibrium expectation value. In the framework of our first-order approximation we obtain

$$\langle A(t) \rangle_{\mathrm{ne}} = \mathrm{Tr} \, \rho^{\mathcal{H}} \left[1 + \frac{\mathrm{i}}{\hbar} \int_{t_0}^{t} H_1^{\mathcal{I}}(t') \, \mathrm{d}t' \right] A^{\mathcal{I}}(t) \left[1 - \frac{\mathrm{i}}{\hbar} \int_{t_0}^{t} H_1^{\mathcal{I}}(t') \, \mathrm{d}t' \right]$$

$$= \mathrm{Tr} \, \rho^{\mathcal{H}} A^{\mathcal{I}}(t) + \frac{\mathrm{i}}{\hbar} \mathrm{Tr} \, \rho^{\mathcal{H}} \int_{t_0}^{t} \left[A^{\mathcal{I}}(t), B^{\mathcal{I}}(t') \right] f(t') \, \mathrm{d}t'$$

$$+ \frac{1}{\hbar^2} \mathrm{Tr} \, \rho^{\mathcal{H}} A^{\mathcal{I}}(t) \left[\int_{t_0}^{t} B^{\mathcal{I}}(t') f(t') \, \mathrm{d}t' \right]^2. \tag{2.24}$$

The last term arising is of second order in $H_{1t}^{\mathcal{I}}$ and has to be neglected in first-order perturbation theory. The other terms can be identified as equilibrium averages as defined in (2.22). We thus write

$$\langle A(t) \rangle_{\mathrm{ne}} = \langle A(t) \rangle_{\mathrm{eq}} + \frac{\mathrm{i}}{\hbar} \int_{t_0}^{t} \left\langle \left[A^{\mathcal{I}}(t), B^{\mathcal{I}}(t') \right] \right\rangle_{\mathrm{eq}} f(t') \, \mathrm{d}t' \tag{2.25}$$

or in terms of the deviation of $A(t)$

$$\delta\langle A(t)\rangle = \frac{\mathrm{i}}{\hbar} \int_{t_0}^{t} \left\langle \left[A^{\mathcal{I}}(t), B^{\mathcal{I}}(t')\right]\right\rangle_{\mathrm{eq}} f(t')\,\mathrm{d}t'. \tag{2.26}$$

We define the arising equilibrium average as the *response function*

$$\chi''_{AB}(t,t') := \frac{1}{2\hbar} \left\langle \left[A^{\mathcal{I}}(t), B^{\mathcal{I}}(t')\right]\right\rangle_{\mathrm{eq}}. \tag{2.27}$$

The deviation in terms of the response function reads

$$\delta\langle A(t)\rangle = 2\mathrm{i} \int_{t_0}^{t} \chi''_{AB}(t,t')\, f(t')\,\mathrm{d}t'. \tag{2.28}$$

We notice that the response function (2.27) does not depend on $f(t)$ in any way. Rather it is constructed from the equilibrium configuration of the system and from the information that the quantity B is perturbed and the effects on the quantity A are observed. The response function therefore represents properties of the considered equilibrium system only and hence is often related to material constants and similar quantities.

2.3.2 General Properties

We now proof some important properties of the response function (2.27). It is clear that the properties of χ''_{AB} are only governed by the involved operators H, A and B in the Interaction picture. We will therefore use the notation $G(t) := G^{\mathcal{I}}(t)$ and $G := G^{\mathcal{I}}(t_0) = G^{\mathcal{S}}$.

We first state that $\chi''_{AB}(t,t')$ does only depend on time differences $t-t'$. Looking at the definition

$$\chi''_{AB}(t,t') = \frac{1}{2\hbar} \left\langle \left[A(t), B(t')\right]\right\rangle_{\mathrm{eq}} = \frac{1}{2\hbar} \left[\left\langle A(t)B(t')\right\rangle_{\mathrm{eq}} - \left\langle B(t')A(t)\right\rangle_{\mathrm{eq}}\right] \tag{2.29}$$

we analyze the equilibrium average

$$\begin{aligned}
\left\langle A(t)\,B(t')\right\rangle_{\mathrm{eq}} &= \mathrm{Tr}\,\rho\, A(t)B(t') \\
&= \mathrm{Tr}\,\rho\, U_0^\dagger(t-t_0)A U_0(t-t_0)\, U_0^\dagger(t'-t_0)B U_0(t'-t_0) \\
&= \mathrm{Tr}\,\rho\, U_0(t'-t_0)U_0^\dagger(t-t_0)\, A\, U_0(t-t_0)U_0^\dagger(t'-t_0)\, B,
\end{aligned} \tag{2.30}$$

where we used the cyclic invariance of the trace and assumed that H_0 is Hermitian and therefore commutes with ρ. Using the explicit form of $U_0(t-t_0)$ from equation (2.11) we obtain

$$U_0(t-t_0)U_0^\dagger(t'-t_0) = U_0(t-t'). \tag{2.31}$$

Thus, equation (2.30) can be written as

$$\begin{aligned}
\left\langle A(t)\,B(t')\right\rangle_{\mathrm{eq}} &= \mathrm{Tr}\,\rho U_0(t-t')^\dagger A U_0(t-t')\, B \\
&= \mathrm{Tr}\,\rho A(t-t')\, B = \left\langle A(t-t')\, B\right\rangle_{\mathrm{eq}}.
\end{aligned} \tag{2.32}$$

We therefore can rewrite the response function as a function of the time difference $t - t'$ only

$$\chi''_{AB}(t - t') = \frac{1}{2\hbar}\left[\langle A(t - t')B\rangle_{\text{eq}} - \langle BA(t - t')\rangle_{\text{eq}}\right],\tag{2.33}$$

which also implies that the response function is invariant under time translations.

Keeping in mind, that the response function always depends on a time difference $t - t'$, we write $\chi''_{AB}(\tau)$ for simplicity in the following, where τ has to be replaced by $t - t'$ for explicit calculations again.

Applying the cyclic invariance of the trace in equation (2.32) we can also move the time dependence from one operator to the other in the form

$$\langle A(\tau)B\rangle_{\text{eq}} = \langle AB(-\tau)\rangle_{\text{eq}}.\tag{2.34}$$

This result can now be used to calculate the symmetry property

$$\begin{aligned}\chi''_{AB}(-\tau) &= \frac{1}{2\hbar}\left[\langle A(-\tau)B\rangle_{\text{eq}} - \langle BA(-\tau)\rangle_{\text{eq}}\right]\\&= \frac{1}{2\hbar}\left[\langle AB(\tau)\rangle_{\text{eq}} - \langle B(\tau)A\rangle_{\text{eq}}\right] = -\chi''_{BA}(\tau).\end{aligned}\tag{2.35}$$

We further compute the complex conjugation of the response function. Using the definition of the density matrix (2.1) we find

$$\begin{aligned}\chi''^{*}_{AB}(\tau) &= \frac{1}{2\hbar}\,\text{Tr}\left[B\rho A(\tau) - A(\tau)\rho B\right]^{*}\\&= \frac{1}{2\hbar}\sum_{i,j}p_j\left[\langle i|B|j\rangle^{*}\langle j|A(\tau)|i\rangle^{*} - \langle i|A(\tau)|j\rangle^{*}\langle j|B|i\rangle^{*}\right]\\&= \frac{1}{2\hbar}\sum_{i,j}p_j\left[\langle i|A^{\dagger}(\tau)|j\rangle\langle j|B^{\dagger}|i\rangle - \langle i|B^{\dagger}|j\rangle\langle j|A^{\dagger}(\tau)|i\rangle\right] = -\chi''_{A^{\dagger}B^{\dagger}}(\tau).\end{aligned}\tag{2.36}$$

This result becomes more important if we consider the case that A and B are observables. In that case A, B are Hermitian and the identity (2.36) trivially reduces to

$$\chi''^{*}_{AB}(\tau) = -\chi''_{AB}(\tau).\tag{2.37}$$

From this identity we can conclude that the response function must be purely imaginary in case of Hermitian operators.

2.3.3 Fourier Transform

In order to analyze the frequency spectrum of the response function, we define the Fourier transform

$$\tilde{\chi}''_{AB}(\omega) := \int_{-\infty}^{\infty}\chi''_{AB}(\tau)\,e^{i\omega\tau}\,d\tau,\tag{2.38}$$

as well as the corresponding inverse Fourier transform

$$\chi''_{AB}(\tau) := \frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{\chi}''_{AB}(\omega)\,e^{-i\omega\tau}\,d\omega.\tag{2.39}$$

For the derivation of equations (2.33) and (2.35) we only used linear operations. Therefore these identities also hold for $\tilde{\chi}''_{AB}(\omega)$, as the Fourier transformation only affects the isolated time dependence of the operator $A(\tau)$. Namely we have

$$\tilde{\chi}''_{AB}(\omega) = \frac{1}{2\hbar}\left[\langle A(\omega)B\rangle_{\text{eq}} - \langle BA(\omega)\rangle_{\text{eq}}\right] \tag{2.40}$$

and

$$\tilde{\chi}''_{AB}(-\omega) = -\tilde{\chi}''_{BA}(\omega). \tag{2.41}$$

Furthermore, if A, B are Hermitian we can use identity (2.37) to obtain

$$\tilde{\chi}''^{*}_{AB}(\omega) = \int_{-\infty}^{\infty}\left(e^{i\omega\tau}\right)^{*}\chi''^{*}_{AB}(\tau)\,d\tau = -\int_{-\infty}^{\infty}e^{-i\omega\tau}\chi''_{AB}(\tau)\,d\tau = -\tilde{\chi}''_{AB}(-\omega). \tag{2.42}$$

Next we write down the response function in a more explicit form to finally obtain a different representation of its Fourier transform. Using identity (2.34) and the definition (2.1) we find

$$\begin{aligned}
\chi''_{AB}(\tau) &= \frac{1}{2\hbar}\operatorname{Tr}\rho\left[A(\tau)B - BA(\tau)\right] \\
&= \frac{1}{2\hbar}\sum_{m,i}p_m\langle i|m\rangle\left[\langle m|A(\tau)B|i\rangle - \langle m|B(-\tau)A|i\rangle\right] \\
&= \frac{1}{2\hbar}\sum_m p_m\left[\langle m|A(\tau)B|m\rangle - \langle m|B(-\tau)A|m\rangle\right] \\
&= \frac{1}{2\hbar}\sum_{m,n}p_m\left[\langle m|A(\tau)|n\rangle\langle n|B|m\rangle - \langle m|B(-\tau)|n\rangle\langle n|A|m\rangle\right]. \tag{2.43}
\end{aligned}$$

In the last line we introduced intermediate states $\text{Id} = \sum_n|n\rangle\langle n|$. We choose all states $|n\rangle$ to be eigenstates of the unperturbed Hamiltonian H_0^S with eigenvalues $E_n = \hbar\omega_n$. Inserting the Interaction picture time dependence $U_0(\tau)$ of the operators A, B we obtain

$$\begin{aligned}
\chi''_{AB}(\tau) =& \frac{1}{2\hbar}\sum_{m,n}p_m\Big[\langle m|e^{iH_0\tau/\hbar}Ae^{-iH_0\tau/\hbar}|n\rangle\langle n|B|m\rangle \\
&\qquad\qquad - \langle m|e^{-iH_0\tau/\hbar}Be^{iH_0\tau/\hbar}|n\rangle\langle n|A|m\rangle\Big] \\
=& \frac{1}{2\hbar}\sum_{m,n}p_m\Big[\langle m|e^{i\omega_m\tau}Ae^{-i\omega_n\tau}|n\rangle\langle n|B|m\rangle \\
&\qquad\qquad - \langle m|e^{-i\omega_m\tau}Be^{i\omega_n\tau}|n\rangle\langle n|A|m\rangle\Big]. \tag{2.44}
\end{aligned}$$

With this rather explicit expression we are now in the position to calculate the Fourier

transform to

$$
\begin{aligned}
\tilde{\chi}''_{AB}(\omega) &= \frac{1}{2\hbar} \int_{-\infty}^{\infty} e^{i\omega\tau} \chi''_{AB}(\tau) \, d\tau \\
&= \frac{1}{2\hbar} \sum_{m,n} p_m \left[\langle m|A|n\rangle \langle n|B|m\rangle \int_{-\infty}^{\infty} e^{i(\omega-\omega_{nm})\tau} \, d\tau \right. \\
&\qquad\qquad \left. - \langle m|B|n\rangle \langle n|A|m\rangle \right) \int_{-\infty}^{\infty} e^{i(\omega+\omega_{nm})\tau} \, d\tau \Big] \\
&= \frac{\pi}{\hbar} \sum_{m,n} p_m \left[\langle m|A|n\rangle \langle n|B|m\rangle \, \delta(\omega - \omega_{nm}) \right. \\
&\qquad\qquad \left. - \langle m|B|n\rangle \langle n|A|m\rangle \, \delta(\omega + \omega_{nm}) \right].
\end{aligned}
\tag{2.45}
$$

Here the abbreviation $\omega_{nm} := \omega_n - \omega_m$ is used. Apparently the frequency spectrum of the response function consists of sharp peaks at $\pm\omega_{nm}$.

2.4 Dynamic Susceptibility

In this section some essential tools of the Kubo formalism will be briefly outlined. To this end we turn back to the point where we have defined the response function. We found in (2.28) that the deviation from equilibrium in first oder is given by

$$
\delta\langle A(t)\rangle = 2i \int_{t_0}^{t} \chi''_{AB}(t - t') f(t') \, dt'.
\tag{2.46}
$$

The next aim is to extend the lower and upper boundary of the integral to minus and plus infinity. We recall that the system is in equilibrium prior to the disturbance induced by the external field $f(t)$. Therefore, we assume that $f(t)$ is chosen such that it is zero until time t_0 and replace the lower boundary by $-\infty$. To replace the upper boundary by $+\infty$ we have to adjust the integrand such that it vanishes for all times $t' > t$. We do so by introducing the *dynamic susceptibility*

$$
\chi_{AB}(t - t') := 2i\,\theta(t - t')\,\chi''_{AB}(t - t'),
\tag{2.47}
$$

where θ denotes the Heaviside step function. The definition of the dynamic susceptibility can be interpreted as an explicit implementation of causality [16]. The deviation (2.46) can then be written in terms of the dynamic susceptibility

$$
\delta\langle A(t)\rangle = \int_{-\infty}^{\infty} \chi_{AB}(t - t') f(t') \, dt' = (\chi_{AB} * f)(t),
\tag{2.48}
$$

where $(\cdot * \cdot)(t)$ denotes the convolution of two functions.

Although the definition of the dynamic susceptibility was at first technically motivated, the Fourier transform gives rise to a further physical interpretation. Using the convolution theorem we find

$$\delta\langle A(\omega)\rangle = \tilde{\chi}_{AB}(\omega)f(\omega).\tag{2.49}$$

This means that if we observe the deviation $\delta\langle A(\omega)\rangle$ for a perturbation with the known frequency spectrum $f(\omega)$, we can measure the Fourier transform of the dynamic susceptibility $\tilde{\chi}_{AB}(\omega)$.

Next we relate the Fourier transforms $\tilde{\chi}_{AB}(\omega)$ and $\tilde{\chi}''_{AB}(\omega)$ in a direct manner. Using the integral representation of the Heaviside step function

$$\theta(x) = \lim_{\eta\downarrow 0}\frac{1}{2\pi\mathrm{i}}\int\limits_{-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}x\gamma}}{\gamma - \mathrm{i}\eta}\,\mathrm{d}\gamma,\tag{2.50}$$

the dynamic susceptibility reads

$$\tilde{\chi}_{AB}(\omega) = \lim_{\eta\downarrow 0}\frac{1}{\pi}\iint\limits_{-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}\tau\gamma}}{\gamma - \mathrm{i}\eta}\,\mathrm{e}^{\mathrm{i}\omega\tau}\chi''_{AB}(\tau)\,\mathrm{d}\gamma\,\mathrm{d}\tau.\tag{2.51}$$

We express $\chi''_{AB}(\tau)$ in terms of its Fourier transform $\tilde{\chi}''_{AB}(\omega)$ by using the inverse Fourier transform. Then we have

$$\tilde{\chi}_{AB}(\omega) = \lim_{\eta\downarrow 0}\frac{1}{2\pi^2}\iint\limits_{-\infty}^{\infty}\frac{1}{\gamma - \mathrm{i}\eta}\,\tilde{\chi}''_{AB}(\omega'')\int\limits_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}t(\gamma+\omega-\omega'')}\,\mathrm{d}t\,\mathrm{d}\omega''\mathrm{d}\gamma,\tag{2.52}$$

where the integration over τ yields $2\pi\delta(\gamma + \omega - \omega'')$. This enables us to also execute the integration over γ. Finally we obtain

$$\tilde{\chi}_{AB}(\omega) = \lim_{\eta\downarrow 0}\frac{1}{\pi}\int\limits_{-\infty}^{\infty}\frac{\tilde{\chi}''_{AB}(\omega'')}{\omega'' - \omega - \mathrm{i}\eta}\,\mathrm{d}\omega''.\tag{2.53}$$

We will turn back to this identity later on.

A spectral representation can be obtained by inserting the equation (2.45) into equation (2.53) yielding

$$\begin{aligned}\tilde{\chi}_{AB}(\omega) &= \lim_{\varepsilon\downarrow 0}\frac{1}{\hbar}\int\limits_{-\infty}^{\infty}\sum_{m,n}p_m\left(\frac{\langle m|A|n\rangle\,\langle n|B|m\rangle\,\delta(\omega''-\omega_{nm})}{\omega'' - \omega - \mathrm{i}\eta}\right.\\ &\qquad\qquad\qquad\qquad\left.-\frac{\langle m|B|n\rangle\,\langle n|A|m\rangle\,\delta(\omega''-\omega_{mn})}{\omega'' - \omega - \mathrm{i}\eta}\right)\mathrm{d}\omega''\\ &= -\lim_{\varepsilon\downarrow 0}\frac{1}{\hbar}\sum_{m,n}p_m\left(\frac{\langle m|A|n\rangle\,\langle n|B|m\rangle}{\omega - \omega_{nm} + \mathrm{i}\eta} - \frac{\langle m|B|n\rangle\,\langle n|A|m\rangle}{\omega - \omega_{mn} + \mathrm{i}\eta}\right).\end{aligned}\tag{2.54}$$

This expression can be used as a starting point for explicit calculations as is e.g. done for Bose–Einstein condensates [17].

Using methods of complex analysis and distribution theory it can be shown that the Fourier transform of the dynamic susceptibility can be written in the form

$$\tilde{\chi}_{AB}(\omega) = \tilde{\chi}'_{AB}(\omega) + i\,\tilde{\chi}''_{AB}(\omega)\,, \tag{2.55}$$

where $\tilde{\chi}''_{AB}(\omega)$ is the previously discussed response function. Both $\tilde{\chi}'_{AB}(\omega)$ and $\tilde{\chi}''_{AB}(\omega)$ can be shown to be real. This leads to the conclusion that $\tilde{\chi}''_{AB}(\omega)$ represents the dissipative part of the dynamic susceptibility. The underlying mathematics and derivations are extensively discussed in Ref. [18] as well as the specific requirements to the involved functions that have to be regarded. A comprehensive summary of statical physics including the Kubo formalism can be found in Ref. [19].

2.5 Sum Rules

In this section we develop a simplified method to calculate the energy weighted moments of the response function's Fourier transform

$$\omega_{AB}^{(n)} := \frac{1}{\pi} \int\limits_{-\infty}^{\infty} (\hbar\omega)^n \tilde{\chi}''_{AB}(\omega)\, \mathrm{d}\omega\,. \tag{2.56}$$

Inserting the spectral representation (2.45) we immediately obtain

$$\omega_{AB}^{(n)} = \frac{1}{\hbar} \sum_{m,l} p_l\, (\hbar\omega_{lm})^n \left[\langle m|A|l\rangle \langle l|B|m\rangle - (-1)^n \langle m|B|l\rangle \langle l|A|m\rangle \right]\,. \tag{2.57}$$

The moments of a function can be used to explore its distribution characteristics. Also the moments of a function represent the coefficients of the corresponding Laurent series and, in principle, enable us to approximately reconstruct the function in the radius of convergence around $\omega = 0$.

In order to obtain a direct way to calculate the nth moment of $\tilde{\chi}''_{AB}(\omega)$, we rewrite the definition (2.56) in the terms of the nth time derivative as

$$(-i)^n \omega_{AB}^{(n)} = \frac{\hbar^n}{\pi} \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}^n}{\mathrm{d}t^n} e^{-i\omega(t-t_0)}\, \tilde{\chi}''_{AB}(\omega)\, \mathrm{d}\omega \bigg|_{t=t_0} = 2\hbar^n \frac{\mathrm{d}^n}{\mathrm{d}t^n} \chi''_{AB}(t) \bigg|_{t=t_0}\,. \tag{2.58}$$

For the second equal sign we have identified the inverse Fourier transform (2.39) of the response function at time t_0. Inserting the definition of $\chi''_{AB}(t)$ from equation (2.33) we obtain

$$(-i)^n \omega_{AB}^{(n)} = \hbar^{n-1} \frac{\mathrm{d}^n}{\mathrm{d}t^n} \langle [A(t), B] \rangle_{\mathrm{eq}} \bigg|_{t=t_0} = \hbar^{n-1} \left\langle \left[\frac{\mathrm{d}^n A}{\mathrm{d}t^n}(t_0), B \right] \right\rangle_{\mathrm{eq}}\,. \tag{2.59}$$

We now have reduced the calculation of the nth moment to a calculation of the nth time derivative of the operator A in the Heisenberg representation. We confine our theory to observable operators A, B that are not explicitly time dependent. The Interaction picture

Heisenberg equation is given by (2.17). Using this equation we first calculate the second derivative of $A(t)$ at time t_0

$$\frac{d^2 A}{dt^2} = \frac{i}{\hbar}\left[H_0, \frac{dA}{dt}\right] = \frac{i^2}{\hbar^2}[H_0, [H_0, A]] . \tag{2.60}$$

We recall that per definition operators without time argument have to be evaluated at time t_0 i.e. $dG/dt \equiv dG/dt|_{t_0}$.

Accordingly, we can write the nth derivative as the n-fold commutator

$$\frac{d^n A}{dt^n} = \frac{i^n}{\hbar^n}[H_0, \cdots [H_0, \cdots [H_0, A] \cdots] \cdots]] , \tag{2.61}$$

where H_0 appears n times in front of the operator A. In order to obtain the same prefactor as in equation (2.59), the anticommutativity of the commutator is used to get

$$\frac{d^n A}{dt^n} = \frac{(-i)^n}{\hbar^n}[[\cdots[\cdots[A, H_0]\cdots, H_0]\cdots, H_0] . \tag{2.62}$$

Combining equations (2.59) and (2.62) we finally have

$$\omega_{AB}^{(n)} = \frac{1}{\hbar}\left\langle[[\cdots[\cdots[A, H_0]\cdots, H_0]\cdots, H_0], B]\right\rangle_{\text{eq}} = \frac{1}{\hbar}\left\langle[\mathcal{L}^n A, B]\right\rangle_{\text{eq}} , \tag{2.63}$$

where we introduced the superoperator

$$\mathcal{L}G := [G, H_0] . \tag{2.64}$$

Like equation (2.57) this representation of the function's moments does not include any operators in Fourier space. Also all the calculations take place at time t_0 or, in other words, only Schrödinger picture operators and states are involved.

We also present a slightly different way to calculate the moments that often allows for the calculation of moments in the first place. Rewriting equation (2.59) we find

$$
\begin{aligned}
(-i)^n \omega_{AB}^{(n)} &= \hbar^{n-1}\frac{d^n}{dt^n}\left\langle[A(t), B]\right\rangle_{\text{eq}}\bigg|_{t=t_0} \\
&= \hbar^{n-1}\frac{d^n}{dt^n}\left[\left\langle A(t) B\right\rangle_{\text{eq}} - \left\langle BA(t)\right\rangle_{\text{eq}}\right]\bigg|_{t=t_0} \\
&= \hbar^{n-1}\frac{d^{n-k}}{dt^{n-k}}\left[\left\langle\frac{d^k A}{dt^k}(t) B\right\rangle_{\text{eq}} - \left\langle B\frac{d^k A}{dt^k}(t)\right\rangle_{\text{eq}}\right]\bigg|_{t=t_0} , \tag{2.65}
\end{aligned}
$$

where we moved k of n time derivatives into the average. The idea is now to shift the time dependence from the time derivatives of A to the operator B and then calculate the $n - k$ remaining time derivatives. Corresponding to equation (2.34) we can shift the time dependence to the operator B, if the time derivatives of $A(t)$ give a valid Interaction picture operator as defined via (2.13). This can be easily verified by looking at the Heisenberg equation (2.17). Therefore we can write

$$(-i)^n \omega_{AB}^{(n)} = \hbar^{n-1}(-1)^l\left[\left\langle\frac{d^k A}{dt^k}\frac{d^l B}{dt^l}(t)\right\rangle_{\text{eq}} - \left\langle\frac{d^l B}{dt^l}(t)\frac{d^k A}{dt^k}\right\rangle_{\text{eq}}\right]\bigg|_{t=t_0} , \tag{2.66}$$

where we introduced the abbreviation $l := n - k$. The minus signs in front arise from the fact that we have to take the time derivatives of $B(-t)$. Inserting equation (2.62) and using the definition (2.64), the nth moment reads

$$\omega_{AB}^{(n)} = \frac{1}{\hbar}(-1)^l \left[\left\langle \left(\mathcal{L}^k A\right) \left(\mathcal{L}^l B\right) \right\rangle_{\text{eq}} - \left\langle \left(\mathcal{L}^l B\right) \left(\mathcal{L}^k A\right) \right\rangle_{\text{eq}} \right]. \tag{2.67}$$

Until now we only dealt with positive moments and the zeroth moment. For negative moments the time derivatives in (2.59) become inverse operators of the time derivative. We take the Heisenberg equation for an operator F and act with the inverse time derivative on both sides of the equation to obtain

$$F = \frac{\text{i}}{\hbar} \frac{\text{d}^{-1}}{\text{d}t^{-1}} [H_0, F]. \tag{2.68}$$

If we require that

$$\frac{\text{i}}{\hbar} [H_0, F] = A \tag{2.69}$$

we have to solve equation (2.69) to find the operator F that gives the inverse time derivative of A. This concept can be easily generalized to further negative moments. But equation (2.69) is hardly solvable for practical purposes [17].

However, applications of the sum-rule formalism can be found in Refs. [15–17]. A slightly different form of sum rules and their application will be discussed below in Section 3.1.2.

3 Correlation Functions and Related Estimates

In this section we will turn to the field of correlation functions. We will briefly discuss the properties of these functions and relate them to the response functions. Finally we will use the obtained identities to derive estimates between moments of the correlation function at zero temperature.

3.1 Correlation Functions

In the following we will define correlation functions and treat them in a similar manner as the response functions in Section 2.3 and also derive sum rules as in Section 2.5. In addition, we will derive the seminal fluctuation dissipation theorem.

3.1.1 Definition and Relation to Linear Response Theory

A further approach to deal with time dependent quantum mechanical systems is to consider time correlation functions of the form

$$C_{AB}(t, t') := \langle A(t)B(t') \rangle_{\text{eq}} .\tag{3.1}$$

Again we use the convention that $G(t)$ denotes an operator in the Interaction picture and G in the Schrödinger picture. An important example of a correlation function is the dynamic structure factor which is essential in scattering theory [16]. Although the calculation and interpretation of correlation functions represents a huge area of modern physics, we restrict ourselves to some specific properties of these functions.

Obviously the response function, as defined in (2.27), can be expressed in terms of correlation functions via

$$\chi''_{AB}(t, t') = \frac{1}{2\hbar} \left[C_{AB}(t, t') - C_{BA}(t', t) \right] .\tag{3.2}$$

This result is very instructive as we can read off that the operators $A(t)$ and $B(t)$ have to be time correlated to obtain a nonzero response function. In other words, the deviation $\delta\langle A(t)\rangle$ is zero if $A(t)$ and $B(t)$ are not correlated in time.

The calculations performed in Sections 2.3.2 and 2.3.3 can be used to derive similar identities for correlation functions, i.e. we find

$$C_{AB}(t, t') = C_{AB}(t - t') = C_{AB}(\tau).\tag{3.3}$$

For the Fourier transform

$$\tilde{C}_{AB}(\omega) := \int_{-\infty}^{\infty} C_{AB}(\tau) \, \mathrm{e}^{\mathrm{i}\omega\tau} \, \mathrm{d}\tau,\tag{3.4}$$

we obtain

$$\tilde{C}_{AB}^*(\omega) = \tilde{C}_{B^\dagger A^\dagger}(\omega). \tag{3.5}$$

In a similar calculation as for equation (2.45) we find the spectral representation

$$\tilde{C}_{AB}(\omega) = 2\pi \sum_{m,n} p_m \braket{m|A|n} \braket{n|B|m} \delta(\omega - \omega_{nm}) \tag{3.6}$$

with $\omega_{nm} := \omega_n - \omega_m$. For a Hermitian operator A and choosing $A = B$ we have

$$\tilde{C}_A(\omega) = 2\pi \sum_{m,n} p_m |\braket{m|A|n}|^2 \delta(\omega - \omega_{nm}). \tag{3.7}$$

We notice that the summands take the form of Fermi's golden rule [20].

3.1.2 Sum Rules

In Section 2.5 we developed a way to calculate the moments of the response function also referred to as sum rules. Again we can trivially adopt the result to correlation functions. To this end we define the nth energy weighted moment of the correlation function

$$m_{AB}^{(n)} := \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} (\hbar\omega)^n \tilde{C}_{AB}(\omega) \, d\omega. \tag{3.8}$$

The equivalent result to equation (2.67) reads

$$m_{AB}^{(n)} = (-1)^l \left\langle \left(\mathcal{L}^k A\right)\left(\mathcal{L}^l B\right)\right\rangle_{\text{eq}}, \tag{3.9}$$

with arbitrary $k,l \in \mathbb{Z}$, where $k + l = n$ and again $\mathcal{L}G := [G, H_0]$.

Next we consider the special case that $A = B$. We rewrite equation (3.9) by combining two different choices of k, l. First in the form as written down in equation (3.9) and second with k, l interchanged. The nth energy weighted moment then reads

$$m_A^{(n)} = \frac{1}{2}(-1)^l \left[\left\langle \left(\mathcal{L}^k A\right)\left(\mathcal{L}^l A\right)\right\rangle_{\text{eq}} + (-1)^{k+l} \left\langle \left(\mathcal{L}^l A\right)\left(\mathcal{L}^k A\right)\right\rangle_{\text{eq}} \right]. \tag{3.10}$$

Thus, the odd moments of the correlation function are given via the commutator

$$m_A^{(n)} = \frac{1}{2}(-1)^l \left\langle \left[\mathcal{L}^k A, \mathcal{L}^l A\right]\right\rangle_{\text{eq}}, \tag{3.11}$$

and the even moments via the anticommutator

$$m_A^{(n)} = \frac{1}{2}(-1)^l \left\langle \left\{\mathcal{L}^k A, \mathcal{L}^l A\right\}\right\rangle_{\text{eq}}. \tag{3.12}$$

The specific result (3.11) has been presented in the context of nuclear excitations [2].

3.1.3 Identities in Canonical Ensemble

In this section we examine correlation functions with the specific density matrix of the canonical ensemble. This density matrix reads

$$\rho = \frac{e^{-\beta H_0}}{Z}, \tag{3.13}$$

where $1/\beta := k_B T$ is the inverse temperature and Z denotes the partition function

$$Z := \operatorname{Tr} e^{-\beta H_0}. \tag{3.14}$$

Inserting the density matrix into the definition of the correlation function (3.1) we find

$$
\begin{aligned}
C_{AB}(\tau) &= \operatorname{Tr} \rho\, U_0^\dagger(\tau) A(\tau) U_0(\tau)\, B \\
&= \frac{1}{Z} \operatorname{Tr} e^{-\beta H_0}\, e^{iH_0\tau/\hbar} A e^{-iH_0\tau/\hbar} e^{\beta H_0} e^{-\beta H_0} B \\
&= \frac{1}{Z} \operatorname{Tr} e^{iH_0(\tau+i\hbar\beta)/\hbar} A e^{-iH_0(\tau+i\hbar\beta)/\hbar} e^{-\beta H_0} B.
\end{aligned}
\tag{3.15}
$$

If we now allow the time to be complex, we can identify the time evolution operator $U_0(\tau + i\hbar\beta)$ that transforms A to the Interaction picture at the corresponding complex time. Using the same arguments as for equation (2.32), we obtain the identity

$$C_{AB}(\tau) = \operatorname{Tr} e^{-\beta H_0} B A(\tau + i\hbar\beta) = \langle B(-\tau - i\hbar\beta) A \rangle_{\mathrm{eq}} = C_{BA}(-\tau - i\hbar\beta). \tag{3.16}$$

Combining the identities above and inserting twice the definition of the Fourier transform, we obtain

$$
\begin{aligned}
\tilde{C}_{AB}(\omega) &= \int_{-\infty}^{\infty} e^{i\omega\tau} C_{AB}(\tau)\, d\tau = \int_{-\infty}^{\infty} e^{i\omega\tau} C_{BA}(-\tau - i\hbar\beta)\, d\tau \\
&= \int_{-\infty}^{\infty} e^{i\omega\tau} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega'(-\tau - i\hbar\beta)} \tilde{C}_{BA}(\omega')\, d\omega'\, d\tau \\
&= \int_{-\infty}^{\infty} e^{-\hbar\omega'\beta} \tilde{C}_{BA}(\omega') \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\tau(\omega+\omega')}\, d\tau\, d\omega' \\
&= \int_{-\infty}^{\infty} e^{-\hbar\beta\omega'} C_{BA}(\omega')\, \delta(\omega + \omega')\, d\omega' = e^{\hbar\beta\omega} \tilde{C}_{BA}(-\omega), \tag{3.17}
\end{aligned}
$$

taken together

$$\tilde{C}_{AB}(\omega) = e^{\hbar\beta\omega} \tilde{C}_{BA}(-\omega). \tag{3.18}$$

This identity has a similar form as equation (2.41) for the response function's Fourier transform, which can not be obtained for correlation functions.

3.2 Fluctuation-Dissipation Theorem

We already discussed the relation between correlation and response functions. The identity (3.2) also holds for the Fourier transforms

$$\tilde{\chi}''_{AB}(\omega) = \frac{1}{2\hbar} \left[\tilde{C}_{AB}(\omega) - \tilde{C}_{BA}(-\omega) \right] . \tag{3.19}$$

It seems natural to relate the two quantities $\tilde{\chi}''_{AB}(\omega)$ and $\tilde{C}_{AB}(\omega)$ in a direct way. We can express $\tilde{C}_{BA}(-\omega)$ via (3.18) and therefore write the response function in terms of the correlation function

$$\tilde{\chi}''_{AB}(\omega) = \frac{1}{2\hbar} \left[\tilde{C}_{AB}(\omega) - e^{-\hbar\beta\omega}\tilde{C}_{AB}(\omega) \right] = \frac{1 - e^{-\hbar\beta\omega}}{2\hbar}\tilde{C}_{AB}(\omega) . \tag{3.20}$$

This important relation between the correlation function and the response function is called *fluctuation-dissipation theorem*. Attention should by paid to the fact that this result has been obtained by using the explicit form of the density matrix in the canonical ensemble.

An extensive discussion of the interpretation of the fluctuation-dissipation theorem as a relation between scattering and linear response experiments can be found in Ref. [16]. Considerations with emphasis on stochastic aspects can be found in Ref. [21].

3.3 Related Estimates at zero Temperature

In the following we will discuss estimates for minimal excitation energies and ordering relations between correlation functions at zero temperature. By zero temperature we mean that only the ground state $|0\rangle$ with the corresponding energy eigenvalue $\hbar\omega_0$ is occupied. In other words the density matrix reads $\rho = |0\rangle \langle 0|$. We will also rely on this concept to describe ultracold quantum gases, although the assumption, that only the ground state is occupied, is an approximation due to the existence of quantum fluctuations.

3.3.1 Estimates for Elementary Excitations

In this section we derive a method to estimate the lowest excitation energy at zero temperature. To this end we consider the spectral representation (3.7) of $\tilde{C}_A(\omega)$ which, for zero temperature, reduces to

$$\tilde{C}_A(\omega) = 2\pi \sum_m |\langle 0|A|m\rangle|^2 \, \delta(\omega - \omega_{m0}) . \tag{3.21}$$

Inserting this expression into the definition (3.8) of $m_A^{(n)}$ we obtain

$$m_A^{(n)} = \sum_m (\hbar\omega_{m0})^n |\langle 0|A|m\rangle|^2 = \sum_m \epsilon_m^n \Gamma_m , \tag{3.22}$$

where we defined $\epsilon_m := \hbar\omega_{m0}$ and $\Gamma_m := |\langle m|A|0\rangle|^2$. We assume that there exists at least one excited state $m \neq 0$ with $\langle 0|A|m\rangle \neq 0$. We define the lowest excitation energy as

$$\omega_{\min} := \inf_{\epsilon_m \Gamma_m \neq 0} \omega_{m0} , \tag{3.23}$$

also referred to as elementary excitation. The infimum arises due to the fact that the summation over all eigenvalues in equation (3.22) has to be replaced by an integration in the case that H_0 has unbound eigenstates. Then a definition using the minimum might be undefined which coincides with the case of gapless excitations. Certainly in this case it is unclear, whether the moments themselves are well defined.

To make quantitative predictions for the elementary excitations, we can estimate the nth moment via

$$(\hbar\omega_{\min})^l \sum_m (\hbar\omega_{m0})^{n-l} |\langle 0|A|m\rangle|^2 \leq \sum_m (\hbar\omega_{m0})^n |\langle 0|A|m\rangle|^2, \tag{3.24}$$

where $l \in \mathbb{Z}$ can be chosen arbitrarily. The inequality also holds in the case of integrals replacing the sums. The latter follows directly from the common proof of the first mean value theorem for integration.

We can simplify the inequality (3.24) by identifying the nth and $(n-l)$th moment using equation (3.22):

$$(\hbar\omega_{\min})^l \, m_A^{(n-l)} \leq m_A^{(n)}. \tag{3.25}$$

If the $(n-l)$th moment is nonzero we can rewrite the inequality as

$$(\hbar\omega_{\min})^l \leq m_A^{(n)} \big/ m_A^{(n-l)}, \tag{3.26}$$

which defines a strict upper bound for the lowest excitation energy $\hbar\omega_{\min}$ at zero temperature [17]. In the case of exactly one elementary excitation energy, i.e. for all $m \neq 0$ where $\langle 0|A|m\rangle \neq 0$, the excitation energy $\hbar\omega_{m0}$ is exactly the same, equation (3.26) trivially becomes an identity.

It should be emphasized that the moments arising in the estimate (3.26) can be calculated using the sum rules (3.11) and (3.12).

3.3.2 Estimates between Moments

Whereas the calculation of some moments might be impracticable, every moment can be estimated by two other moments via the inequality [17]:

$$\left(m_A^{(n)}\right)^2 \leq m_A^{(n-1)} m_A^{(n+1)}. \tag{3.27}$$

We proof this inequality using the notation introduced in equation (3.22).

All addends in the series (3.22) are positive and thus the series is absolutely convergent. Therefore the Cauchy product of two moments converges to the product of both moments. Hence we can write

$$\left(m_A^{(n)}\right)^2 = \sum_{k=0}^{\infty} \sum_{p=0}^{k} \epsilon_p^n \Gamma_p \, \epsilon_{k-p}^n \Gamma_{k-p}, \tag{3.28}$$

$$\left(m_A^{(n-1)}\right)\left(m_A^{(n+1)}\right) = \sum_{k=0}^{\infty} \sum_{p=0}^{k} \epsilon_p^{n-1} \Gamma_p \, \epsilon_{k-p}^{n+1} \Gamma_{k-p}. \tag{3.29}$$

We now compare the sum over k in both equations. If the kth addend in (3.28) is smaller then the kth addend in (3.29) for all k then the whole expression (3.28) is smaller than (3.29). In general a sum over p can be rewritten as

$$\sum_{p=0}^{k} x_p \equiv \begin{cases} x_0 & k = 0 \\ \sum_{s=0}^{(k-1)/2} (x_s + x_{k-s}) & \text{odd } k \\ \sum_{s=0}^{(k-2)/2} (x_s + x_{k-s}) + x_{k/2} & \text{even } k. \end{cases} \tag{3.30}$$

Considering the corresponding terms x of (3.28) and (3.29) we can also state that, if $x_s + x_{k-s}$ fulfills the desired inequality for all s, the whole inequality has to be valid. The single term arising for $k = 0$ and k even, i.e. $s = k/2$, can be treated in the same manner, as the term $x_s + x_s$ only gives a factor of two on both sides of the inequality. Therefore we proof the inequality $x_s + x_{k-s} \le y_s + y_{k-s}$, where x represents the right-hand side terms of equation (3.28) and y the ones of equation (3.29). Then we have

$$2\epsilon_s^n \epsilon_{k-s}^n \, \Gamma_s \Gamma_{k-s} \le \left(\epsilon_s^{n-1} \epsilon_{n-s}^{n+1} + \epsilon_s^{n+1} \epsilon_{n-s}^{n-1} \right) \Gamma_s \Gamma_{k-s}$$
$$\Leftrightarrow \; 2\epsilon_s^n \epsilon_{k-s}^n \le \epsilon_s^{n-1} \epsilon_{k-s}^{n+1} + \epsilon_s^{n+1} \epsilon_{k-s}^{n-1}$$
$$\Leftrightarrow \; 0 \le (\epsilon_s - \epsilon_{k-s})^2 , \tag{3.31}$$

which is, indeed, always fulfilled. Using the identity $a^{2k} + b^{2k} - 2a^k b^k = (a^k - b^k)^2$ we can easily generalize the result (3.27) to

$$\left(m_A^{(n)} \right)^2 \le m_A^{(n-l)} m_A^{(n+l)} , \tag{3.32}$$

where l must be an integer number.

4 Application to Collective Excitations of Ultracold Quantum Gases

In the following, we will apply the estimates for elementary excitation energies derived in Section 3.3.1 to ultracold quantum gases. In order to demonstrate the applicability of the procedure we restrict ourselves to investigate the monopole excitation also referred to as *breathing mode* with an isotropic harmonic trapping potential. The moments relevant for these estimates are calculated via the sum rules presented in Section 3.1.2. The results obtained are expressed in terms of the specific ground-state energies of the system, i.e. kinetic, trapping and, if present, interaction energy.

Supplementary we will derive virial identities that enable us to avoid the calculation of one of the specific ground-state energies. Exemplary, the monopole excitation energy for a delta interacting Bose gas as well as for a dipolar Fermi gas is calculated in detail.

4.1 Description of Ultracold Quantum Gases

We consider the time independent Hamiltonian

$$H_0 = H_{\text{kin}} + H_{\text{trap}} + H_{\text{int}}, \tag{4.1}$$

with

$$H_{\text{kin}} := -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \Delta_i, \qquad H_{\text{trap}} := \sum_{i=1}^{N} V(\boldsymbol{r}_i), \qquad H_{\text{int}} := \sum_{i=1}^{N} \sum_{j\,(>i)}^{N} U(\boldsymbol{r}_{ij}), \tag{4.2}$$

where $\boldsymbol{r}_{ij} := \boldsymbol{r}_i - \boldsymbol{r}_j$. This Hamiltonian can in general describe the full features of a trapped quantum gas with the fixed particle number N. To allow for any dimension $\mathcal{D}$ the position operator takes the form

$$\boldsymbol{r}_i = \sum_{\nu=1}^{\mathcal{D}} q_{i_\nu} \boldsymbol{e}_\nu \tag{4.3}$$

with $\boldsymbol{e}_\nu$ denoting the canonical unit vectors. We notice that, using this canonical approach, no assumptions have been made about the underlying statistics of the particles. Thus, the following considerations are valid for both bosonic and fermionic species.

We assume that our system is situated at zero temperature as defined in Section 3.3. Referring to Section 3.3.1 we can estimate the elementary excitation energy for the excitation operator A via

$$(\hbar\omega_{\text{min}})^l \leq m_A^{(n)} \big/ m_A^{(n-l)}. \tag{4.4}$$

Using the sum rules (3.11) and (3.12) the first four moments can be explicitly written as

$$m_A^{(0)} = \tfrac{1}{2} \langle \{A, A\} \rangle_{\text{eq}} = \langle A^2 \rangle_{\text{eq}} \, , \tag{4.5a}$$

$$m_A^{(1)} = \tfrac{1}{2} \langle [[A, H_0], A] \rangle_{\text{eq}} \, , \tag{4.5b}$$

$$m_A^{(2)} = \tfrac{1}{2} \langle \{[A, H_0], [H_0, A]\} \rangle_{\text{eq}} = \langle [H_0, A]^2 \rangle_{\text{eq}} \, , \tag{4.5c}$$

$$m_A^{(3)} = \tfrac{1}{2} \langle [[[A, H_0], H_0], [H_0, A]] \rangle_{\text{eq}} \, . \tag{4.5d}$$

We notice that by using the fluctuation dissipation theorem (3.20) at zero temperature

$$\tilde{\chi}''_{AB}(\omega) = \frac{1}{2\hbar} \tilde{C}_{AB}(\omega) \, , \tag{4.6}$$

we can relate the moments of $\tilde{\chi}''$ and $\tilde{C}$ via

$$\varpi_A^{(n)} = \frac{1}{2\hbar} m_A^{(n)} \, . \tag{4.7}$$

With only the ground state occupied at zero temperature, equilibrium averages cut down to the pure ground-state average

$$\langle G \rangle_{\text{eq}} = \frac{\langle 0|G|0 \rangle}{\langle 0|0 \rangle} \, . \tag{4.8}$$

We stress again that the moments expressed via sum rules are calculated in the equilibrium configuration.

4.2 Sum-Rule Approach to Breathing Mode

In this section we will explore the breathing mode of ultracold quantum gases in isotropic harmonic trapping potentials. We will first derive results, that are valid without any further assumptions. For interacting gases we will regard a specific class of interaction potentials. Finally we derive exact results for the limit of non-interacting gases.

4.2.1 General Results

We consider an arbitrary one-component gas in a harmonic trap

$$H_{\text{ho}} |0\rangle = \sum_{i=1}^{N} V_{\text{ho}}(\boldsymbol{r}_i) |0\rangle = E_{\text{ho}} |0\rangle \tag{4.9}$$

with the rotational symmetric potential

$$V_{\text{ho}}(\boldsymbol{r}_i) = \frac{1}{2} m \Omega_{\text{ho}}^2 r_i^2 \, . \tag{4.10}$$

The gas can be excited by a modulation of the trapping frequency [5] that we can describe by the time dependent perturbation Hamiltonian

$$H_{1t} = -\frac{1}{2} m \Omega^2(t) \sum_{i=1}^{N} r_i^2 = -f(t) M \, , \tag{4.11}$$

where $M := \sum_{i=1}^{N} r_i^2$ denotes the monopole operator that couples to the c-number

$$f(t) = \frac{1}{2} m \Omega^2(t) \,. \tag{4.12}$$

As M is Hermitian, we can calculate the first moments of the correlation function via (4.5a–d). We require that $[M, H_{\text{int}}] = 0$ and find that $[M, H_{\text{ho}}] = 0$, hence the arising commutator $[M, H_0]$ has only contributions from the kinetic term H_{kin}. One easily finds

$$[M, H_0] = [M, H_{\text{kin}}] = \frac{\hbar^2}{m} \sum_{i=1}^{N} \left(\mathcal{D} + 2\boldsymbol{r}_i \cdot \boldsymbol{\nabla}_i \right) \,, \tag{4.13}$$

and from that

$$[[M, H_0], M] = \frac{4\hbar^2}{m} \sum_{i=1}^{N} r_i^2 \,. \tag{4.14}$$

This result is rather general as the calculation of these commutators does not depend on the interaction except for the requirement that the interaction Hamiltonian commutes with the monopole operator M.

Using equations (4.5a–c) we can now write the first three moments as

$$m_M^{(0)} = N \langle r^4 \rangle_{\text{eq}} \,, \tag{4.15}$$

$$m_M^{(1)} = \frac{2N\hbar^2}{m} \langle r^2 \rangle_{\text{eq}} = \frac{4N\hbar^2}{m^2 \Omega_{\text{ho}}^2} \langle H_{\text{ho}} \rangle_{\text{eq}} \,, \tag{4.16}$$

$$m_M^{(2)} = \frac{N\hbar^4}{m^2} \left[\mathcal{D}^2 + 4\mathcal{D} \langle \boldsymbol{r} \cdot \boldsymbol{\nabla} \rangle_{\text{eq}} + \left\langle (\boldsymbol{r} \cdot \boldsymbol{\nabla})^2 \right\rangle_{\text{eq}} \right] \,, \tag{4.17}$$

where we used that, for indistinguishable particles, the operator averages can not depend on the specific particle. Although the interaction potential did not enter the calculation of these commutators, the corresponding equilibrium averages do depend on the interaction.

Theoretically each ratio of two moments (4.15) to (4.17) can be used to obtain an upper bound for the minimal excitation frequency via equation (4.4). We notice that the first moment can be expressed in terms of the potential energy $E_{\text{ho}} = \langle H_{\text{ho}} \rangle_{\text{eq}}$ and some given constants. As the averages within the 0th and 2th moment have no straightforward physical interpretation, we try to find a higher moment that can be expressed in terms of energies. But for the calculation of commutators appearing for higher moments we have to take the explicit form of the interaction into account.

4.2.2 Non-Interacting Gases

We first consider the simplest case of a non-interacting gas. Contributions due to non zero interaction will emerge as additional terms in the moments, that can be calculated subsequently. The commutators

$$[[M, H_0], H_0] = [[M, H_0], H_{\text{kin}} + H_{\text{ho}}] = \frac{2\hbar^4}{m^2} \sum_{i=1}^{N} \Delta_i + 2\hbar^2 \Omega_{\text{ho}}^2 \sum_{i=1}^{N} r_i^2 \,, \tag{4.18}$$

$$[[[M, H_0], H_{\text{kin}} + H_{\text{ho}}], [H_0, M]] = -\frac{8\hbar^6}{m^3} \sum_{i=1}^{N} \Delta_i + \frac{8\hbar^4 \Omega_{\text{ho}}^2}{m} \sum_{i=1}^{N} r_i^2 \tag{4.19}$$

can be found by a straight forward calculation. Inserting these results into (4.5d) we find

$$
\begin{aligned}
m_M^{(3)} &= -\frac{4N\hbar^6}{m^3}\left\langle \Delta \right\rangle_{\text{eq}} + \frac{4\hbar^2\Omega_{\text{ho}}^2}{m}\left\langle r^2 \right\rangle_{\text{eq}} \\
&= \frac{8N\hbar^4}{m^2}\left\langle H_{\text{kin}} \right\rangle_{\text{eq}} + \frac{8N\hbar^4}{m^2}\left\langle H_{\text{ho}} \right\rangle_{\text{eq}}.
\end{aligned}
\tag{4.20}
$$

According to the inequality (4.4) the ratio of the third moment (4.20) and the first moment (4.16) defines a rigorous upper bound for the elementary excitation of the breathing mode [14]:

$$
(\hbar\omega_{\text{min}})^2 \le m_M^{(3)}\big/ m_M^{(1)} = \hbar^2\Omega_{\text{ho}}^2 \frac{4E_{\text{kin}} + 4E_{\text{ho}}}{2E_{\text{ho}}}.
\tag{4.21}
$$

We have now achieved to express the upper bound in terms of energies. Further aspects of this result will be discussed in Section 4.2.4.

4.2.3 Interacting Gases

Next we study the contributions of the interaction potential to the third moment. The commutator

$$
[[M, H_0], H_{\text{int}}] = \frac{2\hbar^2}{m}\sum_{i=1}^{N}\sum_{j(>i)}^{N}\left(r_i \cdot \nabla_i + r_j \cdot \nabla_j\right)U(r_{ij})
\tag{4.22}
$$

can then be rewritten as

$$
[[M, H_0], H_{\text{int}}] = \frac{2\hbar^2}{m}\sum_{i=1}^{N}\sum_{j(>i)}^{N} r_{ij} \cdot \nabla_{ij}U(r_{ij}),
\tag{4.23}
$$

where nabla is only acting on U. We now specify to an effective dipole–dipole interaction potential

$$
U_{\text{dd}}(r_{ij}) = \frac{D^2}{r_{ij}^3} - \frac{\left(D \cdot r_{ij}\right)^2}{r_{ij}^5},
\tag{4.24}
$$

where we have $D = m\sqrt{\mu_0/4\pi}$ or $D = d/\sqrt{4\pi\epsilon_0}$ for magnetic or electric dipoles, respectively. Here m denotes the magnetic moment in units of the Bohr magneton and d the electric moment in units of Debye. Via a straight forward calculation one finds

$$
r_{ij} \cdot \nabla_{ij}U_{\text{dd}}(r_{ij}) = -3\,U_{\text{dd}}(r_{ij}).
\tag{4.25}
$$

Therefore the additional commutator for the third moment reads

$$
[[[M, H_0], H_{\text{dd}}], [H_0, M]] = \frac{36N\hbar^4}{m^2}H_{\text{dd}}.
\tag{4.26}
$$

Combining the results for the non-interacting case (4.20) and equation (4.26) we obtain

$$
(\hbar\omega_{\text{min}})^2 \le m_M^{(3)}\big/ m_M^{(1)} = \hbar^2\Omega_{\text{ho}}^2 \frac{4E_{\text{kin}} + 4E_{\text{ho}} + 9E_{\text{dd}}}{2E_{\text{ho}}}
\tag{4.27}
$$

as an upper bound for the excitation energy of the breathing mode.

The result obtained for the dipole–dipole interaction was essentially governed by the identity

$$\boldsymbol{r} \cdot \boldsymbol{\nabla}\, U(\boldsymbol{r}) = n\, U(\boldsymbol{r}) \tag{4.28}$$

where $n = -3$. It is recognized that equation (4.28) is nothing else than an equivalent definition for the positive homogeneity of $U(\boldsymbol{r})$, formally

$$U(\lambda\boldsymbol{r}) = \lambda^n U(\boldsymbol{r})\ \forall \lambda > 0 \quad \Leftrightarrow \quad \boldsymbol{r} \cdot \boldsymbol{\nabla}\, U(\boldsymbol{r}) = n\, U(\boldsymbol{r})\,, \tag{4.29}$$

known as *Euler's theorem* [22]. Thus we are in the position to generalize the commutator (4.26) for potentials $U(\boldsymbol{r}_{ij})$ which are homogenous of degree n to

$$[[[M, H_0], H_{\text{int}}], [H_0, M]] = \frac{4\hbar^4}{m^2} \sum_{i=1}^{N} \sum_{j\,(>i)}^{N} \left\{ \boldsymbol{r}_{ij} \cdot \boldsymbol{\nabla}_{ij} \left[\boldsymbol{r}_{ij} \cdot \boldsymbol{\nabla}_{ij} U(\boldsymbol{r}_{ij}) \right] \right\}$$

$$= \frac{4n^2\hbar^4}{m^2} \sum_{i=1}^{N} \sum_{j\,(>i)}^{N} U(\boldsymbol{r}_{ij})\,. \tag{4.30}$$

This yields the upper bound

$$(\hbar\omega_{\min})^2 \leq m_M^{(3)} \Big/ m_M^{(1)} = \hbar^2 \Omega_{\text{ho}}^2 \frac{4E_{\text{kin}} + 4E_{\text{ho}} + n^2 E_{\text{int}}}{2E_{\text{ho}}}\,. \tag{4.31}$$

This rather general result can now be applied to the case of a delta interaction

$$U_\delta(\boldsymbol{r}_{ij}) = g\, \delta(\boldsymbol{r}_{ij}) = g \prod_{\nu=1}^{\mathcal{D}} \delta(q_{i_\nu} - q_{j_\nu})\,. \tag{4.32}$$

Using the well-known relation $\delta(\lambda q) = \delta(q)/|\lambda|$ we can write

$$\delta(\lambda\boldsymbol{r}) = |\lambda|^{-\mathcal{D}} \delta(\boldsymbol{r})\,, \tag{4.33}$$

where $\mathcal{D}$ represents the number of dimensions involved in the problem. This shows immediately that $U_\delta(\boldsymbol{r}_{ij})$ is positive homogenous of degree $-\mathcal{D}$ and therefore

$$(\hbar\omega_{\min})^2 \leq m_M^{(3)} \Big/ m_M^{(1)} = \hbar^2 \Omega_{\text{ho}}^2 \frac{4E_{\text{kin}} + 4E_{\text{ho}} + \mathcal{D}^2 E_\delta}{2E_{\text{ho}}}\,. \tag{4.34}$$

We notice that for $\mathcal{D} = 3$ this result takes exactly the same form as in the case of dipole interaction (4.27), with E_δ replaced by E_{dd}. Of course the specific energies E_{kin} and E_{ho} differ from system to system.

We can finally combine both previous results to the expression

$$\omega_{\min} \leq \Omega_{\text{ho}} \sqrt{\frac{4E_{\text{kin}} + 4E_{\text{ho}} + \mathcal{D}^2 E_\delta + 9E_{\text{dd}}}{2E_{\text{ho}}}}\,, \tag{4.35}$$

which would be applicable for the breathing mode frequency of a dipolar Bose gas [23]. We stress again that this result provides a rigorous upper bound for the elementary excitations at zero temperature irrespective of the underlying quantum statistics. Examples of explicit results for the entering energies will be provided in Section 4.4.

4.2.4 Exact Solution for Non-Interacting Case

To derive an exact solution for the excitation energy in the non-interacting case we regard the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\prod_{j=1}^{N}|\psi\rangle_j = \left\{-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i + \frac{1}{2}m\left[\Omega_{\mathrm{ho}}^2 + \Omega^2(t)\right]\sum_{i=1}^{N}r_i^2\right\}\prod_{j=1}^{N}|\psi\rangle_j. \tag{4.36}$$

Self-evidently for $\Omega^2(t) = 0$ this equations describes nothing else then N independent $\mathcal{D}$-dimensional harmonic oscillators. For this problem the moments of the correlation function can be directly evaluated via equation (3.22).

The position operator q can be expressed through the well-known lowering and raising operators α and $\alpha^\dagger$ [24]. Accordingly the excitation operator M can be rewritten in the form

$$M = \sum_{i=1}^{N}r_i^2 = \sum_{i=1}^{N}\sum_{\nu=1}^{\mathcal{D}}q_{i\nu}^2 = \frac{\hbar}{2m\Omega_{\mathrm{ho}}}\sum_{i=1}^{N}\sum_{\nu=1}^{\mathcal{D}}\left(\alpha_{i\nu} + \alpha_{i\nu}^\dagger\right)^2. \tag{4.37}$$

We omit all prefactors for simplicity, as they will not be relevant in the end. Utilizing the rotational symmetry we can further rewrite

$$M = \sum_{i=1}^{N}\left(\alpha_i + \alpha_i^\dagger\right)^2. \tag{4.38}$$

For the direct evaluation we have to calculate the moment

$$m_M^{(n)} = \sum_{\{h\}}\omega_{\{h\}0}\left|\langle 0\,|\,M\,|\,\{h\}\rangle\right|^2, \tag{4.39}$$

where we have defined the energy eigenstate

$$|\{h\}\rangle := S_\pm\prod_{j=1}^{N}|h_j\rangle_j, \tag{4.40}$$

where S_+ denotes the symmetrization operator for bosons and S_- the antisymmetrizing operator for fermions, respectively. The ket $|0\rangle$ denotes the ground state configuration. We now choose to represent our problem in Fock space. The operator M in the Fock space reads [15]:

$$\mathfrak{M} = \sum_{i,j}\left\langle i\,\left|\,\left(\alpha + \alpha^\dagger\right)^2\,\right|\,j\right\rangle a_i^\dagger a_j. \tag{4.41}$$

Here, $a_i^\dagger, a_i$ denote the operators that create or annihilate a bosonic or fermionic particle with the energy $\hbar\omega_i$ in Fock space. We write $|F\rangle$ to denote a Fock state of the harmonic oscillator.

For further calculations we have to distinguish between fermionic and bosonic systems. We first regard the Bose gas at zero temperature. The state $|s, t\rangle$ labels the Fock state where

s particles are in the lowest energy state and t particles are in the state with the energy $\hbar\omega_2$. Thus the ground state reads $|N,0\rangle$. The nth moment expressed in the Fock space reads

$$m_M^{(n)} = \sum_F \omega_{F0}^n \, |\langle N,0 \,|\, \mathfrak{M} \,|\, F\rangle|^2 \,. \tag{4.42}$$

We calculate the matrix element

$$\langle N,0 \,|\, \mathfrak{M} \,|\, F\rangle = \sum_{i,j} \left\langle i \,\middle|\, (\alpha + \alpha^\dagger)^2 \,\middle|\, j \right\rangle \left\langle N,0 \,\middle|\, a_i^\dagger a_j \,\middle|\, F \right\rangle \tag{4.43}$$

$$= \sqrt{N} \sum_j \left\langle 0 \,\middle|\, (\alpha + \alpha^\dagger)^2 \,\middle|\, j \right\rangle \langle N-1,0 \,|\, a_j \,|\, F\rangle \tag{4.44}$$

$$= \sqrt{N} \left(\sqrt{2}\,\langle N-1,0 \,|\, a_2 \,|\, F\rangle + \langle N-1,0 \,|\, a_0 \,|\, F\rangle \right). \tag{4.45}$$

We recall that ω_{F0} denotes the difference between the total ground-state energy and the total energy of the state $|F\rangle$. Since the term $\langle N-1,0 \,|\, a_0 \,|\, F\rangle = \sqrt{n}\,\langle N,0 \,|\, F\rangle$ does only contribute if $|F\rangle$ is the ground state, but ω_{00} is zero, this term does not contribute to the sum at all. The second matrix element $\langle N-1,0 \,|\, a_2 \,|\, F\rangle = \langle N-1,1 \,|\, F\rangle$ contributes with the energy difference $\hbar\omega_{(N-1,1)\,0} = 2\hbar\Omega_{\text{ho}}$.

But the most important fact is, that finally only the Fock state $|N-1,0\rangle$ contributes to the calculation of the moment (4.42). As discussed in Section 3.3.1 this implies that the sum-rule estimate for the non-interacting case (4.21) is an equality rather than an inequality. For the sum-rule estimate we are interested in the ratio $m_M^{(n)}/m_M^{(n-l)}$ of two moments. Inspecting equation (4.42) we can see that the single contributing matrix element cancels out of the ratio. A posteriori this also justifies the neglected prefactors. The ratio reads

$$m_M^{(n)} \Big/ m_M^{(n-l)} = (2\hbar\Omega_{\text{ho}})^l \,. \tag{4.46}$$

We therefore have the result

$$\omega_{\min} = 2\Omega_{\text{ho}} \,, \tag{4.47}$$

which is exact in the regime of linear response theory. We also notice that the result for $\omega_{\min}$ is, indeed, independent of the choice of l.

We now turn to fermionic gases, where all states below the Fermi energy are occupied. For a neat representation we assume spinless particles, however all arguments can be carried out for particles with arbitrary spin. We denote the fermionic ground state by $|\tilde{0}\rangle$ and regard again the nth moment

$$m_M^{(n)} = \sum_F \omega_{F\tilde{0}}^n \, |\langle \tilde{0} \,|\, \mathfrak{M} \,|\, F\rangle|^2 = \sum_F \omega_{F\tilde{0}}^n \left| \sum_{i,j} \left\langle i \,\middle|\, (\alpha + \alpha^\dagger)^2 \,\middle|\, j \right\rangle \left\langle \tilde{0} \,\middle|\, a_i^\dagger a_j \,\middle|\, F \right\rangle \right|^2 . \tag{4.48}$$

The matrix element $\left\langle i \,\middle|\, (\alpha + \alpha^\dagger)^2 \,\middle|\, j \right\rangle$ yields two terms contributing with $\langle i|j\rangle = \delta_{ij}$. We notice that the matrix element $\left\langle \tilde{0} \,\middle|\, a_i^\dagger a_i \,\middle|\, F \right\rangle$ is only nonzero if $|F\rangle = |\tilde{0}\rangle$, but again since

$\omega_{\tilde{0}\tilde{0}} = 0$ these matrix elements do not contribute at all. The nth moment then reads

$$\sum_F \omega_{F\tilde{0}}^n \left| \langle \tilde{0} \,|\, \mathfrak{M} \,|\, F \rangle \right|^2 =$$

$$= \sum_F \omega_{F\tilde{0}}^n \left| \sum_{i,j} \left[\langle i \,|\, j+2 \rangle \sqrt{j^2 + 3j + 2} + \langle i+2 \,|\, j \rangle \sqrt{i^2 + 3i + 2} \right] \left\langle \tilde{0} \,\middle|\, a_i^\dagger a_j \,\middle|\, F \right\rangle \right|^2. \quad (4.49)$$

The term $\left\langle \tilde{0} \,\middle|\, a_i^\dagger a_j \,\middle|\, F \right\rangle$ is only nonzero if $j > i$, since otherwise an energy state is removed from the ground state that is above the Fermi energy or a state below i is added, which is already fully occupied. Since $j + 2 = i$ contradicts $j > i$, equation (4.49) can be rewritten as

$$\sum_F \omega_{F\tilde{0}}^n \left| \langle \tilde{0} \,|\, \mathfrak{M} \,|\, F \rangle \right|^2 = \sum_F \omega_{F\tilde{0}}^n \left| \sum_{i,j} \langle i+2 \,|\, j \rangle \sqrt{i^2 + 3i + 2} \left\langle \tilde{0} \,\middle|\, a_i^\dagger a_j \,\middle|\, F \right\rangle \right|^2$$

$$= \sum_F \omega_{F\tilde{0}}^n \left| \sum_j \sqrt{j^2 - j} \left\langle \tilde{0} \,\middle|\, a_{j-2}^\dagger a_j \,\middle|\, F \right\rangle \right|^2. \quad (4.50)$$

We can read off that we have to excite a fermion out of the ground state to an energy that is $\hbar\omega_{20}$ higher then the ground state, or formally $|F\rangle = a_j^\dagger a_{j-2} |\tilde{0}\rangle$. This is only possible for a few configurations around the Fermi energy. However, the energy difference $\omega_{F\tilde{0}}$ is the same for every excitation as the harmonic oscillator energies are equidistant. Thus all the results presented for Bose gases are also valid for Fermi gases.

4.3 Virial Identities

Virial identities are useful to reduce the effort for calculating specific energy contributions in a system as they provide a possibility to avoid the calculation of one specific ground-state energy. We will prove rather general virial identities for canonical Hamiltonians and exemplarily show the validity in case of a mean-field theory.

We point out, that for the approximative approaches in Section 4.4 the derived virial identities are still valid as is shown in Sections 4.4.1 and 4.4.2.

4.3.1 Canonical Hamiltonians with Homogenous Potentials

The generalization of the classical virial theorem is already known since the very beginning of quantum mechanics. The following derivation follows the historical approach by Born, Heisenberg, and Jordan from 1926 [25].

We consider a Hamiltonian of the form

$$H = H_{\text{kin}} + H'(r_1, \dots, r_N) \quad (4.51)$$

where H' should only consist of a potential which is positive homogenous of degree n' without explicit time dependence. We consider the *virial* defined by

$$G := \sum_{i=1}^N p_i \cdot r_i. \quad (4.52)$$

The average of the total time derivative can be written in the form

$$
\left\langle \frac{\mathrm{d}G}{\mathrm{d}t} \right\rangle_{\mathrm{eq}} = \left\langle \sum_{i=1}^{N} \frac{\mathrm{d}\boldsymbol{p}_i}{\mathrm{d}t} \cdot \boldsymbol{r}_i \right\rangle_{\mathrm{eq}} + \left\langle \sum_{i=1}^{N} \boldsymbol{p}_i \cdot \frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t} \right\rangle_{\mathrm{eq}}.
\tag{4.53}
$$

Next we analyze the terms of equation (4.53) subsequently. First we define the kinetic-energy operator from the classical expression

$$
T := \frac{m}{2} \sum_{i=1}^{N} \left(\frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t} \right)^2 = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m}
\tag{4.54}
$$

whereas the last equal sign is justified by the Heisenberg equation

$$
\frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar} [H, \boldsymbol{r}_i] = \frac{\boldsymbol{p}_i}{m}.
\tag{4.55}
$$

Using equations (4.54), (4.55) we can write

$$
\sum_{i=1}^{N} \boldsymbol{p}_i \cdot \frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t} = 2T.
\tag{4.56}
$$

To evaluate the second addend of equation (4.53) we calculate the Heisenberg equation

$$
\frac{\mathrm{d}\boldsymbol{p}_i}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar} [H, \boldsymbol{p}_i] = -\boldsymbol{\nabla}_i H'.
\tag{4.57}
$$

Using theorem (4.29) we have

$$
\sum_{i=1}^{N} \frac{\mathrm{d}\boldsymbol{p}_i}{\mathrm{d}t} \cdot \boldsymbol{r}_i = - \sum_{i=1}^{N} \boldsymbol{r}_i \cdot \boldsymbol{\nabla}_i H' = -n' H'.
\tag{4.58}
$$

As shown for equation (4.23) this argument can also be applied to interaction potentials $H'(\boldsymbol{r}_{ij})$ which are positive homogenous of degree n'.

Finally, we regard the first term of equation (4.53). Considering the case where the density matrix ρ commutes with H and using the cyclic invariance of the trace we have

$$
\left\langle \frac{\mathrm{d}G}{\mathrm{d}t} \right\rangle_{\mathrm{eq}} = \frac{\mathrm{i}}{\hbar} \langle [H, \boldsymbol{p} \cdot \boldsymbol{r}] \rangle_{\mathrm{eq}} = \frac{\mathrm{i}}{\hbar} \left(\langle H\boldsymbol{p} \cdot \boldsymbol{r} \rangle_{\mathrm{eq}} - \langle \boldsymbol{p} \cdot \boldsymbol{r}H \rangle_{\mathrm{eq}} \right) = 0.
\tag{4.59}
$$

Inserting these identities into equation (4.53) we find

$$
2 \langle T \rangle_{\mathrm{eq}} = n' \langle H' \rangle_{\mathrm{eq}}
\tag{4.60}
$$

which trivially generalizes to the case of multiple potentials via

$$
2 \langle T \rangle_{\mathrm{eq}} = n' \langle H' \rangle_{\mathrm{eq}} + n'' \langle H'' \rangle_{\mathrm{eq}} + \cdots.
\tag{4.61}
$$

Using the positive homogeneity of the potentials $V_{\mathrm{ho}}(\boldsymbol{r})$, $U_\delta(\boldsymbol{r}_{ij})$ and $U_{\mathrm{dd}}(\boldsymbol{r}_{ij})$ we thus obtain the result

$$
2E_{\mathrm{kin}} - 2E_{\mathrm{ho}} + \mathcal{D}E_\delta + 3E_{\mathrm{dd}} = 0.
\tag{4.62}
$$

As we have used a canonical approach, this result is valid regardless of the underlying statistics.

4.3.2 Explicit Derivation for Gross–Pitaevskii Theory

Many of the essential properties of ultracold quantum gases can be covered by a mean-field theory [17, 26]. For bosons at zero temperature we regard the Gross–Pitaevskii equation that takes into account both the contact and the dipole–dipole interaction

$$\left\{ -\frac{\hbar^2}{2m}\Delta + \frac{m\Omega_{\text{ho}}^2}{2}r^2 + g\left|\psi(\boldsymbol{r})\right|^2 + \int V_{\text{dd}}(\boldsymbol{r}-\boldsymbol{r}')\left|\psi(\boldsymbol{r}')\right|^2 \mathrm{d}^{\mathcal{D}}r' \right\}\psi(\boldsymbol{r}) = \mu\,\psi(\boldsymbol{r})\,. \qquad (4.63)$$

Although the results obtained for the breathing mode like equation (4.27) have been derived from a canonical Hamiltonian, we expect that the respective energies can also be calculated within a mean-field theory. We also expect that the virial identity holds for the mean-field theory as well.

We introduce the abbreviations

$$n(\boldsymbol{r}) \equiv n := \left|\psi(\boldsymbol{r})\right|^2\,, \qquad\qquad n(\boldsymbol{r}') \equiv n'\,. \qquad (4.64)$$

The energy functional decomposes into the following contributions

$$E(n) = E_{\text{kin}}(n) + E_{\text{ho}}(n) + E_{\delta}(n) + E_{\text{dd}}(n)\,, \qquad (4.65)$$

where

$$E_{\text{kin}}(n) = \int \frac{\hbar^2}{8m}(\partial_{q_\nu}n)(\partial_{q_\nu}n)\,n^{-1}\,\mathrm{d}^{\mathcal{D}}r\,, \qquad E_{\text{ho}}(n) = \int \frac{m\Omega_{\text{ho}}^2}{2}(q_\sigma q_\sigma)\,n\,\mathrm{d}^{\mathcal{D}}r\,, \qquad (4.66a)$$

$$E_{\text{dd}}(n) = \frac{1}{2}\iint V_{\text{dd}}(\boldsymbol{r}-\boldsymbol{r}')\,n\,n'\,\mathrm{d}^{\mathcal{D}}r'\mathrm{d}^{\mathcal{D}}r\,, \qquad E_{\delta}(n) = \int \frac{g}{2}n^2\,\mathrm{d}^{\mathcal{D}}r\,. \qquad (4.66b)$$

Here we use Einstein notation to sum over all coordinates. Note that an extremization of (4.65) with respect to n yields the Gross–Pitaevskii equation (4.63). If $\psi_0(\boldsymbol{r})$ is a solution of the Gross–Pitaevskii equation, the energy functional $E(n)$ has to be stationary at $n_0 := |\psi_0|^2$. Choosing the scaling transformation [17, p. 167]

$$n(\boldsymbol{r}) \rightarrow (1+\epsilon)^{\mathcal{D}}\,n_0(\boldsymbol{r}+\epsilon\boldsymbol{r})\,, \qquad (4.67)$$

the stationarity of $E(n)$ requires

$$\left.\frac{\partial E(n)}{\partial \epsilon}\right|_{\epsilon=0} = 0\,. \qquad (4.68)$$

Before we calculate the left-hand side of this equation, we note the result

$$\left.\frac{\partial n}{\partial \epsilon}\right|_{\epsilon=0} = \mathcal{D}n_0 + \boldsymbol{r}\cdot\boldsymbol{\nabla}n_0\,. \qquad (4.69)$$

For a space-saving presentation we replace n_0 with n in the following. We find

$$\left.\frac{\partial E_{\text{kin}}}{\partial\epsilon}\right|_{\epsilon=0} =$$

$$= \frac{\hbar^2}{8m}\int 2n^{-1}(\partial_{q_v}n)\,\partial_{q_v}(\mathcal{D}n + q_\sigma\partial_{q_\sigma}n) - n^{-2}(\partial_{q_v}n)(\partial_{q_v}n)(\mathcal{D}n + q_\sigma\partial_{q_\sigma}n)\,\mathrm{d}^{\mathcal{D}}r$$

$$\overset{(4.71)}{=} \mathcal{D}E_{\text{kin}} + 2E_{\text{kin}} + \frac{\hbar^2}{8m}\int 2n^{-1}(\partial_{q_v}n)(q_\sigma\partial_{q_\sigma}\partial_{q_v}n) - n^{-2}(\partial_{q_v}n)(\partial_{q_v}n)(q_\sigma\partial_{q_\sigma}n)\,\mathrm{d}^{\mathcal{D}}r$$

$$= \mathcal{D}E_{\text{kin}} + 2E_{\text{kin}} + \frac{\hbar^2}{8m}\int n^{-1}(\partial_{q_v}n)(q_\sigma\partial_{q_\sigma}\partial_{q_v}n) - n^{-2}(\partial_{q_v}n)(\partial_{q_v}n)(q_\sigma\partial_{q_\sigma}n)\,\mathrm{d}^{\mathcal{D}}r$$

$$- \frac{\hbar^2}{8m}\int [\partial_{q_\sigma}(n^{-1}q_\sigma\partial_{q_v}n)](\partial_{q_v}n)\,\mathrm{d}^{\mathcal{D}}r \overset{(4.71)}{=} 2E_{\text{kin}} \quad (4.70)$$

where we used twice the identity

$$\partial_{q_v}(q_\sigma\partial_{q_\sigma}n) = q_\sigma\partial_{q_\sigma}\partial_{q_v}n + \partial_{q_v}n. \quad (4.71)$$

By further straight forward calculations we find

$$\left.\frac{\partial E_{\text{ho}}}{\partial\epsilon}\right|_{\epsilon=0} = \frac{m\Omega_{\text{ho}}^2}{2}\int (q_\sigma q_\sigma)(\mathcal{D}n + q_v\partial_{q_v}n)\,\mathrm{d}^{\mathcal{D}}r = \mathcal{D}E_{\text{ho}} + \frac{m\Omega_{\text{ho}}^2}{2}\int (q_\sigma q_\sigma)q_v\partial_{q_v}n\,\mathrm{d}^{\mathcal{D}}r$$

$$= \mathcal{D}E_{\text{ho}} - \frac{m\Omega_{\text{ho}}^2}{2}\int n\partial_{q_v}(q_\sigma q_\sigma q_v)\,\mathrm{d}^{\mathcal{D}}r = \mathcal{D}E_{\text{ho}} - \mathcal{D}E_{\text{ho}} - 2E_{\text{ho}} = -2E_{\text{ho}}, \quad (4.72)$$

$$\left.\frac{\partial E_{\delta}}{\partial\epsilon}\right|_{\epsilon=0} = \frac{g}{2}\int 2n(\mathcal{D}n + q_v\partial_{q_v}n)\,\mathrm{d}^{\mathcal{D}}r$$

$$= 2\mathcal{D}E_{\delta} + \frac{g}{2}\int nq_v\partial_{q_v}n\,\mathrm{d}^{\mathcal{D}}r - \frac{g}{2}\int [\partial_{q_v}(nq_v)]n\,\mathrm{d}^{\mathcal{D}}r = \mathcal{D}E_{\delta} \quad (4.73)$$

and

$$\left.\frac{\partial E_{\text{dd}}}{\partial\epsilon}\right|_{\epsilon=0} = \iint V_{\text{dd}}(\mathcal{D}n + q_v\partial_{q_v}n)n'\,\mathrm{d}^{\mathcal{D}}r'\,\mathrm{d}^{\mathcal{D}}r = 2E_{\text{dd}} - \iint n\,\partial_{q_v}(V_{\text{dd}}n'q_v)\,\mathrm{d}^{\mathcal{D}}r'\,\mathrm{d}^{\mathcal{D}}r$$

$$= -\iint n(q_v\partial_{q_v}V_{\text{dd}} + V_{\text{dd}}q_v\partial_{q_v}n')\,\mathrm{d}^{\mathcal{D}}r'\,\mathrm{d}^{\mathcal{D}}r$$

$$= -\frac{1}{2}\iint [(q_v\partial_{q_v} + q'_v\partial_{q'_v})V_{\text{dd}}]\,n\,n'\,\mathrm{d}^{\mathcal{D}}r'\,\mathrm{d}^{\mathcal{D}}r = 3E_{\text{dd}}. \quad (4.74)$$

For the last equal sign we have used again the identity (4.25). Inserting equations (4.70) and (4.72)–(4.74) into the stationarity condition (4.68) gives the virial identity

$$2E_{\text{kin}} - 2E_{\text{ho}} + \mathcal{D}E_{\delta} + 3E_{\text{dd}} = 0, \quad (4.75)$$

which is identical to the result (4.62) obtained in the previous section.

4.4 Exemplary Calculations of Breathing Modes

Next we investigate the sum-rule expression (4.35) obtained for the breathing mode of an ultracold quantum gas in an isotropic harmonic trap. Assuming only the presence of contact interaction and using the virial identity (4.62) an upper bound to the lowest excitation frequency in a Bose gas is given by

$$\omega_{\min} \le \Omega_{\mathrm{ho}} \sqrt{2 + \mathcal{D} + (2 - \mathcal{D}) \frac{E_{\mathrm{kin}}}{E_{\mathrm{ho}}}} \,, \tag{4.76}$$

where $\mathcal{D}$ denotes the dimension. For the dipolar Fermi gas with $E_\delta = 0$ the upper bound reads

$$\omega_{\min} \le \Omega_{\mathrm{ho}} \sqrt{5 - \frac{E_{\mathrm{kin}}}{E_{\mathrm{ho}}}} \tag{4.77}$$

in any dimension. In this section we will exemplarily calculate the respective energies of the estimates (4.76) and (4.77) for a Bose gas with contact interaction and for a dipolar Fermi gas.

4.4.1 Bose Gas with Delta Interaction

We consider a three-dimensional Bose gas with delta interaction. An upper bound for the frequency of the breathing mode then follows from equation (4.76) and reads

$$\frac{\omega_{\min}}{\Omega_{\mathrm{ho}}} \le \sqrt{5 - \frac{E_{\mathrm{kin}}}{E_{\mathrm{ho}}}} \,. \tag{4.78}$$

We introduce the dimensionless parameter for the strength of the interaction energy

$$P := \sqrt{\frac{2}{\pi}} \frac{Na}{a_{\mathrm{ho}}} \,, \tag{4.79}$$

where a denotes the s-wave scattering length and $a_{\mathrm{ho}} := \sqrt{\hbar/(m\Omega_{\mathrm{ho}})}$ is referred to as the oscillator length. In the non-interacting case $P \to 0$ we have $E_{\mathrm{kin}} = E_{\mathrm{ho}}$ and we recover the exact result $\omega_{\min}/\Omega_{\mathrm{ho}} = 2$ found previously in equation (4.47). In the hydrodynamic limit $P \gg 1$, also referred to as the Thomas–Fermi limit, the kinetic energy can be neglected [14]. Then we have $\omega_{\min}/\Omega_{\mathrm{ho}} \le \sqrt{5}$. This result can also be obtained as an exact solution of the hydrodynamic equations [17].

In order to calculate both the kinetic and the trapping energy of the system beyond the discussed limits, we consider the stationary Gross–Pitaevskii equation (4.63), which can also be derived by minimizing the Lagrange density $\mathcal{L}(n) = -E(n)$. The corresponding energy functional $E(n)$ is given by equation (4.65). The eigenfunction of the stationary Gross–Pitaevskii equation in the non-interacting case is nothing else than the harmonic oscillator ground state, i.e. a Gaussian function. To implement the features of an interacting
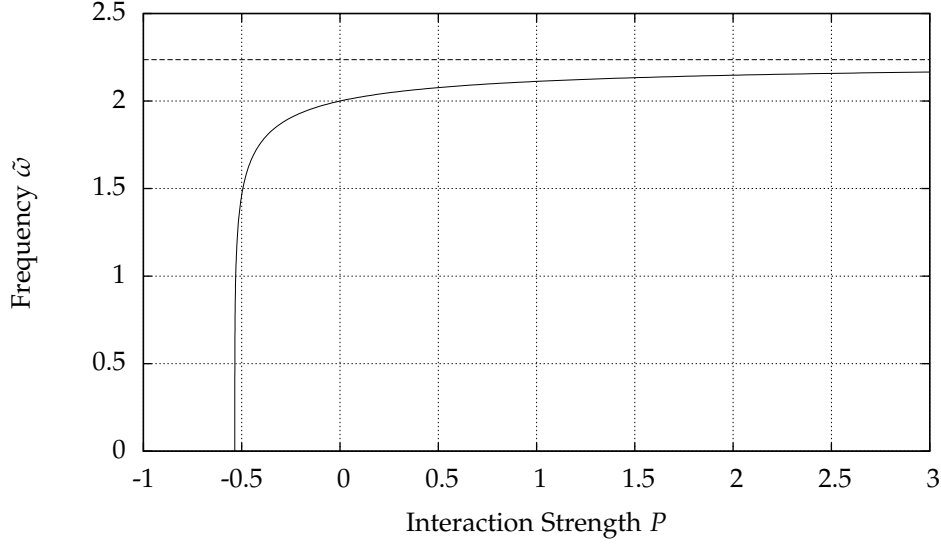
Fig. 4.1: Breathing mode frequency of a Bose gas with contact interaction as function of the dimensionless interaction strength P. The dashed line shows the frequency in the Thomas–Fermi limit valid for $P \gg 1$, at $P = 0$ we have the non-interacting case, and the zero-crossing in the second quadrant coincides with the set in of an instability. An equivalent result has been presented by Stringari [14].

Bose gas we introduce the width of the Gaussian as an artificial variational parameter Ξ. Then the wave function reads [27]

$$\psi_0(\boldsymbol{r}) = \frac{N^{1/2}}{\pi^{3/2}\Xi^{3/2}}\mathrm{e}^{-\frac{3}{2}\Xi^{-2}r^2}. \tag{4.80}$$

This approach implies the assumption that the wave function in the interacting case takes a similar form as in the non-interacting case. Next we minimize the Lagrange density $\mathcal{L}$ with respect to Ξ. Introducing the dimensionless width $\zeta := \Xi/a_{\mathrm{ho}}$, we obtain the defining equation

$$\zeta^2 - \zeta^{-2} - P\zeta^{-3} = 0 \tag{4.81}$$

by inserting the resulting Lagrange density into the Euler–Lagrange equation.

The system specific energies (4.66a–b) in terms of ζ read

$$E_{\mathrm{kin}} = \frac{3}{4}\hbar\Omega_{\mathrm{ho}}N\,\zeta^{-2}\,, \qquad E_{\mathrm{ho}} = \frac{3}{4}\hbar\Omega_{\mathrm{ho}}N\,\zeta^2\,, \qquad E_\delta = \frac{1}{2}\hbar\Omega_{\mathrm{ho}}N\,P\zeta^{-3}\,. \tag{4.82}$$

If we multiply equation (4.81) with $\hbar\Omega_{\mathrm{ho}}N$ and compare the result with the energies (4.82) we immediately identify the virial identity (4.62). This means that we have shown that the virial identity even holds in the regime of this specific variational approach. Thus, the defining equation (4.81) for ζ is equivalent to the requirement that the virial identity (4.62) should be valid.

The upper bound for the lowest excitation frequency in terms of ζ reads

$$\frac{\omega_{\mathrm{min}}}{\Omega_{\mathrm{ho}}} \leq \tilde\omega := \sqrt{5 - \zeta^{-4}}\,. \tag{4.83}$$

This upper bound coincides with the breathing-mode frequency which follows from a time-dependent generalization of the above used variational approach [27]. Calculating numerical solutions of equation (4.81) we obtain the breathing mode frequency (4.83) as shown in Figure 4.1.

4.4.2 Dipolar Fermi Gas

Next we investigate a three-dimensional dipolar Fermi gas. The effective dipole–dipole interaction potential is given by equation (4.24). An upper bound for the frequency of the breathing mode is given by (4.77). For the calculation of the kinetic and trapping energy we employ again a variational approach. For a detailed discussion of dipolar Fermi gases and an extensive review of the used variational approach within a Hartree–Fock theory we refer to Ref. [26, 28, 29]. We choose for the semiclassical Wigner function the ansatz of a Fermi–Dirac distribution at zero temperature with the artificial dimensionless variational parameters $R_{x,y,z}$ and $K_{x,y,z}$ which represent the extension of density and momentum distribution in the corresponding directions. As we work with an isotropic trapping potential we have the trap aspect ratio $\lambda = 1$. Nevertheless due to the dipole–dipole interaction the gas tends to be stretched along the polarization direction. Yet, perpendicular to the polarization direction rotational symmetry is conserved and we can, therefore, choose $R_x = R_y$ and $K_x = K_y$. It is convenient to introduce the notation

$$R_x = R_z \kappa, \quad K_z = K_x \delta, \tag{4.84}$$

where now R_x, κ, K_z and δ represent the only remaining variational parameters. Extremizing the corresponding action yields the following system of equations

$$R_z^3 \kappa^2 K_x^3 \delta = 0, \tag{4.85}$$

$$-R_z^2 \kappa^2 + \frac{K_x^2}{3}\left(2 + \delta^2\right) - \frac{\epsilon_{dd} c_d}{R_z^3 \kappa^2}\left[\mathfrak{F}(\kappa) - \kappa\, \mathfrak{F}'(\kappa) - \mathfrak{F}(\delta)\right] = 0, \tag{4.86}$$

$$-R_z^2 + \frac{K_x^2}{3}\left(2 + \delta^2\right) - \frac{\epsilon_{dd} c_d}{R_z^3 \kappa^2}\left[\mathfrak{F}(\kappa) + 2\kappa\, \mathfrak{F}'(\kappa) - \mathfrak{F}(\delta)\right] = 0, \tag{4.87}$$

$$K_x^2\left(\delta^2 - 1\right) = \frac{3\epsilon_{dd} c_d}{R_z^3 \kappa^2}\left[-1 + \frac{2 + \delta^2}{2 - \delta^2}\mathfrak{f}(\delta)\right]. \tag{4.88}$$

The associated energy reads

$$E = E_{kin} + E_{ho} + E_{dd}, \tag{4.89}$$

where

$$E_{kin} = \frac{N E_F}{8} K_z^2\left(2\kappa^2 + 1\right), \quad E_{ho} = \frac{N E_F}{8} K_x^2\left(2 + \delta^2\right), \tag{4.90a}$$

$$E_{dd} = \frac{N E_F \epsilon_{dd} c_d}{4 R_z^3 \kappa^2}\left[\mathfrak{F}(\kappa) - \mathfrak{F}(\delta)\right]. \tag{4.90b}$$

The function $\mathfrak{F}$ denotes the cylinder-symmetric anisotropy function

$$\mathfrak{F}(a) := \frac{3a^2}{1 - a^2}\left(1 - \frac{\operatorname{artanh}\sqrt{1 - a^2}}{\sqrt{1 - a^2}}\right) + 1. \tag{4.91}$$
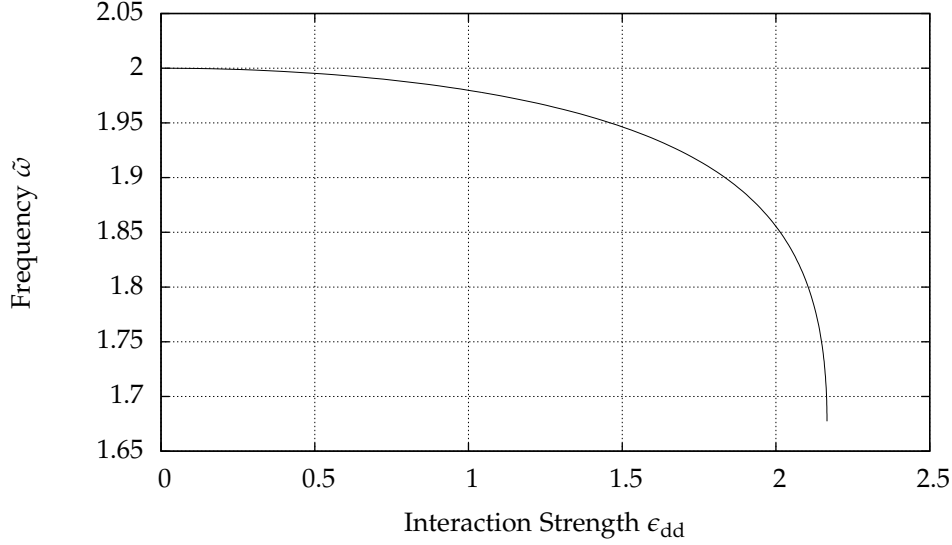
Fig. 4.2: Breathing mode frequency of a dipolar Fermi gas as function of dimensionless interaction strength ϵ_{dd}. The ending of the graph denotes the set in of instability.

We have further defined the dimensionless parameter for the dipole–dipole interaction strength

$$\epsilon_{dd} := D^2 \left(\frac{m^3 \Omega_{ho}}{\hbar^5} \right)^{1/2} N^{1/6} \tag{4.92}$$

and the constant

$$c_d := \frac{2^{38/3}}{3^{23/6} \cdot 35 \cdot \pi^2} . \tag{4.93}$$

The Fermi energy of the non-interacting gas is denoted by E_F and reads

$$E_F = \hbar \Omega_{ho} (6N)^{1/3} . \tag{4.94}$$

Summing up equation (4.87) and two times (4.86) yields

$$- R_z^2 \left(2\kappa^2 + 1 \right) + K_x^2 \left(2 + \delta^2 \right) - \frac{\epsilon_{dd} c_d}{R_z^3 \kappa^2} \left[3\mathfrak{F}(\kappa - 3\mathfrak{F}(\delta) \right] = 0 . \tag{4.95}$$

By multiplying with NE_F we can identify the energies (4.90a–b) and obtain the virial identity (4.62). The upper bound for the breathing-mode frequency (4.77) in terms of K_x, δ, R_z and κ then reads

$$\frac{\omega_{min}}{\Omega_{ho}} \leq \tilde{\omega} := \sqrt{5 - \frac{K_x^2(2 + \delta^2)}{R_z^2(1 + 2\kappa^2)}} . \tag{4.96}$$

Calculating the required parameters numerically, we obtain the results as shown in Figure 4.2. The numerical calculation of the breathing-mode frequency via the equations of motion from the time-dependent variational approach [28, 29] results in practically identical results. We therefore conclude that the sum-rule approach is again equivalent to the time-dependent variational approach in this particular case.

5 Conclusion and Outlook

In this thesis we presented a comprehensive and detailed derivation of the sum-rule approach for collective excitations of ultracold quantum gases and demonstrated its applicability by investigating the breathing mode. We started by looking at the foundations of quantum mechanical linear response theory referred to as Kubo formalism. The main concept of this formalism is that the reaction of the system to a corresponding external perturbation can be described in terms of response functions. One of the advantages of these response functions is that they can be calculated in terms of thermal averages. We discussed some general properties of response functions, thereby we focused on results relevant for further derivations in this thesis. Especially, we derived a method to calculate the energy-weighted moments of the response function's Fourier transform via nested commutators which is referred to in the literature as sum rule.

Furthermore, we investigated time-correlation functions and their relation to response functions. This relation also manifests itself in the derived fluctuation dissipation theorem. Similarly, as for response functions, we discussed some important properties of time-correlation functions and presented sum rules for the calculation of their energy-weighted moments. The obtained results were used to derive strict upper bounds for the lowest excitation energies in the sense of linear response theory. The derived inequalities could be expressed in terms of energy-weighted moments which could be calculated via the derived sum rule. We also discussed in which case the equality is exact. Additionally, we proved ordering relations between correlation functions. Although most of the presented results are mentioned in the present literature, the detailed derivation of equations (2.67), (3.11), and (3.12) as well as the explicit discussions in Section 3.3 were not found to be available.

In Section 4 we explored the properties of the breathing mode in an ultracold quantum gas in an isotropic harmonic trap at zero temperature. We did so by combining the estimates and the sum rules derived before. The application of the sum rules yielded expressions that could be identified as the specific ground-state energies of the system, i.e. the kinetic, the trapping and the interaction energy. These results are rather general as they apply to both bosonic and fermionic gases in any dimension and are valid for any positive homogenous interaction potential, e.g. contact or dipole-dipole interaction. The non-interacting case was also investigated without using the sum rules. By doing so, we showed that the sum-rule approach in that case delivers a result which is exact in the sense of linear response theory.

In order to reduce the effort required for the calculation of the particular ground-state energies, we proved well-known virial identities for systems described by a canonic Hamiltonians, which enabled us to avoid the calculation of one arbitrary energy. We also verified the validity of these virial identities in the Gross–Pitaevskii theory.

Finally, exemplary results for the breathing mode frequency of a delta interacting Bose gas as well as of a dipolar Fermi gas were provided for an isotropic harmonic trap. For the calculation of the particular ground-state energies we used a time-independent variational

ansatz for solving the respective mean-field theories. We verified the validity of virial identities in the regime of this ansatz. A comparison of the breathing mode frequency obtained by the sum-rule approach with the result of the corresponding time-dependent variational approach resulted in a trivial analytical equivalence in the case of the delta interacting Bose gas. For the dipolar Fermi gas the equivalence could only be verified via numerical calculations.

The whole thesis was essentially governed by the linear approximation of the formal solution of the evolution operator (2.19). In general, it is also possible to calculate the system response more accurately by including higher order terms. These terms can be still calculated via equilibrium averages [30]. It is unknown to the author of this thesis whether corresponding sum rules or energy estimates exist for these higher orders.

Furthermore, only the excitation of a breathing mode via a modulation of the trapping frequency [5] was discussed in this thesis. As the use of Feshbach resonance evokes a similar excitation [6, 7], it should be discussed how the sum-rule approach fits into this experimental setup. Especially for choosing the interaction potential $U(\boldsymbol{r}_{ij})$ as the excitation operator, one expects to obtain a similar excitation frequency.

In this thesis we have restricted ourselves to an application of sum rules for quantum gases in an isotropic harmonic trapping potential. In general, it is worthwhile to investigate how an anisotropic trapping potential can enter the sum-rule approach. In particular, it is unclear wether in this case the ratio of two moments can also be expressed in terms of particular energies. However, using a variational approach like in Section 4.4, where the eigenstates of the Hamiltonian are given, the sum-rule commutator averages might be directly evaluable.

It is also of interest to investigate further excitation modes, especially the dipole mode with the excitation operator $D := \sum_{i=1}^{N} z_i$ [17, p. 187]. In the isotropic case the first moment reads $m_D^{(1)} = \hbar^2 N/(2m)$, which is well known as f-sum rule or Thomas–Reich–Kuhn sum rule of atomic physics [31, pp. 110–112]. This result is the basis for various results regarding different types of sum rules [32, pp. 86–98].

A rather general result for the excitation energies in a dipolar Fermi gas was discussed in Ref. [33]. The presented sum-rule expressions equal those derived in this thesis in the case of an isotropic trapping potential. Beside further works on dipolar Fermi gases [34], the sum-rule approach was also used to explore boson-fermion mixed condensates [35] and spin-orbit coupled quantum gases [36]. This illustrates the current relevance of the sum-rule approach in the modern field of ultracold quantum gases.

The limitations of the sum-rule approach are discussed e.g. by Li and Stringari who state that the hydrodynamic frequencies of trapped Fermi gases are significantly overestimated by this method [37]. In fact the ground-state energies of a hydrodynamic dipolar Fermi gas in the stationary case [28, 29] do not differ from those in the collisionless regime [33]. Therefore the sum-rule approach predicts the same upper limits for both regimes. Since we have shown that the sum-rule approach is exact for non-interacting gases we conclude that the frequencies calculated in Section 4.4.2 represent the frequencies of the collisionless regime. But we emphasize again that the results of the sum-rule approach stay correct in the sense, that they provide at least a rigorous upper bound to the excitation frequencies in the linear response theory. Apart from that, it would be interesting to investigate which kind of sum rules might be able to represent excitations frequencies in other than the collisionless regime.

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Declaration

I hereby declare that I wrote this thesis on my own and listed all used sources of information in the references.

Michael Herold, Berlin, July 3, 2012