Chapter 7

Long-range order

Learning goals

- What is long-range order?
- What is the order parameter of the BEC phase transition?
- How is the reduced one-particle density matrix changing when the system undergoes a phase transition to a Bose-Einstein condensate?
- What is the difference between the coherence and the correlation length?
- What is the critical region?

We will apply the formalism of second quantization to describe the spatial coherence of an atomic cloud, captured in the reduced single-particle density matrix. In the case of a BEC, the system will show off-diagonal long-range order, where remote parts of the same sample show correlated behavior. The existence of off-diagonal long-range order can hence be used as a condition for BEC. The chapter ends with a general discussion of second order phase transitions. We follow here Pitaevskii/Stringari: BEC, and Pethick/Smith: BEC in dilute gases.

7.1 Reduced one-body density-matrix

The many-body correlations in a system can be very complicated. However, for the estimation of most experimentally relevant properties, knowledge of the reduced one-body density matrix $\rho(\mathbf{r}, \mathbf{r}')$ is already sufficient. It can be expressed with the particle creation and annihilation operators $\hat{\Psi}^{\dagger}(\mathbf{r})$ and $\hat{\Psi}(\mathbf{r})$ as

$$\rho(\mathbf{r},\mathbf{r}') = \langle \hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r}')\rangle.$$
(7.1)

For a pure state, the average $\langle \cdot \rangle$ is the quantum mechanical expectation,

$$\rho(\mathbf{r},\mathbf{r}') = N \int \mathrm{d}\mathbf{r}_2 \mathrm{d}\mathbf{r}_3 \dots \mathrm{d}\mathbf{r}_N \Psi^*(\mathbf{r},\mathbf{r}_2,\mathbf{r}_3,\dots\mathbf{r}_N) \Psi(\mathbf{r}',\mathbf{r}_2,\mathbf{r}_3,\dots\mathbf{r}_N) \,. \tag{7.2}$$

Here we integrated over all except of one degree of freedom of the N-body wave function and significantly reduced the complexity of the problem. For a system in a statistical mixture, the average is an ensemble average taking into account the probability to occupy a certain state.

The reduced one-particle density matrix expresses the probability amplitude to annihilate a particle at location \mathbf{r}' and to create one at location \mathbf{r} . For $\mathbf{r} = \mathbf{r}'$, this describes the local density of the system,

$$n(\mathbf{r}) = \rho(\mathbf{r}, \mathbf{r}) = \langle \hat{\Psi}^{\dagger}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \rangle.$$
(7.3)

From this we see that the one-body density matrix is normalized, such that the total number of particles is $\int d\mathbf{r} \rho(\mathbf{r}, \mathbf{r}) = N$. The density matrix also describes the momentum distribution of

the system

$$n(\mathbf{p}) = \langle \hat{\Psi}^{\dagger}(\mathbf{p}) \hat{\Psi}(\mathbf{p}) \rangle, \qquad (7.4)$$

with the Fourier transform $\hat{\Psi}(\mathbf{p}) = (2\pi\hbar)^{-3/2} \int d\mathbf{r} e^{-i\mathbf{p}\mathbf{r}/\hbar} \hat{\Psi}(\mathbf{r})$. We now consider a homogeneous



Figure 7.1: **One-particle density matrix.** A particle with initial momentum \mathbf{p} is incident on a slab of atomic medium with thickness L. The transmitted wavefunction will acquire a phase shift due to the effective index of refraction.

gas¹ with N particles contained in a volume V and take the thermodynamic limit $N, V \to \infty$ with $n = \frac{N}{V} = \text{const.}$ Under this assumption the system will be translation invariant and the reduced one-body density matrix will only depend on the modulus s of the separation of the two points in space considered, $\rho(\mathbf{r}, \mathbf{r}') = \rho(|\mathbf{r} - \mathbf{r}'|) = \rho(s)$. Bose-Einstein condensation is a phenomenon taking place in momentum space, so it is useful to express the reduced one-body density matrix with help of the momentum distribution:

$$\rho(s) = \frac{1}{V} \int \mathrm{d}\mathbf{p} e^{-i\mathbf{p}\mathbf{s}/\hbar} n(\mathbf{p}) \,. \tag{7.5}$$

A system with $T > T_c$ will have a smooth momentum distribution, and the different contributions to $\rho(s)$ will average out for large s, such that $\lim_{s\to\infty} \rho(s) = 0$. The one-body density matrix will decay to zero over a distance given by the thermal de Broglie length $\lambda_{\rm th}$. The momentum distribution for a BEC however is very different since it exhibits a singular behavior at $\mathbf{p} = 0$,

$$n(\mathbf{p}) = N_0 \delta(\mathbf{p}) + \tilde{n}(\mathbf{p}) \,. \tag{7.6}$$

The corresponding reduced one-body density matrix will thus show a finite value also for very large separations s,

$$\lim_{s \to \infty} \rho(s) = n_0 = \frac{N_0}{V} \,. \tag{7.7}$$

The one-body density matrix for the case of a BEC is decaying over a distance typically given by the thermal de Broglie length to a finite value which is set by the condensate fraction of the gas. The system is then said to show off-diagonal long-range order (ODRLO), i.e. finite values in $\rho(\mathbf{r}, \mathbf{r}')$ for $\mathbf{r} \neq \mathbf{r}'$. This is directly related to the macroscopic occupation of a single-particle state. The criterion for BEC of a macroscopic occupation given by Penrose and Onsager is thus equivalent to the existence of ODLRO.

¹however, this concept holds equally for trapped systems, as described in detail in M. Naraschewski and R. Glauber, *Spatial coherence and density correlations of trapped Bose gases*. Physical Review A, 59(6), 4595 (1999)

A non-interacting Bose gas at T = 0 in which all N particles occupy the single particle wave function $|\phi\rangle$ can be described by the many-body wave function $\psi(\mathbf{r}) = \sqrt{N} \langle \mathbf{r} | \phi \rangle$, and will have a constant one-body density matrix for all separations s. If interactions are present, even at T = 0 not all particles will be in the ground state but the system will show quantum depletion, and the one-body density matrix decays to the constant value n_0 .

First order correlation function. The reduced one-body density matrix is closely related to the concept of correlation functions. It is indeed given by the first order correlation function $G^{(1)}(\mathbf{r}, \mathbf{r}')$,

$$G^{(1)}(\mathbf{r}, \mathbf{r}') = \rho(\mathbf{r}, \mathbf{r}').$$
(7.8)

The first order correlation function is often used in its normalized form $g^{(1)}(\mathbf{r}, \mathbf{r}')$,

$$g^{(1)}(\mathbf{r}, \mathbf{r}') = \frac{G^{(1)}(\mathbf{r}, \mathbf{r}')}{\sqrt{G^{(1)}(\mathbf{r}, \mathbf{r})}\sqrt{G^{(1)}(\mathbf{r}', \mathbf{r}')}},$$
(7.9)

such that perfect correlations correspond $g^{(1)}(\mathbf{r}, \mathbf{r}') = 1$.

Coherence length vs. correlation length. It is important to distinguish between the correlation length and the coherence length. The coherence length is referring to the length scale in the gas over which the system shows a certain degree of coherence. For a thermal gas, this length scale is given by the thermal de Broglie wavelength $\lambda_{\rm th}$. It diverges to the system size at the phase transition to BEC, where global coherence throughout the system is built up. In contrast, the correlation length describes the length scale in the system over which fluctuations are correlated. In a thermal gas, this length scale is identical to the coherence length and given by $\lambda_{\rm th}$. Again, this length scale is diverging towards the critical point of the phase transition. However, once the phase transition has taken place and coherence is built up in the system, the correlation length will decay again.

7.2 Order parameter and wave function of the condensate

Applying the definition of the field operator $\hat{\Psi}(\mathbf{r})$ to the situation of a BEC, where the state $\phi_0(\mathbf{r})$ is macroscopically populated, one can write

$$\hat{\Psi}(\mathbf{r}) = \sum_{i} \phi_i(\mathbf{r})\hat{a}_i = \phi_0(\mathbf{r})\hat{a}_0 + \sum_{i\neq 0} \phi_i(\mathbf{r})\hat{a}_i.$$
(7.10)

We here separated the contribution of the BEC (first term) from the non-condensed part (second term). At this point, we make use the Bogoliubov approximation, which we introduced formally previously. It boils down to replacing the operators \hat{a}_0 and \hat{a}_0^{\dagger} by the value $\sqrt{N_0}$. This ignores the non-commutativity of these operators, but the introduced errors are on the order of $1/N_0$ and thus small. With help of this step, we can write

$$\tilde{\Psi}(\mathbf{r}) = \psi(\mathbf{r}) + \delta \tilde{\Psi}(\mathbf{r}), \qquad (7.11)$$

where we defined $\psi(\mathbf{r}) = \sqrt{N_0}\phi_0(\mathbf{r})$ and $\delta\hat{\Psi}(\mathbf{r}) = \sum_{i\neq 0}\phi_i(\mathbf{r})\hat{a}_i$. For a pure BEC, this corresponds to $\hat{\Psi}(\mathbf{r}) = \psi(\mathbf{r})$, such that the field operator is described by a wave function and thus can be regarded as classical object. This wave function $\psi(\mathbf{r})$ is generally a complex function which can be written as

$$\psi(\mathbf{r}) = |\psi(\mathbf{r})|e^{i\varphi(\mathbf{r})}.$$
(7.12)

The modulus of $\psi(\mathbf{r})$ is describing the density (diagonal density) of the gas, while the phase is characterizing the coherence (off-diagonal density) of the gas.

The function $\psi_0(\mathbf{r})$ is the order parameter of the normal-to-superfluid phase transition. It is zero in the normal phase $(T > T_c)$, and takes a finite value for the condensed phase $(T < T_c)$. It is defined only up to an arbitrary, fixed phase constant, as the wavefunction can be multiplied with a factor $e^{i\alpha}$ without changing a physical property of the system. An explicit choice for the phase will break the given continuous symmetry, which is a feature of this second order phase transition.

7.3 Phase transitions and critical behavior

7.3.1 Order Parameter

A system undergoing a continuous phase transition from the high-temperature side to the lowtemperature side will reduce its symmetry. For example, a ferromagnet below its critical temperature shows spontaneous magnetization into a certain direction, thereby destroying rotational invariance. Because of this reduction in symmetry, an extra parameter is needed for the description of the thermodynamics below T_c , and one introduces the order parameter Φ . The order parameter is a certain thermodynamic quantity of a system; its thermal average vanishes on one side of the phase transition, and has a non-zero value on the other side. It is a quantity which can fluctuate both in space and in time, so we can write $\Phi(\mathbf{r}, t)$.

In the above example of the ferromagnet one chooses the magnetization vector \mathbf{M} as an order parameter, whereas for a Bose-Einstein condensate the wave function $\psi(\mathbf{r})$ is the order parameter. The choice of the order parameter is not at all obvious, but has to be made afresh for every new system. The *n*-dimensional order parameter can be a scalar (like the density for the liquid gas transition), a vector as in the above examples or a tensor. The higher the dimensionality of the order parameter is, the more complex the phase diagram will be.

7.3.2 Critical Exponents

Although no latent heat is involved in second order phase transitions, this does not mean that the heat capacity is a smooth function of temperature. In fact it shows in many cases a divergence according to $\sim \left|\frac{T-T_c}{T_c}\right|^{-\alpha}$, where α is a so-called critical exponent. This kind of non-analytic dependence is a crucial property of continuous phase transitions. It is not limited to the behavior of the specific heat, but there are many other quantities which show a singular behavior around the critical temperature, like the susceptibility, the compressibility, the equation of states, the order parameter itself or the correlation length. Each of these properties shows a divergence at the critical temperature of the form

$$\sim \left| \frac{T - T_c}{T_c} \right|^{-c} \,. \tag{7.13}$$

The critical exponents c are typically labeled by Greek letters (α for heat capacity, β for order parameter, γ for compressibility, δ for equation of states ...). For a convenient description of these phenomena we introduce the reduced temperature

$$t = \frac{T - T_c}{T_c} = \frac{T}{T_c} - 1.$$
(7.14)

The above definition (Equation 7.13) refers only to the singular part of the interesting quantity, which is symbolized with "~". It can happen, that a critical exponent is zero, so there is no singularity. For example, $\alpha = 0$ tells us that there is no singularity in the heat capacity, which nevertheless can have a finite discontinuity at t = 0.

The first order correlation function behaves for large r in the proximity of the critical temperature like

$$g^{(1)}(r) \to \frac{e^{-r/\xi}}{r^p}$$
. (7.15)

Here we introduced the correlation length ξ , which is the typical length scale over which the fluctuations of the order parameter are correlated. The exponent $p = d-2+\eta$ in the denominator depends on the dimensionality d of the system and on the critical exponent η . The correlation length ξ diverges, when T approaches T_c according to

$$\xi \sim |t|^{-\nu} \,, \tag{7.16}$$

where ν is the critical exponent for the correlation length. Combining (7.15) and (7.16) it becomes clear that right at the critical temperature $\xi \to \infty$ and the nominator in (7.15) becomes unity. The first order correlation function $g^{(1)}(r)$ will thus show for large r a power-law decay at $T = T_c$,

$$g^{(1)}(r) \to \frac{1}{r^p}$$
. (7.17)

It is worth noting why critical exponents have proven to be very helpful in the description of phase transitions. It would of course be preferable to obtain a complete functional form for the behavior of a quantity as the specific heat or the correlation length, instead of only a number describing the singular part. However, near the critical point, the singular part is the dominating one.

Another, more important, reason for focusing on critical exponents is that they are universal, which means that they are not only valid for a specific system, but for a whole set of physical systems that can be grouped in universality classes. In addition, the critical exponents are not independent from each other, but there exists a number of scaling relations between them, arising from statistical and thermodynamical considerations.

7.3.3 Landau and Landau-Ginzburg theory

Landau Theory

Landau theory can be understood as a unification of earlier mean-field theories such as the van der Waals theory or Weiss' molecular field theory. It is a phenomenological approach, avoiding the underlying microscopic structure and dealing only with macroscopic quantities. Landau theory is meant to describe a system in proximity of the critical point only, where the order parameter Φ is small.

This theory is based on the assumption that the free energy \mathcal{F} of the system can be expanded in powers of the order parameter Φ . We can write the Landau expansion of the free energy for a system at temperature T and in an external field h (which is always zero for a Bose-Einstein condensate) as

$$\mathcal{F}(T,\Phi,h) = \mathcal{F}_0 - h\Phi + \frac{1}{2}a(T)\Phi^2 + \frac{1}{4}b(T)\Phi^4 + \dots$$
(7.18)

Except of the term with the external field h, the expansion includes only even powers of Φ , which corresponds to the case of a second order phase transition. To find an equilibrium situation, the free energy has to show a minimum with respect to Φ :

$$\frac{\partial \mathcal{F}(T,\Phi)}{\partial \Phi} = 0, \frac{\partial^2 \mathcal{F}(T,\Phi)}{\partial \Phi^2} > 0.$$
(7.19)

	n	d	α	β	γ	δ	ν	η
Ising 2D	1	2	0	1/8	7/4	15	1	1/4
Ising 3D	1	3	0.110(1)	0.3265(3)	1.2372(5)	4.789(2)	0.6301(4)	0.0364(5)
			-0.025		1.27		0.65	0.026
XY	2	3						
			+0.05		1.371		0.700	0.07
				0.3535	1.270	4.68	0.642	0.030
Heisenberg	3	3		•••	•••			•••
				0.388	1.465	4.85	0.747	0.06
Landau	-	4	0	1/2	1	3	1/2	0

Table 7.1: Theoretical values for the critical exponents.

If a(T), b(T) > 0 and h = 0, the only minimum is $\Phi_0 = 0$, corresponding to a situation where the system is in the non-ordered phase. The situation changes for the case where a(T) < 0 and b(T) > 0, where we find the non-trivial solution

$$\Phi_0^2 = -a(T)/b(T) \,. \tag{7.20}$$

In Landau theory the expansion coefficients a(T), b(T) are in turn themselves expanded in the reduced temperature t (7.14), where to lowest order $a(T) = \alpha_0 t$ and b is considered constant in the vicinity of T_c . Now the solution (7.20) can be written as

$$\Phi_0 = \pm \left(-\frac{\alpha_0 t}{b}\right)^{1/2}, \quad \text{for } t < 0.$$
(7.21)

With the last equation the critical exponent for the order parameter has been found: $\beta = 1/2$. From similar arguments all critical exponents can be determined. They are listed in the lowest row in Table 7.1. The other values in this table are results from more refined theories like renormalization group theory.

Equation (7.21) gives two solutions for the minima of the free energy of the system. In the absence of an external field h, it is not clear in which minimum the system will evolve. The situation is illustrated for the case of a one-dimensional (n = 1) (Figure 7.2 a) and of a two-dimensional (n = 2) (Figure 7.2 b) order parameter in Figure 7.2. For n = 1 the system has two equivalent free energy minima and is thus twofold degenerate, whereas for n > 1 the system shows a continuous degeneracy. A system undergoing a phase transition will be driven by fluctuations into one of the minima—the symmetry is spontaneously broken. Comparing the behavior of the order parameter to that of the free energy around the critical temperature, it becomes clear why second order phase transitions are very sensitive to fluctuations: Around the critical temperature, the minimum of the free energy changes only weakly with T, while the order parameter Φ changes rapidly, and thus fluctuations which involve a large change in Φ require only a small change of free energy.

Landau theory is a mean-field theory, assuming a uniform order parameter and neglecting the fluctuations of the order parameter around its average value. Even though Landau theory provides a good understanding of phase transitions and symmetry breaking, this must lead to quantitatively wrong predictions. The influence of the fluctuations on the behavior at a phase transition was found to depend on dimensionality. Fluctuation have a decreasing effect with increasing dimensionality of both the system, d, and the order parameter, n. In fact, one can define a lower critical dimension d^- and an upper critical dimension d^+ . For dimensions $d \ge d^+$,



Figure 7.2: Free energy as function of order parameter. Dependence of the free energy \mathcal{F} on the value of the order parameter Φ . (a) shows the situation for a one-dimensional (n = 1) order parameter for three different temperatures. Above T_c , the free energy has only one minimum, which becomes very broad for $T = T_c$. For temperatures below T_c there is a two-fold degeneracy and the system is driven by fluctuations into one realization. (b) shows the situation $T < T_c$ for a two-dimensional (n = 2) order parameter, where the degeneracy is continuous.

the fluctuations can be neglected, and the behavior is correctly predicted by Landau theory. In contrast, for $d \leq d^-$ the fluctuations are so strong that they completely destroy the ordered phase, thereby inhibiting the phase transition. If the dimensionality of the system is between the critical dimensions, $d^- < d < d^+$, a phase transition will occur, but the behavior is different from Landau theory. The values for the critical dimensions depend on the universality class. For the XY-universality class (n = 2), to which Bose-Einstein condensation belongs, the lower critical dimension is $d^- = 2$, whereas the upper critical dimension is $d^+ = 4$.

Landau-Ginzburg Theory

Landau theory does not take any fluctuations into account. The influence of fluctuations is included by Landau-Ginzburg theory which is an extension of Landau theory. Landau-Ginzburg theory contains a fluctuating field in form of a spatially varying order parameter $\Phi(\mathbf{r})$. The theory bases on the Landau-Ginzburg free energy functional \mathcal{F}_{LG} which is a generalization of the Landau free energy (7.18). Due to the spatial dependence of $\Phi(\mathbf{r})$, also derivatives of the order parameter have to be included in the expansion. For an isotropic system, there is no term linear in $\nabla \Phi(\mathbf{r})$, because it would depend on the direction of the change in $\Phi(\mathbf{r})$. Thus the simplest possible term is quadratic in $\nabla \Phi(\mathbf{r})$ and the Landau-Ginzburg free energy functional is given by

$$\mathcal{F}_{\mathrm{LG}}(\Phi(\mathbf{r})) = \int \mathcal{F}_0 - h\Phi(\mathbf{r}) + \frac{1}{2}\alpha_0 t\Phi(\mathbf{r})^2 + \frac{1}{4}b(T)\Phi(\mathbf{r})^4 + c\left(\nabla\Phi(\mathbf{r})\right)^2 \mathrm{d}\mathbf{r} \,.$$
(7.22)

The Landau-Ginzburg free energy functional is often also called Φ^4 -model. Although this model describes a phase transition in principle very well, it turns out that calculations are highly complicated because higher orders have to be included in the functional (7.22) when T approaches T_c . Knowing that Landau-Ginzburg theory is correct for systems with dimensions higher than the upper critical dimension d^+ , one introduces a continuous dimensionality d and tries to expand the energy functional for dimensions smaller, but close to the critical dimension. This approach is called ϵ -expansion, where $\epsilon = d^+ - d$ is the deviation from the upper critical dimension. This method can surprisingly be extended to lower dimensions, even if ϵ then is not a small parameter any more. Similar to the ϵ -expansion one can apply a 1/n-expansion according to the dimensionality of the order parameter n. Landau theory is correct for $n = \infty$, that is why an expansion in 1/n was shown to be successful. The ϵ - and the 1/n-expansion are used to reliably calculate critical exponents for the physically interesting dimensions.

Critical Region

To estimate the importance of fluctuations it is useful to compare the magnitude of the fluctuations with the mean value of the order parameter. Landau theory is correct as long as the fluctuations in the system are much smaller than the mean value of the order parameter. The amplitude of the fluctuations increases when the temperature approaches the transition temperature. One can define a temperature region around the critical temperature, the so-called critical region, in which the fluctuations dominate and thus Landau theory breaks down. The size of this region is determined by the Ginzburg criterion

$$\frac{b^2 T_c^2}{\alpha_0^{4-d} c^d} \ll |t| \ll 1,$$
(7.23)

where α_0 , b and c are the expansion coefficients from (7.22) and d is the dimensionality. This means that Landau theory is only applicable in a temperature range which is sufficiently close to T_c , but not so close that fluctuations are dominating. On the other hand, this criterion also determines how close to T_c the temperature has to be in order to experimentally observe the effects of fluctuations and thus beyond mean-field behavior.

The actual calculation of the critical region is not trivial, because it depends on the microscopic details of the system. The size of the critical region is thus not universal. For a conventional superconductor it can be small (10^{-14}) , whereas for a high- T_c superconductor the critical region is 10^{-2} . For the case of Bose-Einstein condensation in dilute gases, the critical region has been estimated in terms of the correlation length to be

$$\xi \ge \frac{\lambda_{\rm dB}^2}{\sqrt{128}\pi^2 a} \tag{7.24}$$

with the scattering length a, which yields for typical experimental parameters $\xi \ge 0.36 \ \mu m$. From this one can find via $\xi \sim |t|^{-\nu}$ the temperature range of the critical region to be on the order of 10^{-2} .

7.3.4 The Correlation Function near the Phase Transition

In the following we want to concentrate on the correlation function $g^{(1)}(\mathbf{r}, \mathbf{r}')$ of a system in proximity of a phase transition. As introduced in Section 7.3.2, the correlation function in the critical region has the asymptotic form

$$g^{(1)}(r) \xrightarrow[r > \lambda_{\rm dB}]{} \frac{e^{-r/\xi}}{r^{d-2+\eta}} \xrightarrow[T = T_c]{} \frac{1}{r^{d-2+\eta}}, \qquad (7.25)$$

which means that it changes its shape from a mainly exponential decay to a pure power law decay when approaching the critical temperature. The correlation length ξ is a measure for the size of the regions in which the fluctuations of the order parameter are correlated. The order parameter fluctuates in domains of all sizes up to ξ . When $T \to T_c$, the correlation length grows without limits and thus the order parameter has correlated fluctuations on all length scales.

This behavior is nicely illustrated by snapshots of the Ising model taken at different temperatures as shown in Figure 7.3. Black pixels correspond to spin down, white to spin up. For high temperatures there are many small black and white regions, generating a pepper-and-salt effect, and there is no preferred direction of the spins, i.e. there is no net magnetization. When the temperature is lowered towards T_c , the typical size of the monochrome regions steadily increases, until the critical temperature is reached. At this point fluctuations from infinitesimally small



Figure 7.3: **2D** Ising across critical point. Snapshots of the two-dimensional Ising model at different temperatures. Black pixels correspond to spin down, white to spin up. At high temperatures (top left) there is no net magnetization, and the fluctuating regions are very small. Going to the right in the upper row the temperature is decreased, until around T_c (top right), the fluctuating regions are correlated over the whole system, but there is still no net magnetization. In the lower row the temperature is below T_c and the system has chosen to be by the majority spin down. Going to the right in the lower row, for even lower temperatures the size of the fluctuating regions decreases.

to infinite similar length ξ corresponds in this example to the typical size of the white regions. It diverges at T_c and falls off again when the temperature moves away from the critical temperature.