Density fluctuations in the 1D Bose gas

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Chapter 2

Many-body Physics in 1D

This chapter provides an introduction to the physics of the 1D Bose gas and its correlation functions. We start with a construction of exact wave functions of the gas by means of the Coordinate Bethe Ansatz. This creates a firm basis on which further discussions in this chapter rely. After highlighting a few properties of the wavefunctions of the 1D Bose gas and connecting them with physical phenomena we will jump to the topic of correlation functions. The main focus here, as well as in the rest of the thesis, lies on the density-density correlation function which we discuss throughout the second part of this chapter. We conclude by reviewing different available methods to study correlation functions in the 1D Bose gas and discussing the relation between theoretical studies and experimental realizations.

2.1 1D Bose Gas

Let us start with a simple problem involving two particles of the same mass $m$ moving along a line. We assume the particles interact through a short-ranged repulsive potential and thus whenever they are far from each other their energy is purely kinetic. In order to build a bit of intuition it is instructive to consider the classical case. Then the momentum and energy conservation in 1D yield that the only possible effect of a short-ranged interaction is an exchange of momenta (velocities) (see Fig. 2.1). If we close the line by placing two walls from which particles bounce elastically then they will keep on exchanging momenta every time they collide and beside that nothing more will ever happen. Interestingly even after increasing number of particles $N$ but without reaching too high densities $n = N/L$ the conclusions do not change\(^1\). Although we have more particles all the collisions still lead only to exchange of momenta and that is it. Thus

\(^1\)We assume here that the density is small enough that we can neglect chances of 3-body collisions.
the classical 1D gas is not the most interesting system to devote attention to\textsuperscript{2}. And if there is anything that emerges out of such studies, it is a curiosity to see whether the quantum nature of particles modifies this picture.

In fact, it modifies it drastically. The 1D Bose gas has such rich physics with so many beautiful phenomena that are neatly expressible in the mathematical language that despite 50 years of studies only recently we have started to be able to grasp many of them. It is worth remembering that the complexity that we will encounter during these studies is all due to quantum effects. Therefore studying 1D gases we learn a lot not only about them but also about quantum many-body physics.

\section{2.1.1 Coordinate Bethe Ansatz}

Therefore without further delay let us start immediately with a quantum version of the 1D gas. In order to be more specific let us write down the general Hamiltonian describing a one-dimensional system of massive, bosonic particles with two-body interactions. Usually in the context of cold atoms the interaction is due to spontaneous polarization and results in a short-ranged Van der Waals potential \cite{16}. In the field theory language we write

\begin{equation}
H = \int_0^L dx \partial_x \Psi^\dagger(x) \partial_x \Psi(x) + \int_0^L dxdy V(|x - y|) \Psi^\dagger(x) \Psi^\dagger(y) \Psi(y) \Psi(x),
\end{equation}

with the bosonic fields $\Psi(x)$, $\Psi^\dagger(x)$ obeying the canonical commutation relations ($\{\Psi(x), \Psi^\dagger(y)\} = \delta(x - y)$ and zero otherwise). We also assume the existence of the vacuum state $|\Psi(x)|0\rangle = 0$ and its dual. Moreover we impose periodic boundary conditions: $\Psi(x + L) = \Psi(x)$. As usual we define the particle number and the total momentum

\textsuperscript{2}This rather harsh statement should be understood in the context of correlations: 1D classical gases with short interactions do not exhibit any long-range correlations \cite{19}.
operators as follows

\[ \hat{N} = \int_0^L dx \Psi^\dagger(x)\Psi(x), \quad (2.2a) \]
\[ \hat{P} = -i \int_0^L dx \Psi^\dagger \partial_x \Psi(x). \quad (2.2b) \]

Both operators commute with the Hamiltonian and therefore the particle number and the total momentum are conserved quantities. Conservation of momentum does not depend on the specific form of the interaction potential \( V(x, y) \) as long as the potential is a function of the relative distance only, that is \( V(x, y) = V(|x - y|) \).

In what follows we assume that the range of the potential is extremely short and for all practical purposes at low enough temperatures the potential is proportional to the Dirac \( \delta(x) \) function\(^3\). The strength of interaction depends not only on the intrinsic properties of the atoms but actually can be tuned by various experimental methods (see section 2.4). This in principle allows us to study values of interaction strength extending from minus to plus infinity. For simplicity in this chapter we assume repulsive interactions unless otherwise stated. For a complete discussion of both cases we refer to Chapter 3.

Coming back to the Hamiltonian describing the 1D Bose gas we write

\[ H = \int_0^L dx \left( \partial_x \Psi^\dagger(x)\partial_x \Psi(x) + c\Psi^\dagger(x)\Psi^\dagger(x)\Psi(x)\Psi(x) \right), \quad (2.3) \]

where \( c \) sets the aforementioned interaction strength and is positive for repulsive interactions. This Hamiltonian was first introduced by E. Lieb and W. Liniger [21] as a generalization of the Tonks-Girardeau gas [22] which is a strongly repulsive limit of (2.3). Varying the density \( n = N/L \) of the gas the effective interaction strength changes and thus the correct parameter describing the thermodynamics is \( \gamma = c/n \). This leads to a counter-intuitive conclusion that the particles are more free for larger densities contrary to the 3D gases. The Tonks-Girardeau gas corresponds to \( \gamma \to \infty \).

Employing the conservation of particle number one can recast the Hamiltonian on a fixed particle number subspace. To this end we write a general state as

\[ |\Psi_N\rangle = \int_0^L d^N x \Psi_N (\{x_i\}_{i=1}^N) \prod_{i=1}^N \Psi^\dagger(x_i) |0\rangle, \quad (2.4) \]

\(^3\)This assumption is easily justifiable by noting that the scattering length produced by a \( \delta \)-potential is the same as the scattering length produced by the Van der Waals potential in the low energy limit. Thus this simplification can be viewed as a projection of the original Hamiltonian on a low energy subspace of the Hilbert space. [20]
where $\Psi_N(\{x_i\}_{i=1}^N)$ is an N-particle wave function. Then an action of $H$ on $|\Psi_N\rangle$ is equivalent to an action of the following Hamiltonian

$$H_N = -\sum_{i=1}^N \partial_x^2 + 2c \sum_{i>j} \delta(x_i - x_j),$$

(2.5)
on the wave function $\Psi_N(\{x_i\}_{i=1}^N)$ and thus the eigenvalue problems for $H$ and $H_N$ are equivalent. Amazingly the eigenvalue problem

$$H_N \Psi_N(\{x_i\}_{i=1}^N) = E_N \Psi_N(\{x_i\}_{i=1}^N)$$

(2.6)
can be solved exactly [21].

The main idea, which goes back to Bethe’s solution of the 1D magnet [23], follows from the observation that because interactions are point-like, scattering is already asymptotic for any nonzero separation. Moreover since particles are in 1D they can be labeled with respect to their ordering in $x$. Thus if we restrict ourselves to the domain where $x_1 < x_2 < \cdots < x_N$ then the wavefunction can be guessed using the following reasoning. Let us start with set of N rapidities $\{\lambda_j\}_{j=1}^N$ entering the ansatz function (which is not yet an eigenfunction) formed as a product of plane waves

$$\Psi(x_1 < x_2 < \cdots < x_N) \sim \exp \left( \sum_{j=1}^N \lambda_i x_i \right).$$

(2.7)

The conservation of energy and momentum in 1D implies that after collisions the particles keep or interchange rapidities. Thus after all possible collisions the initial set of rapidities will get permuted among all the particles. Thus refining the ansatz we write

$$\Psi_N(x_1 < x_2 < \cdots < x_N) = \sum_P A(P) \exp \left( i \sum_{j=1}^N \lambda_j x_j \right),$$

(2.8)
where the sum is taken over all permutations of set of $N$ elements. $A(P)$ are functions of permutation and of rapidities $\{\lambda_j\}_{j=1}^N$ but do not depend on spatial variables. The meaning of $A(P)$ is clear, it captures the effect of interactions. Indeed consider two permutations $P$ and $P'$ that differ only by transposition of the first two rapidities. We can write

$$A(P) = S(\lambda_1, \lambda_2) A(P'),$$

(2.9)
where $S(\lambda_1, \lambda_2)$ describes the interaction (scattering) of two particles with rapidities $\lambda_1$ and $\lambda_2$. Since the collisions are elastic $S(\lambda_1, \lambda_2)$ must be a purely phase function.
Moreover translational invariance implies that it must be a function of the rapidity difference only. Therefore we write (the minus signs are for convenience only)

\[ S(\lambda_1, \lambda_2) = -\exp(-i\theta(\lambda_1 - \lambda_2)). \] (2.10)

The function \( \theta(\lambda) \) can be easily found. To do this we only need to consider a two-body problem which can be further simplified by noting that the interaction term in the Hamiltonian (2.5) is equivalent to the following boundary condition on the wave function

\[ \partial_x \frac{\delta(x_1 < x_2)}{|x_1 - x_2|} - \partial_x \frac{\Psi(x_1 < x_2)}{|x_1 - x_2|} = c \Psi(x_1, x_2). \] (2.11)

Thus substituting the two-body wave function of the form (2.8) in eq. (2.11) we find

\[ \theta(\lambda) = 2 \arctan(\lambda/c). \] (2.12)

The function \( \theta(\lambda) \) describes a phase shift caused by interactions. It has two simple limits: for \( c \to 0 \) it equals \( \pi \text{sgn}(\lambda)/2 \) which is consistent with absence of interactions as then \( S(\lambda) = 1 \) and all \( A(P) \)'s are the same. In the other limit, \( c \to \infty \), it also becomes constant but this time equals 0. In this case \( S(\lambda) = -1 \) which causes the wave function to vanish each time \( x_i = x_j, \ i \neq j \).

The factors \( A(P) \) fulfill an interesting relation that in the present context can be viewed as a consistency check. Let us consider two factors \( A(P) \) and \( A(P'') \) that differ by transposition of the first and third element instead of the first and the second (see Fig. 2.2). We can obtain \( A(P'') \) from \( A(P) \) by successive application of eq. (2.9). Consistency requires that two ways in which we can do it yield the same result. This is guaranteed...
once the following relation (Yang-Baxter) is fulfilled

\[ S(\lambda_1 - \lambda_2)S(\lambda_1 - \lambda_3)S(\lambda_2 - \lambda_3) = S(\lambda_2 - \lambda_3)S(\lambda_1 - \lambda_3)S(\lambda_1 - \lambda_2). \]  (2.13)

In the present context, with \( S(\lambda) \) given by eq. (2.10), this is naturally the case.

The factors \( A(P) \) are fully determined once we choose their value for an identity permutation. In the end this choice is physically irrelevant since it is equivalent to multiplying the whole wavefunction by a constant (recall the \( U(1) \) symmetry). Motivated by the simplicity of the final expression, we choose

\[ A(I) = \exp \left( \frac{i}{2} \sum_{i>j} N \theta(\lambda_i - \lambda_j) \right) , \]  (2.14)

from which all the others readily follow

\[ A(P) = (-1)^{[P]} \exp \left( \frac{i}{2} \sum_{i>j} \theta(\lambda_{P_i} - \lambda_{P_j}) \right) . \]  (2.15)

This specifies the wave function in the fundamental domain (eq. (2.8)). Extension of the wave function to the full domain follows simply from symmetrization of the wave function (as is required for bosonic particles) and yields

\[ \Psi \left( \{x_j\}_{j=1}^N \right) = \prod_{j<k} \text{sgn}(x_j - x_k) \]

\[ \times \sum_{P} (-1)^{[P]} \exp \left( \sum_{j=1}^N \lambda_{P_j} x_j + \frac{1}{2} \sum_{i>j} \text{sgn}(x_i - x_j) \theta(\lambda_{P_i} - \lambda_{P_j}) \right) . \]  (2.16)

The eigenvalues of the energy and the total momentum are now easy to calculate

\[ E_N = \sum_{j=1}^N \lambda_j^2 , \]  (2.17a)

\[ P_N = \sum_{j=1}^N \lambda_j , \]  (2.17b)

where we used that the total momentum in the wave function representation reads

\[ \hat{P} = -i \sum_{j=1}^N \partial_x . \]  (2.18)

Finally the periodic boundary conditions imply constraints on the possible values of
rapidities. The equality $\Psi(x_1,\ldots,x_j,\ldots,x_N) = \Psi(x_1,\ldots,x_j+L,\ldots,x_N)$ yields the Bethe equations

$$\lambda_j = \frac{2\pi}{L} I_j - \frac{1}{L} \sum_{k=1}^{N} \theta(\lambda_j - \lambda_k), \quad j = 1,\ldots,N, \quad (2.19)$$

with quantum numbers $I_j$ being integers ($N$ odd) or half-odd integers ($N$ even). In terms of quantum numbers the total momentum of the system is easily expressible

$$P_N = \frac{2\pi}{L} \sum_{j=1}^{N} I_j, \quad (2.20)$$

which follows from the antisymmetry of $\phi(\lambda) = -\phi(-\lambda)$. The energy stays as an implicit function of quantum numbers.

Finally let us comment on the name rapidities instead of momenta as the letter sounds plausible in view of eq. (2.17b). The reason is that although the sum of rapidities is an eigenvalue of the total momentum operator, a single rapidity is not an eigenvalue of a momentum operator of a single particle ($\hat{p}_i = -i\partial_{x_j}$). In fact $\hat{p}_i$ does not even commute with the Hamiltonian (because of the interaction part) and thus the concept of momentum of a single particle does not carry on from the free theories to interacting ones. In order to avoid confusion using the name rapidities instead of momenta seems appropriate.

Empowered now with an exact solution of the Lieb-Liniger model we can discuss some of the physical implications. Leaving the completeness of the discussion for the next chapters (mainly Chapter 3) we focus here just on three aspects: the structure of the ground state and two types of excitations that reign over the low energy sector of 1D Bose gas.

### 2.1.2 Physical Picture

First of all the quantum numbers $\{I_j\}$ obey a Pauli principle since the wave function vanishes identically whenever any two quantum numbers coincide. We will prove this important result in the next chapter. What is important for now is that the Pauli principle significantly restricts the structure of eigenstates and yields that the ground state is formed by a Fermi sea (Fig. 2.3). The following choice of quantum numbers minimizes the energy

$$I_j^{GS} = -\frac{N+1}{2} + j, \quad j = 1,\ldots,N. \quad (2.21)$$
This can be easily seen when one notices that rapidities are strictly monotonic functions of quantum numbers (see the Bethe equations (2.19)) and the energy (2.17a) is quadratic in rapidities. Therefore the ground state is achieved by the most compact, allowed choice of quantum numbers, hence the Fermi sea structure.

Now let us consider low momentum excitations above the ground state (see Fig. 2.3). For simplicity let us start with the $c \to \infty$ case in which the phase shifts $\phi(\lambda)$ vanish and the Bethe equations (2.19) decouple from each other

$$\lambda_j^\infty = \frac{2\pi}{L} I_j, \quad j = 1, \ldots, N. \quad (2.22)$$

Then the energy $\omega$ of a low-momentum $k$ excitation over the ground state is proportional to the momentum: $\omega = v_s k$ with $v_s = v_F$ where $v_F = \pi n/m$ is the Fermi velocity\textsuperscript{4}. In the presence of finite interactions the equality between the sound velocity and the Fermi velocity is broken and in general $0 < v_s < v_F$. The non-zero value of the sound velocity implies that the 1D Bose gas has a liquid like behavior, the low energy excitations are given by sound waves, collective waves of density spreading over the whole system and involving all particles.

Finally there is also a group of very special excitations with finite momentum but with a very small energy (i.e. with the energy vanishing in the thermodynamic limit). These excitations can be created by shifting all the ground state quantum numbers by a constant integer $m$. From the form of the Bethe equations (2.19) it follows that the rapidities with

\textsuperscript{4}It can be defined as a velocity of the fastest particle in the ground state of the spinless free Fermi gas.
shifted quantum numbers are related to the ground state rapidities by $\lambda_j = \lambda_{j}^{GS} + 2\pi m/L$. It is easy to see that it leads to a state with momentum larger by $k = 2\pi mN/L = 2mk_F$ on one hand, on the other hand the energy is larger only by $\omega = k^2/(2Nm)$ and vanishes in the thermodynamic limit. The system thus has low energy excitations also with finite momentum (the umklapp excitations). The appearance of umklapp excitations is a peculiarity of 1D, in higher dimensions there are low-energy excitations with arbitrary momentum, not only $2mk_F$. It is only in 1D, when the Fermi sea is a line, that an excitation from one edge to the other is connected through high energy excitations (see Fig. 2.3).

This structure of the low-lying excitations is not only specific to the 1D Bose gas but is general for the 1D models with gapless (thus linear at small momentum) spectrum. It forms a basis for an effective theory of 1D quantum liquids (Luttinger liquid theory, see Chapter 4).

In the next chapter we extend and supplement the sketched here solution of the 1D Bose gas with an algebraic method.

### 2.2 The Density-density Correlation Function

The main topic of this dissertation is correlations between particles in the 1D gas. Since we assume that there is no external potential acting on the gas we expect particles to homogeneously spread over the length $L$: the density of the gas $n = N/L$ does not depend on the position. Still the gas is a dynamic system and the density is subject to fluctuations. In order to quantify these fluctuations we can ask the following question: What is the correlation between the expectation value of the density operator at position $x_2$ and time $t_2$ and expectation value of the density operator at position $x_1$ and time $t_1$. The answer to this question is given by the density-density correlation functions (thus the function that describes correlations between density fluctuations, also known as dynamical structure factor or DSF). The pursuit to compute this function for the 1D Bose gas in different physical situations occupies most of what follows in this and the next chapters.

#### 2.2.1 Real Space Correlation Function

Let us start by studying some general properties of the correlation functions (We have already introduced one correlation function, the one-body function, in the first Chapter 1, eq. (1.18)). First of all since all the positions are equivalent (the system is homogeneous)
and there is no reference in time the correlation functions are actually functions of the relative distance \( x = x_2 - x_1 \) and elapsed time \( t = t_2 - t_1 \). Thus we define the density-density correlation function as follows

\[
S(x, t) = \langle \hat{\rho}(x, t)\hat{\rho}(0, 0) \rangle,
\]

(2.23)

where \( \hat{\rho}(x, t) = \Psi^\dagger(x, t)\Psi(x, t) \) is the density operator. Since the interaction between particles is short ranged we expect the fluctuations to be uncorrelated for large \( x \) or \( t \): \( S(x, t) \xrightarrow{\ x, t \to \infty} n^2 \). Moreover in the maximally correlated case \( S(x, t) = 2n^2 \) and in the completely anticorrelated case \( S(x, t) = 0 \). The averaging symbol \( \langle \ldots \rangle \) in the definition (2.23) represents expectation value with respect to either some state \( |\Omega\rangle \) of the Hamiltonian \( \langle \ldots \rangle = \langle \Omega | \ldots | \Omega \rangle \) or to an ensemble of states. The most important example of the later is the thermal ensemble following the Gibbs weight (1.1):

\[
\langle \ldots \rangle = \frac{1}{Z} \sum_\Omega e^{-\left(\langle \hat{H}_\Omega \rangle - hN_\Omega / T\right)}/\langle \Omega | \ldots | \Omega \rangle \quad \text{with the partition function } Z \quad \text{(see eq. (1.2))}.
\]

**Equal-time Correlation**

For simplicity let us focus on the equal-time correlation function \( S(x) \equiv S(x, t = 0) \) also known as the pair correlation function. It supplies us with information about the spatial patterns (are lack thereof) in the density fluctuations. For example looking at small \( x \) we can infer whether particles are likely to be spatially separated and how it is influenced by interaction or temperature.

Exactly at \( x = 0 \) this correlation function can be computed by employing the Hellmann-Feynman theorem\(^5\). Indeed we have

\[
S(0) = \langle \Psi^\dagger(0)\Psi^\dagger(0)\Psi(0)\Psi(0) \rangle + \delta(0)\langle \Psi^\dagger(0)\Psi(0) \rangle = \frac{1}{L} \frac{\partial E}{\partial c} + n\delta(0),
\]

(2.24)

where \( E = \langle \hat{H} \rangle \). In general the expectation value of the energy (and its derivative) depends on both the interaction parameter and the temperature. As compared with the large distance limit, the short distance correlation function carries a lot of information about the interplay between quantum correlations (coming from the quantum statistics of the particles), thermal correlations and the effect of the interactions.

For convenience one usually considers the correlation function \( S(x) \) minus the disconnected part \( n\delta(0) \)

\[
g_2(x) \equiv (S(x) - n\delta(0)) / n^2.
\]

(2.25)

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\(^5\)The theorem says that the expectation value of any operator appearing in the Hamiltonian is equal to the derivative of energy with respect to a parameter multiplying this operator (in our case the parameter is \( c \)).
Figure 2.4: Local correlation function at zero temperature computed using eq. (2.24). The energy of the ground state followed from numerical solution to the Bethe equations (2.19) and formula (2.17a). The derivative with respect to the interaction strength was also computed numerically. The dot is an exact result for free bosons.

In Fig. 2.4 we plot $g_2(0)$ at zero temperature. One clearly sees that by changing the value of $c$ the local ($x = 0$) pair correlation function interpolates between uncorrelated value at small $c$ towards completely anti-correlated, fermionic like behavior of the Tonks-Girardeau gas. It is also worth pointing out that exactly at $c = 0$ the free bosons exhibit the bunching phenomenon and $g_2(x) = 2$. This effect vanishes immediately at any finite value of $c$ and signals a quantum phase transition between the $c = 0$ gas with a broken phase symmetry and $c \neq 0$ gas with a fluctuating phase. Increase of this fluctuation ultimately leads to an anti-bunching phenomenon for $c = \infty$.

To get more intuition about the correlation function it is instructive to consider two limiting situations: weakly interacting gas $\gamma < 1$ and strongly interacting gas ($\gamma > 1$). Both cases are solvable by referring to either the Bogolyubov approximation (for weakly interacting gas) or by mapping to free fermions (for the strongly interacting case). Let us start with the former case.

The above-observed discontinuity in $g_2(0)$ at $c = 0$ disqualifies immediately any perturbative expansion at small $c$. However progress can be made by following the Bogolyubov approximation. To this end we write the field operator as a sum of a small momentum ($\sim 0$) component and the rest

$$
\Psi(x) = \frac{1}{L} \Psi_0 + \frac{1}{L} \sum_{k \neq 0} e^{ikx} \Psi_k.
$$

(2.26)
Noting that the Hamiltonian is minimized by maximizing to occupancy of the lowest momentum mode we replace $\Psi_0$ with a c-number $\langle \Psi_0 \rangle \sim L\sqrt{n}$. This allows for diagonalization of the Hamiltonian and computation of the correlation functions. The computation itself is shown in the Appendix C, here we show only the final results. Before that however let us consider the opposite limit.

When $c \to \infty$ the Bethe wavefunctions (2.19) start to resemble the wave functions of a fermionic system. Indeed up to a symmetrization factor the wave function can be written as a Slater determinant

$$
\Psi_c=\infty (x_1, \ldots, x_N) = \prod_{j<k} \text{sgn}(x_j - x_k) \det_N \exp \left( \frac{2\pi i}{L} L_j x_k \right).
$$

Now since the density operator does not depend on the statistic of the particles its expectation values will be the same for a fermionic and bosonic system. Therefore the symmetrization factor does not play any role and the density-density correlation function of the 1D Bose gas at $c = \infty$ is identical to the density-density correlation function of free fermions. This allows for a straightforward computation of the correlation function which again is performed in the Appendix C.

Fig. 2.5 shows the density-density correlation function of weakly and strongly interacting 1D Bose gases. The small $x$ values agree with the earlier calculations based on the Hellmann-Feynman theorem. Beyond that we see now also the full $x$ dependence together with the large $x$ limit. Interestingly the strong repulsive interaction leads to the formation of a quasi-crystal. The oscillation in $S(x)$ signals the existence of more and less likely
distances between particles. No symmetry breaking occurs but the density fluctuates much more than in the weakly interacting case. Thus the $c \to \infty$ limit is dominated by the density fluctuations whereas the $c \to 0$ limit is dominated by phase fluctuations (sometimes the weakly interacting gas is called a quasi-condensate exactly because the phase still fluctuates so there is no complete condensation). As we should see later in the metastable super Tonks-Girardeau gas the density fluctuations are even stronger.

Now let us move to the momentum space and see what kind of information about the 1D Bose gas we can extract from studying the Fourier transform of $S(x,t)$. This will provide us with a different point of view on the nature of correlations and also allow for deriving a few important relations.

### 2.2.2 Momentum Space

Let us get back to the full distance and time dependent correlation function. Imagine that for some specific values of $x$ and $t$ the correlation function varies significantly from the uncorrelated value. This means that a fluctuation in density is likely to travel a distance $x$ within a time $t$. Therefore we can think about the density fluctuation as a density wave with a wave vector (or momentum) $k$ and a frequency (or energy) $\omega$. Transformation of the correlation function from real space (thus function of $x$ and $t$) to momentum space is simply given by the Fourier transform. Thus we define

$$S(k, \omega) = \int_0^L dx \int_{-\infty}^{\infty} dt \ e^{i(kx - \omega t)} S(x,t), \quad (2.28)$$

where $k = 2\pi m/L$ with $m \in \mathbb{Z}$.

The $S(k, \omega)$ function fulfills a simple sum rule

$$\frac{1}{L} \sum_k \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S(k, \omega) = n^2, \quad (2.29)$$

which follows from $S(x = 0, t = 0) = n^2$. Moreover for parity-invariant systems $S(k, \omega) = S(-k, \omega)$.

A very practical representation of the correlation function in momentum space can be obtained by explicitly carrying out the Fourier transform in (2.28). To this end it is useful to note that since the total momentum operator commutes with the Hamiltonian we have an equality

$$\hat{\rho}(x,t) = e^{i(Ht - \hat{p}x)}\hat{\rho}(0)e^{-i(Ht - \hat{p}x)}. \quad (2.30)$$
Inserting now a resolution of the identity \( \hat{1} = \sum_\lambda |\lambda\rangle \langle \lambda| \) between the density operators in (2.23) we obtain (when averaging is performed with respect to a given eigenstate \( |\Omega\rangle \in \mathcal{H}_N \))

\[
S(x,t) = \sum_{\lambda \in \mathcal{H}_N} e^{i(E_\lambda - E_\Omega)t - (P_\lambda - P_\Omega)x} |\langle \lambda|\hat{\rho}_0(x=0)|\lambda\rangle|^2, \tag{2.31}
\]

where in the last step we used also that the density operator is hermitian. The Fourier transform is easily performed and we obtain

\[
S_\Omega(k,\omega) = \frac{2\pi}{L} \sum_{\lambda \in \mathcal{H}_N} |\langle \lambda|\hat{\rho}_k|\lambda\rangle|^2 \delta (\omega - (E_\lambda - E_\Omega)) \delta_{k, P_\lambda - P_\Omega}. \tag{2.32}
\]

This is the Lehmann representation of the correlation function. In what follows it is convenient to have an expression in terms of the matrix elements of the Fourier transformed density operator. Explicitly inserting the Fourier transform of \( \hat{\rho}(0) = L^{-1} \sum_k \hat{\rho}_k \) we obtain\(^6\)

\[
S_\Omega(k,\omega) = \frac{2\pi}{L} \sum_{\lambda \in \mathcal{H}_N} |\langle \lambda|\hat{\rho}_k|\lambda\rangle|^2 \delta (\omega - (E_\lambda - E_\Omega)). \tag{2.33}
\]

For a thermal correlation function we also need to perform the Gibbs trace with respect to \( |\Omega\rangle \)

\[
S_T(k,\omega) = \frac{2\pi}{LZ} \sum_{\Omega,\lambda \in \mathcal{H}_N} e^{-(E_\Omega - hN\Omega)/T} |\langle \Omega|\hat{\rho}_k|\lambda\rangle|^2 \delta (\omega - (E_\lambda - E_\Omega)), \tag{2.34}
\]

where \( Z \) is the partition function.

The Lehmann representation is useful for a number of reasons. First of all it gives us a nice interpretation of the correlation functions\(^7\). The value of \( S(k,\omega) \) can be easily connected with the probability of creating an excitation in the gas with given \( k \) and \( \omega \) following the Fermi golden rule logic\(^8\).

The Lehmann representation also allows to establish two important equalities fulfilled by the density correlation function: detailed balance and the f-sum rule.

\[^6\]\text{The Kronecker delta} \( \delta_{k, P_\lambda - P_\Omega} \) is absorbed by the form factor of \( \rho_k \) which vanishes for \( k \neq P_\lambda - P_\Omega \).

\[^7\]\text{The Lehmann representation does not depend on the specific choice of the operator (in this case the density operator) and therefore it easily generalizes to any operator which fluctuations one would like to study.}

\[^8\]We remind that according to the Fermi golden rule the probability of excitation from a state \( |A\rangle \) to a state \( |B\rangle \) due to a given perturbation \( \hat{V} \) is proportional to \( \sim |\langle A|\hat{V}|B\rangle|^2 \).
Detailed Balance

Exchanging the meaning of $|\lambda\rangle$ and $|\Omega\rangle$ in the summand of eq. (2.34) and using that, due to the presence of the Dirac delta, $E_\Omega = E_\lambda + \omega$ we obtain an important equality: the detailed balance condition

$$S_T(k, \omega) = e^{-\omega/T} S_T(-k, -\omega) = e^{-\omega/T} S_T(k, -\omega),$$  \hspace{1cm} (2.35)

where the second equality holds for the parity-invariant gas. This relation has a simple interpretation, the negative energy part of the correlation is a dimmed picture of the positive part. The “dimming” factor $e^{-\omega/T}$ depends on both the temperature and the energy. At infinite temperature the correlation function is symmetric around $\omega = 0$ and at any finite temperature becomes exponentially skewed towards positive energies. The region in $\omega$ of the negative part of the correlation shrinks rapidly as the temperature is decreased and at zero temperature the correlation with negative energy is exactly equal to zero. The effect of finite temperatures is visible only for $\omega < T$. For higher $\omega$ the correlation is almost identical to the zero-temperature case. We will get back to this observation and to the detailed balance in Chapter 5 where we consider finite temperature correlation functions.

The f-sum Rule

There is one more relation that is fulfilled by the density-density correlation: the f-sum rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega S_{\Omega}(k, \omega) = nk^2.$$  \hspace{1cm} (2.36)

Starting from the left hand side and performing the integral we obtain

$$I(k) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega S_{\Omega}(k, \omega) = \frac{1}{L} \sum_{\lambda \in H_N} (E_\Omega - E_\lambda) |\langle \lambda | \hat{\rho}_k | \Omega \rangle|^2$$

$$= -\frac{1}{2L} \langle \Omega | [H, \hat{\rho}_{-k}] \hat{\rho}_k - \hat{\rho}_{-k} [H, \hat{\rho}_k] | \Omega \rangle.$$  \hspace{1cm} (2.37)

The expression on the right hand side can be written in terms of double commutators: from $S(k, \omega) = S(-k, -\omega)$ it follows that $I(k) = I(-k)$, thus

$$I(k) = -\frac{1}{4L} \langle \Omega | [[H, \hat{\rho}_{-k}], \hat{\rho}_k] + [[H, \hat{\rho}_k], \hat{\rho}_{-k}] | \Omega \rangle.$$  \hspace{1cm} (2.38)

Since the double commutators are hermitially conjugated it is enough to consider one of them. To this end we write the Hamiltonian and the density operator in momentum
space as

\[ H = \frac{1}{L} \sum_k k^2 \Psi_k^\dagger \Psi_k + \frac{c}{L^3} \sum_{k_1,k_2,q} \Psi_{k_1+q}^\dagger \Psi_{k_2-q}^\dagger \Psi_{k_1} \Psi_{k_2}, \] (2.39a)

\[ \hat{\rho}_k = \frac{1}{L} \sum_q \Psi_{k+q}^\dagger \Psi_k. \] (2.39b)

which follows from the Fourier transform of eq. (2.3) and definition of the density operator \( \hat{\rho}(x) = \Psi^\dagger(x) \Psi(x) \) (see also Appendix A). Evaluation of the commutators simplifies upon noting that the density operator commutes with the interaction part of the Hamiltonian and the kinetic part yields simply

\[ [H, \hat{\rho}_{-k}] = \frac{1}{L} \sum_q (k^2 - 2kq) \Psi_{-k+q}^\dagger \Psi_q. \] (2.40)

The double commutator gives then

\[ [[H, \hat{\rho}_{-k}], \hat{\rho}_k] = -2k^2 \frac{1}{L} \sum_q \Psi_q^\dagger \Psi_q, \] (2.41)

which proves the f-sum rule relation. The f-sum rule states that the average energy of the fluctuations with momentum \( k \) is always the same irrespective of interaction strength (the r.h.s does not depend on \( c \)) and equal to \( k^2 \) just as if it were carried by a single particle. This shows that the only effect of interactions is to change the energy dependence of \( S(k,\omega) \) while keeping the average energy constant. In fact as we will see later this dependence can be modified drastically and one of the purposes of the work presented in this thesis is to give quantitative predictions for \( S(k,\omega) \) in various circumstances.

**The Static Correlation Function**

As for the real space correlator it is also useful to consider correlation functions reduced to one variable. This is achieved by integrating out either \( \omega \) or \( k \) and yields a static correlator (static structure factor) or an autocorrelator

\[ S(k) = \int_{-\infty}^\infty \frac{d\omega}{2\pi} S(k,\omega), \] (2.42)

\[ S(\omega) = \frac{1}{L} \sum_k S(k,\omega). \] (2.43)

This is then consistent with the Fourier transform of static correlator \( S(k) \) which equals the pair correlation function \( S(x) \).
As discussed before, the excitations in the 1D Bose gas are gapless and thus at low momentum they are like sound waves with the sound velocity \( v_s \) that depends on the interaction and temperature. At zero temperature, the gas occupies the lowest energy state and thus only excitations with positive energy are possible. In this case we can write that

\[
S(k, \omega) = A_k \delta(\omega - v_s k),
\]

where \( A_k \) is an unknown function of momentum. This function can be uniquely fixed using the \( f \)-sum rule (2.36), we obtain

\[
S(k) = \frac{|k|}{v_s} + \mathcal{O}(k^2), \quad T = 0.
\]

Thus at zero temperature the static correlator vanishes linearly with \( k \). The proportionality constant is the inverse sound velocity.

The opposite limit of the static structure factor is when \( k \to \infty \). In this case the correlation function becomes independent of temperature and interaction strength and approaches the universal value 1. This can be easily understood. First from the physical point of view very large momentum means that we are looking at the ultra local (in real space) correlation, and this in turn can depend only on a single particle property \(^9\). Thus the static correlator should be equal to this of free bosons (or free fermions) which indeed is equal to 1. Mathematically speaking at large momentum, the Fourier transform of \( S(x) \) (that is \( S(k) \)) depends only on the discontinuity of \( S(x) \) at \( x = 0 \) (see eq. 2.24) what yields 1 for \( S(k \to \infty) \).

Fig. 2.6 summarizes the prediction on the limits of the static structure factor together with the results of Bogolyubov approximation and the Tonks-Girardeau gas (see Appendix B). Similar analysis could be performed for the autocorrelation function however we save it for discussions in further chapters.

### 2.3 How to Compute Correlation Functions

In the previous chapter we have introduced correlation functions, discussed their certain, universal limits, and what is most important showed how understanding of correlation functions enriches our understanding of physical systems. Despite invoking calculations in certain limits when the theory becomes essentially free (the Tonks-Girardeau limit and Bogolyubov approximation) the question how to compute the full dynamical correlation

\(^9\)For short-range interactions and not to large densities there is a region around every particle where it is effectively a free particle.
functions remains open. In this section we would like to address this problem by briefly surveying the most suitable methods that one has at hand.

The available methods can be divided roughly in two groups: the numerical methods or analytic methods. We will start with the first group.

The 1D Bose gas being a continuum model restricts the accessible numerical methods to various types of Monte Carlo algorithms. The other methods relying on a finite basis of the Hamiltonian like Density Matrix Renormalization Group [24, 25] or Stochastic Series Expansion [26] or even straightforward diagonalization are not available since the Hilbert space of a continuum model is strictly infinite dimensional. A method that was successfully used in studies of 1D Bose gas and its variants (such as with an external potential or crossover between 3D and 1D) is the Diffusive Monte Carlo method [27, 28]. Unfortunately the natural limitation of the method is to static properties of the system such as equal-time correlation functions [29, 30]. Similar limitations are also present in the second method that we would like to mention here, the Stochastic P-gauge which was used to compute $g_2(x)$ in the almost full $\gamma - T$ phase space [31].

The second group of methods relies on having some form of an analytic solution of the theory. The full $S(k,\omega)$ function was studied by perturbative expansion around the Tonks-Girardeau limit [32, 33]. The spatial correlation function $g_2(x)$ was studied at various interaction strengths at zero and at finite temperatures by employing either perturbative methods or Bogolyubov approximation [31]. The more complete treatment of the correlation functions but limited only to large-distance and long-time asymptotes
is given by the Luttinger liquid theory. We will briefly summarize the idea behind
this theory and discuss it recent developments that allow to gain insights also in the
momentum dependent correlations in a separate chapter (see Chapter 4). The most
successful attempt in computation of correlation functions starting from the exact $N$–
body Hamiltonian of the 1D Bose gas is presented in the work of Lyon group [34–37].
This method, that relies on the Algebraic Bethe Ansatz (see the next chapter), allows for
capturing the large-distances long-times asymptotes of correlation function and proved
to be consistent with the Luttinger liquid predictions.

2.3.1 The ABACUS

Finally we would like to use the last paragraph briefly describe an alternative approach.
This approach was already used in the past [38, 39] and this thesis documents small
further developments in the same direction. The main idea is as follows. The Lehmann
representation of the correlation function (2.33) that for convenience is repeated here

\[ S(k, \omega) = \frac{2\pi}{L} \sum_{\lambda \in \mathcal{H}_N} |\langle \lambda | \hat{\rho}_k | \Omega \rangle|^2 \delta (\omega - (E_\lambda - E_\Omega)) \]  (2.46)

gives in fact a simple prescription. All that we need to compute a correlation function
is to: (1) Be able to span the Hilbert space, that is enumerate (in some consistent way)
all the eigenstates. (2) Compute their energy. (3) Compute the matrix elements. (4)
Perform summation. This simple prescription relies on two pillars. First computation
of matrix elements of an interesting operator (like density) in an interacting theory is a
challenge on its own. Fortunately for the 1D Bose gas these matrix elements are known
exactly thanks to the Algebraic Bethe Ansatz. The second pillar is the complexity of
the summation problem. The number of states that needs to be considered in order to
achieve good results (the quality of results can be assured by the f-sum rule, for example)
should not be exponentially large in the system size. Fortunately the number of states
contributing significantly to the summation is only polynomial in system size and thus
is relatively small. This makes the method feasible. We will not go here into details of
how the algorithm in fact works and for more information we refer to [40].

2.4 How to Measure Correlation Functions

Finally we would like to conclude this chapter by addressing the experimental relevance
of correlation functions. In this last section we will briefly show how the correlation
functions explicitly enter measurable quantities and we will show also two experimental
configurations that are widely used nowadays to prepare and perform experiments with cold atomic gases and specifically with the 1D Bose gas.

The most straightforward way to measure the density-density correlation function is Bragg spectroscopy \[41, 42\]. In this setup two lasers beams are used to create a time dependent potential

\[
V_{\text{Bragg}} = V_0 \int_0^L dx \cos (kx - \omega t) \hat{\rho}(x,t),
\]  

(2.47)

where \(V_0\) is the intensity of laser beams, \(k\) is the momentum reflecting the geometry of the setup and \(\omega\) is a result of a slight detuning of the beams. The perturbation caused by \(V_{\text{Bragg}}\) couples to the density of atoms and transfers energy and momentum into the system. Within the logic of linear response theory the transferred momentum and energy are directly related to the density-density correlation function and are given by \[41\]

\[
\frac{dP}{dt} = L \left( \frac{V_0}{2} \right)^2 k (S_T(k,\omega) - S_T(k,-\omega)),
\]  

(2.48a)

\[
\frac{dE}{dt} = L \left( \frac{V_0}{2} \right)^2 \omega (S_T(k,\omega) - S_T(k,-\omega)).
\]  

(2.48b)

In principle eq. (2.48) supply us with a direct relation between the density-density correlation function and measurable quantities like change in the momentum or the energy of the gas.

What is left is a problem of creating a 1D gas. There are two popular setups: using an atomic chip, or using a highly anisotropic optical lattice. Let us start with the former.

In an atom chips experiments one uses a pre-manufactured chip with nano wires engraved on its surface. The geometry of the wires together with a control over currents allows for the creation of a magnetic field that acts as a trap for atoms. Leaving out the experimental details this allows for trapping atoms in the effective 1D geometry like a single tube. Unfortunately trapping is realized through magnetic field and thus one cannot use a Feshbach resonance to control the interaction strength. This means that the atom chip experiments are limited to weakly interacting 1D Bose gas \[43, 44\].

The second popular approach is to use optical lattices. Using a configuration of 6 lasers one creates standing waves that trap atoms at the minima

\[
V_{\text{opt}}(x, y, z) = \sum_{i=x,y,z} V_i \sin^2 (q_i x_i).
\]  

(2.49)

By choosing highly anisotropic \(V_i\), for example \(V_z \ll V_x, V_y\), the trap becomes elongated in one direction and narrow in the other two. This results in an array of 1D tubes. Usually
the experimental procedure populates many of these tubes and results of measurements are an average over the whole array. Therefore the signal is not as clear as in atom chip trap experiments especially because different tubes contain different number of atoms. Thus the densities $n$, and as a result also the interaction strength $\gamma$, vary among the tubes and smear the contribution from a single tube at a single value of $\gamma$. The advantage of optical lattices however is that they allow to use the Feshbach or confinement induced resonances. Moreover the optical setting allows for flexible tuning of radial confinement which also influence the interaction strength [20]. Altogether the effective tuning of interactions allows to reach even the Tonks-Girardeau limit [45–47].