Chapter 2

Fundamental Concepts of Bose-Einstein Condensation

This chapter introduces several key features associated with the Bose-Einstein Condensation (BEC) phase transition. The subjects we will study in this chapter include an order parameter, spontaneous symmetry breaking, Nambu-Goldstone bosons, off-diagonal long-range order and higher-order coherence, which are the fundamental concepts in understanding the BEC phase transition physics.

2.1 Order parameter and spontaneous symmetry breaking

The field operator $\hat{\psi}(r)$ that annihilates a particle at the position r can be written in the form

$$\hat{\psi}(r) = \sum_i \varphi_i(r)\hat{a}_i, \tag{2.1}$$

where $\hat{a}_i$ $\left(\hat{a}_i^+\right)$ are the annihilation (creation) operators of a particle in the single particle state $\varphi_i(r)$ and obey the bosonic commutation relations

$$\left[\hat{a}_i, \hat{a}_j^+\right] = \delta_{ij}, \quad [\hat{a}_i, \hat{a}_j] = \left[\hat{a}_i^+, \hat{a}_j^+\right] = 0. \tag{2.2}$$

The $c-$ number wavefunction $\varphi_i(r)$ satisfies an orthonormal condition:

$$\int \varphi_i^*(r)\varphi_j(r)dr = \delta_{ij}. \tag{2.3}$$

The field operator follows the communication relation

$$\begin{aligned}
\left[\hat{\psi}(r), \hat{\psi}^+(r')\right] &= \left[\sum_i \varphi_i(r)\hat{a}_j, \sum_j \varphi_j^*(r')\hat{a}_j^+\right] \\
&= \sum_i \varphi_i(r)\varphi_i^*(r') \\
&= \delta(r - r')
\end{aligned} \tag{2.4}$$

where the completeness (closure) relation of single particle states $|i\rangle$ was used for the last equality,

$$\sum_i |i\rangle\langle i| = \hat{I}. \tag{2.5}$$

If we multiply $\langle r|$ from the left and $|r'\rangle$ from the right of (2.5), we have

$$\sum_i \varphi_i(r)\varphi_i^*(r') = \sum_i \langle r|i\rangle\langle i|r'\rangle = \langle r|r'\rangle = \delta(r - r'). \tag{2.6}$$

If a lowest energy single particle state (ground state) has a macroscopic occupation, we can separate the field operator (2.1) into the condensate term ($i = 0$: lowest energy ground state) and the non-condensate components ($i \neq 0$: excited states):

$$\hat{\psi}(r) = \varphi_0(r)a_0 + \sum_{i\neq 0} \varphi_i(r)\hat{a}_i. \tag{2.7}$$

This expression of the field operator already and implicitly introduced the Bogoliubov approximation [1], in which the operators $\hat{a}_0$ and $\hat{a}_0^+$ are replaced by the c-number $a_0 = \sqrt{N_0}$, where $N_0 = \langle \hat{a}_0^+ \hat{a}_0\rangle$ is the average occupation number of the ground state ($i = 0$). By defining $\psi_0 = \sqrt{N_0}\varphi_0$ and $\delta\hat{\psi} = \sum_{i\neq 0} \varphi_i\hat{a}_i$, we can obtain the Bogoliubov ansatz:

$$\hat{\psi}(r) = \psi_0(r) + \delta\hat{\psi}(r). \tag{2.8}$$

The separation, (2.8), is justified if a lowest energy ground state is occupied by macroscopic number of particles ($N_0 \gg 1$) and is particularly useful to describe the ensemble averaged nonlinear dynamics of the condensate via the closed form equation for the classical field $\psi_0(r)$ and the small fluctuations around the average value.

The classical field $\psi_0(r)$ is called the wave function of the condensate and plays a role of an order parameter. It is characterized by a modulus and a phase:

$$\psi_0(r) = |\psi_0(r)|e^{iS(r)} \tag{2.9}$$

The modulus $|\psi_0(r)|$ determines the particle density $n(r) = |\psi_0(r)|^2$ of the condensate, while the phase $S(r)$ characterizes the coherence and superfluid phenomena. The order parameter $\psi_0 = \sqrt{N_0}\varphi_0$ is defined up to a particular phase factor. However, one can always multiply this function by the arbitrary phase factor $e^{i\alpha}$ without changing any physical property. This is the manifestation of gauge symmetry of the problem. Physically, lack of a phase stabilization force of the system is responsible for the random phase of the condensate. However, in the BEC phase transition, a condensate system spontaneously chooses a particular phase $S(r)$. Making an explicit choice for the phase $S(r)$ in spite of the lack of a preferred phase value is referred to as a spontaneous breaking of gauge symmetry.

The Bogoliubov ansatz (2.8) for the field operator can be interpreted that the expectation value $\langle\hat{\psi}(r)\rangle$ is different from zero. This would not possible if the condensate state is in a particle number eigenstate $|N_0\rangle$. From a quantum field theoretical point of view, this spontaneous symmetry breaking means that the condensate state is in or close to a coherent state defined by [2]

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \tag{2.10}$$

where $|\alpha|^2 = N_0$ is the average particle number of the condensate. The coherent state $|\alpha\rangle$ defined by (2.10) can be expanded by the particle number eigenstates [2]:

$$|\alpha\rangle = \sum_n \frac{e^{-|\alpha|^2/2}}{\sqrt{n!}} \alpha^n |n\rangle \tag{2.11}$$

If we recall that the time dependence of the particle number eigenstate is $e^{-iE(n)t/\hbar}|n\rangle$, where $E(n)$ is a total energy of n particles, we can easily show that the time dependence of the order parameter is given by [2]

$$\psi_0(r,t) \equiv \langle\alpha|\varphi_0(r)\hat{a}_0|\alpha\rangle = \psi_0(r)e^{-i\mu t}, \tag{2.12}$$

if the condensate is in a coherent state. Here $\psi_0(r) = \varphi_0(r)$ and $\hbar\mu = E(n) - E(n-1) \sim \frac{\partial E(n)}{\partial n}$ is the chemical potential of the system. It is important to note that the time evolution of the order parameter is not governed by the total energy $E(n)$ but by the chemical potential μ. This fact is deeply connected to the above mentioned spontaneous symmetry breaking. The difference between the time evolution of a particle number eigenstate $|n\rangle$ and that of a coherent state is schematically shown in Fig. 2.1. A coherent state is a pure state consisting of linear superposition of particle number eigenstates and localizes its phase to a particular value through the destructive and constructive interferences between different particle number eigenstates as shown in Fig. 2.1. Above the BEC phase transition temperature, the ground state is occupied by the statistical mixture of different particle number eigenstates in which an entropy is maximum under the constraint of fixed average occupation number [3]. Below the BEC phase transition temperature, the ground state is approaching to a pure coherent state in which an entropy is zero.

We will quantitatively show how the quantum state of the condensate is approaching to a coherent state rather than a number state in Chapter 8 and 9 using the two different approaches: Heisenberg-Langevin equation and density matrix master equation.

2.2 Nambu-Goldstone bosons and phase stabilization

Bose particles in the condensate interact with each other via repulsive potential. This interaction induces small-energy and long-wavelength fluctuations in the condensate. To see this, we can start with the Gross-Pitaevskii equation for the order parameter:

$$i\frac{d}{dt}\psi(r,t) = \left\{-\frac{\hbar\nabla^2}{2m} + g|\psi(r,t)|^2\right\}\psi(r,t), \tag{2.13}$$

where $g(>0)$ is a repulsive interaction potential. We will derive this equation and discuss the meaning of this potential in detail in chapter 4 but here let us consider g is a mere parameter characterizing the interaction of the system. The solution of (2.13) is expanded as

$$\begin{aligned}
\psi(r,t) &= \psi_0(r)e^{-i\mu t}\left\{1 + \sum_k \alpha_k e^{i(kr-\omega t)} + \beta_k e^{-i(kr-\omega t)}\right\} \qquad (2.14)\\
&= \psi_0(r)e^{-i\mu t} + \sum_k \left\{u_k e^{i(kr-(\mu+\omega)t)} + v_k e^{-i(kr+(\mu-\omega)t)}\right\},
\end{aligned}$$

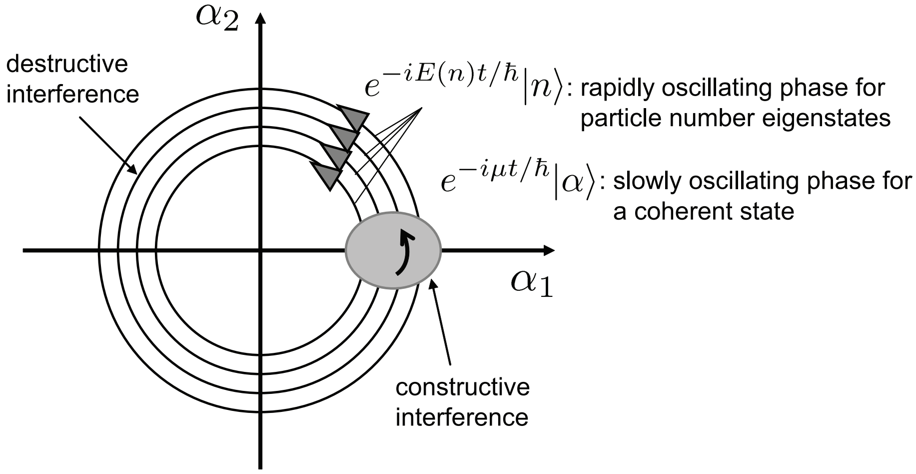

Figure 2.1: The time evolution of particle number eigenstates $|n\rangle$ and a coherent state $|\alpha|$. A coherent state is a pure state consisting of linear superposition of particle number eigenstates. The phase is localized by the destructive and constructive interference among the different particle number eigenstates in a phase space.

where $u_k(r) = \psi_0(r)\alpha_k$ and $v_k(r) = \psi_0(r)\beta_k$ are the excitation amplitudes of forward propagating and backward propagating excitation waves with wavenumber $\pm k$. $\hbar\mu = \hbar g|\psi_0(r)|^2$ is a chemical potential. If we substitute (2.14) into (2.13) and compare the left-hand-side (LHS) and right-hand-side (RHS) for the $e^{i(kr-(\mu+\omega)t)}$ term and $e^{-i(kr-(\mu-\omega)t)}$ term, respectively, we obtain the following eigenvalue equations for the two excitation waves:

$$\begin{pmatrix} \frac{\hbar k^2}{2m} + \mu & \mu \\ -\mu & -\frac{\hbar k^2}{2m} - \mu \end{pmatrix} \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \omega \begin{pmatrix} u_k \\ v_k \end{pmatrix}. \tag{2.15}$$

In order to have a non-trivial solution for u_k and v_k, the eigenvalues ω must satisfy

$$\omega^2 - \left(\mu + \frac{\hbar k^2}{2m}\right)^2 + \mu^2 = 0 \tag{2.16}$$

The solution of (2.16) is easily obtained as

$$\omega = \pm\sqrt{\omega_k\left(\omega_k + 2\mu\right)}, \tag{2.17}$$

where $\hbar\omega_k = \frac{(\hbar k)^2}{2m}$ is the kinetic energy of a non-interacting free particle. Figure 2.2 shows the normalized excitation energy ω/μ vs. normalized wavenumber $k\xi$, where $\xi = \sqrt{\frac{\hbar}{m\mu}}$ is a healing length. At low-energy and small-wavenumber (or long-wavelength) limit, $k\xi < 1$, the excitation modes obey a linear dispersion like a sound wave:

$$\omega = \pm ck, \tag{2.18}$$

where $c = \sqrt{\frac{\hbar\mu}{m}}$ is an effective sound velocity. The important consequence of the linear despersion (2.18) will be discussed in our argument of superfluidity in chapter 5.

The particular formula (2.17) is the celebrating Bogoliubov dispersion law[1], which we will discuss in detail in chapter 4. In general, a long-wavelength fluctuation universally appears in a process of spontaneous symmetry breaking in particle and condensed matter systems, and is called the Nambu-Goldstone modes[4, 5, 6]. The Bogoliubov dispersion law is a special case of the Nambu-Goldstone modes for a weakly interacting Bose particles. A repulsive interaction represented by a parameter $g(>0)$ not only create the Bogoliubov excitations but also introduce the new interaction energy between the condensate and the Bogoliubov excitations. In chapter 7 we will see that this interaction energy forces a condensate to acquire a particular phase as a coherent state rather than to have a random phase as a particle number eigenstate or statistical mixture of them. In this way the Nambu-Goldstone modes play a crucial role in various phase transition physics with spontaneous symmetry breaking.

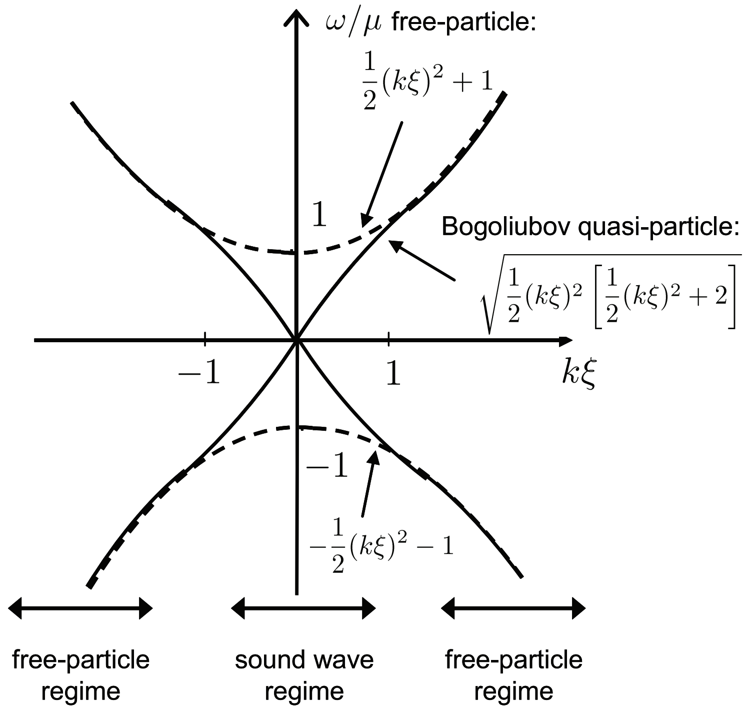

Figure 2.2: The dispersion relations ω/μ vs $k\xi$ for a free-particle and a Bogoliubov quasi-particle.

2.3 Off-diagonal long range order and coherence functions

The first-order coherence function for the field operator is defined by [2]

$$G^{(1)}(r,t;r',t') = \langle \hat{\psi}^{+}(r,t)\hat{\psi}(r',t')\rangle \tag{2.19}$$

Equation (2.19) provides a very general definition of coherence which applies to any system, independent of statistics, in equilibrium as well as out of equilibrium [2]. In an equilibrium system, a time dependence is suppressed so that only concept of a spatial coherence exists.

Because of the commutation relations (2.2) for the boson operators and the orthogonality (2.3) of the single particle state $\varphi_i(r)$, the field operators satisfy (2.4). The first-order spatial coherence function is expressed in terms of single particle wavefunctions:

$$\begin{aligned} G^{(1)}(r,r') &= \langle \hat{\psi}^+(r)\hat{\psi}(r')\rangle \\ &= \sum_i n_i \varphi_i^*(r)\varphi_i(r), \end{aligned} \tag{2.20}$$

where $\langle \hat{a}_i^+ \hat{a}_j \rangle = \delta_{ij} n_i$ is read. From (2.20) we can show the matrix $G^{(1)}$ is Hermitian:

$$G^{(1)}(r',r) = \sum_i n_i \varphi_i^*(r')\varphi_i(r) = G^{(1)}(r,r')^*. \tag{2.21}$$

The particle density is given by the diagonal element of the Hermitian matrix $G^{(1)}(r,r')$:

$$G^{(1)}(r,r) = \sum_i n_i |\varphi_i(r)|^2 = n(r) \tag{2.22}$$

The total number of particles is then given by the spatial integral $N = \int n(r)dr$. The normalized coherence function (or off-diagonal element in the matrix $G^{(1)}$) is defined by

$$g^{(1)}(r,t;r't') = \frac{G^{(1)}(r,t;r',t')}{\left[G^{(1)}(r,t;r,t)G^{(1)}(r',t';r',t')\right]^{1/2}}. \tag{2.23}$$

In a three-dimensional system, the scalar product of the momentum and position eigenstates is written as [7],

$$\begin{aligned} \langle p|r\rangle &= (2\pi\hbar)^{-\frac{3}{2}} \exp\left(-i\frac{p\cdot r}{\hbar}\right) \\ &= \langle r|p\rangle^* \end{aligned} \tag{2.24}$$

Using the completeness relation $\int |r\rangle\langle r|dr = \hat{I}$, the field operator $\hat{\psi}(p)$ in the momentum space is thus written as

$$\begin{aligned} \hat{\psi}(p) = \langle p|\psi\rangle &= \int \langle p|r\rangle dr \langle r|\psi\rangle \\ &= (2\pi\hbar)^{-\frac{3}{2}} \int dr \hat{\psi}(r) \exp\left(i\frac{p\cdot r}{\hbar}\right). \end{aligned} \tag{2.25}$$

The inverse relation to (2.25) is obtained by using the either completeness relation, $\int |p\rangle\langle p|dp = \hat{I}$, as

$$\begin{aligned} \hat{\psi}(r) = \langle r|\psi\rangle &= \int \langle r|p\rangle dp \langle p|\psi\rangle \\ &= (2\pi\hbar)^{-\frac{3}{2}} \int dp \hat{\psi}(p) \exp\left(-\frac{ip\cdot r}{\hbar}\right). \end{aligned} \tag{2.26}$$

Using (2.25) and (2.26), we can calcurate the first-order coherence function as

$$\begin{aligned} G^1(r,r') &= \langle \hat{\psi}^+(r)\hat{\psi}(r')\rangle \\ &= (2\pi\hbar)^{-3} \int dp \int dp' \langle \hat{\psi}^+(p)\hat{\psi}(p')\rangle \exp\left[\frac{i}{\hbar}(pr - p'r')\right] \\ &= \frac{1}{V} \int dp n(p) \exp\left[\frac{i}{\hbar}p(r-r')\right], \end{aligned} \tag{2.27}$$

where the following definition of Dirac delta-function is used:

$$(2\pi\hbar)^{-3}\int dp \exp\left[\frac{ip(r-r')}{\hbar}\right] = \delta(r-r'), \tag{2.28}$$

$$(2\pi\hbar)^{-3}\int dr \exp\left[\frac{i}{\hbar}r(p-p')\right] = \delta(p-p'). \tag{2.29}$$

Here $n(p)$ is the particle distribution over the momentum eigenstates and satisfy the normalization $\int dpn(p) = N$.

Let us consider the case of a uniform and isotropic system of N identical bosons occupying a volume V. In the limit of $N, V \to \infty$ with the density $n = \frac{N}{V}$ kept constant, (2.27) is not dependent on specific positions r, r' but depends on the modulus of the relative position $s = |r - r'|$ and one can write

$$G^{(1)}(r,r') = G^{(1)}(s) = \frac{1}{V}\int dpn(p)e^{-ip\cdot s/\hbar}, \tag{2.30}$$

For a normal state above BEC critical temperature, the momentum distribution is smooth at small momenta and consequently the first-order coherence function $G^{(1)}(r,r')$ (or normalized coherence function $g^{(1)}(r,r')$) vanishes when $s \to \infty$. The situation is different if instead the momentum distribution features the macroscopic occupation N_0 at the single particle ground state with momentum $p = 0$

$$n(p) = N_0\delta(p) + \tilde{n}(p). \tag{2.31}$$

This macroscopic occupation of the single particle state, usually at $p = 0$, is a general definition of BEC and the quantity $N_0/N < 1$ is called the condensate fraction. Using (2.28) in the Fourier transform (2.27), one finds the first-order coherence function does not vanish when $s \to \infty$ but approaches a finite value:

$$G^{(1)}(s)|_{s\to\infty} \longrightarrow \frac{N_0}{V}, \tag{2.32}$$

or

$$g^{(1)}(s)|_{s\to\infty} \longrightarrow \frac{N_0}{N}. \tag{2.33}$$

This asymptotic behavior of the first-order coherence function was discussed by Landau and Lifshitz [8], Penrose [9] and Penrose and Onsager [10], and is often referred to as off-diagonal long-range order (ODLRO), since it involves the off-diagonal elements ($r \neq r'$) of the first-order coherence function. Figure 2.3 shows the typical behavior of $g^{(1)}(s)$ at above and below BEC critical temperature. The initial decrease of $g^{(1)}(s)$ in a small s values is governed by $\tilde{n}(p)$ in (2.28). The low-s expansion of (2.27) results in the following quadratic decrease in $g^{(1)}(s)$ in the limit of $s \to 0$:

$$e^{-ip\cdot s/\hbar} \simeq 1 - i(p\cdot s)/\hbar - \frac{1}{2}(p\cdot s)^2/\hbar^2 + \cdots, \tag{2.34}$$

and

$$g^{(1)}(s)|_{s\to 0} = 1 - \frac{1}{2}\langle\hat{p}^2\rangle\frac{s^2}{\hbar^2} + \cdots, \tag{2.35}$$

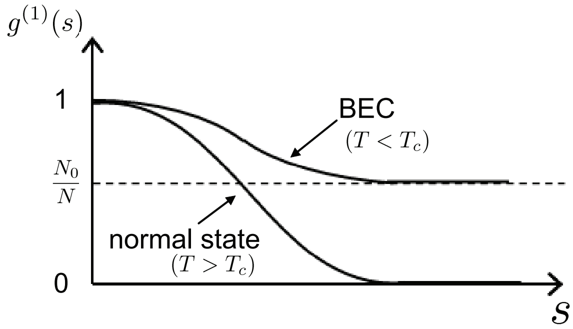

Figure 2.3: The normalized first-order coherence function $g^{(1)}(s)$ vs the relative positions $s = |r - r'|$. For a normal state, $g^{(1)}(s)$ vanishes for large s, but for a BEC, $g^{(1)}(s)$ approaches to the condensate fraction N_0/N for large s.

where $\langle \hat{p}^2 \rangle = \frac{1}{N} \int dpn(p)p^2$ is the second order moment of the momentum distribution and identically equal to the variance of the momentum distribution $\langle \Delta\hat{p}^2 \rangle = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$, since $\langle \hat{p} \rangle = 0$.

The first order coherence function $g^{(1)}(s)$ is measured by various single particle interferometers. A Young's double slit interferometer is one of them. Figure 2.4 shows the measured interference patterns for an exciton-polariton condensate across the BEC critical density [11]. When the particle density is below BEC critical density (or above BEC critical temperature), no interference pattern is observed, while at above BEC critical density (or below BEC critical temperature), the visibility of interference pattern increases with the particle density. This indicates the condensate fraction increases with the particle density. Figure 2.5 shows the measured $g^{(1)}(s)$ vs. s for a trapped Bose gas at below and above BEC critical temperature [12].

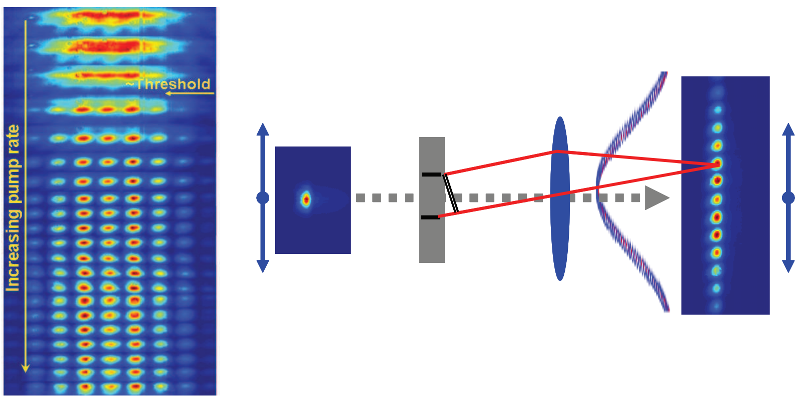

Figure 2.4: The interference patterns of the Young's double slit interferometer vs. the particle density across the BEC critical density for an exciton polariton condensate [11].

If all particles condense into the ground state, i.e. $\frac{N_0}{N} \to 1$, the first-order coherence function $g^{(1)}(s)$ is independent of s and equal to one. The first-order coherence function $g^{(1)}(s)$ is a measure for the degree of condensation in momentum space. If only the ground state is occupied and there is negligible populations in excited states, we always obtain

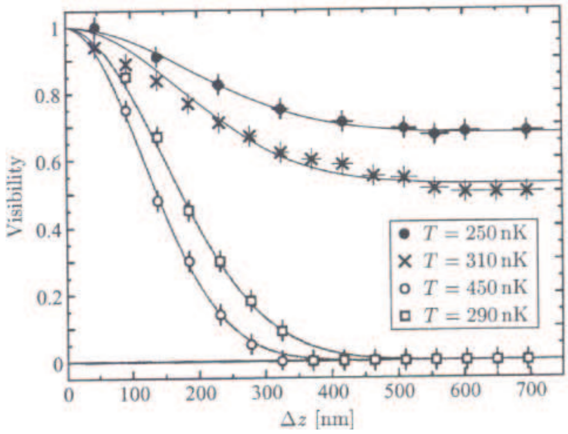

Figure 2.5: Spatial coherence of a trapped Bose gas as a function of slit separation for temperature below (black crosses and circles) and above (white circles and squares) the transition temperature. For temperatures above T_c coherence disappears for distances much smaller than the size of the sample. (The number of atoms in the trap was reduced to prepare a thermal gas at a temperature of 290 nK in the experimental data represented by open squares.

$g^{(1)}(s) \simeq 1$.

However, this measurement does not provide any information about the quantum statistical properties of the condensate itself. In order to distinguish various possible candidate quantum states such as a particle number eigenstate $|N\rangle$, coherent state $|\alpha\rangle$ or thermal state $\hat{\rho}_{\text{mix}} = \sum_n \rho_{nn}|n\rangle\langle n|$ [13], we have to study the higher-order coherence functions defined by [2]

$$\begin{aligned} g^{(n)}(s) &= \frac{G^{(n)}(r_1,t_1;r_2,t_2;\cdots;r_n,t_n)}{\left[G^{(1)}(r_1,t_1)G^{(1)}(r_2,t_2)\cdots G^{(1)}(r_n,t_n)\right]} \\ &= \frac{\langle\hat{\psi}^+(r_1,t_1)\cdots\hat{\psi}^+(r_n,t_n)\hat{\psi}(r_n,t_n)\cdots\hat{\psi}(r_1,t_1)\rangle}{\left[\langle\hat{\psi}^+(r_1,t_1)\hat{\psi}(r_1,t_1)\rangle\cdot\cdots\cdot\langle\hat{\psi}^+(r_n,t_n)\hat{\psi}(r_n,t_n)\rangle\right]^{1/n}} \end{aligned} \tag{2.36}$$

The higher-order coherence function is the joint probability of detecting n particles at $(r_1,t_1),(r_2,t_2)\cdots$ and (r_n,t_n) time-space points, and can be measured by the Hanbury-Brown and Twiss interferometer [14] or its variants. For instance, if a given Bose particle system in a single spatial mode is in a coherent state $|\alpha\rangle$, particle number eigenstate $|N\rangle$ or thermal state $\hat{\rho}_{\text{mix}}$ and there is no excitations, the n-th order coherence function takes the following values [15, 16]:

$$g^{(n)}(\tau=0) = \begin{cases} 1 : \text{coherent state} \\ 1-\frac{n-1}{N} : \text{particle number eigenstate} \\ n! : \text{thermal state} \end{cases}, \tag{2.37}$$

where $\tau = 0$ means the simultaneous detection of n particles, i.e. $t_1 = t_2 = \cdots = t_n$.

In this way, the higher-order coherence functions provide the information on the particular quantum states of the experimentally realized condensate. Figure 2.6 shows the measured $g^{(2)}(\tau = 0)$ and $g^{(3)}(\tau = 0)$ for the exciton-polariton condensate [17]. The experimental results of $g^{(2)}(\tau = 0) = 1.3$ and $g^{(3)}(\tau = 0) = 2.5$ at well above the BEC critical density suggest that the quantum state of the condensate is not a particle number eigenstate for which $g^{(2)}(\tau = 0) = 2$ and $g^{(3)}(\tau = 0) = 6$ nor a coherent state for which $g^{(2)}(\tau = 0) = g^{(3)}(\tau = 0) = 1$. This detailed discussion of this result, including the theoretical results shown by solid lines will be presented within the context of the quantum theory of matter-wave lasers in chapter 9.

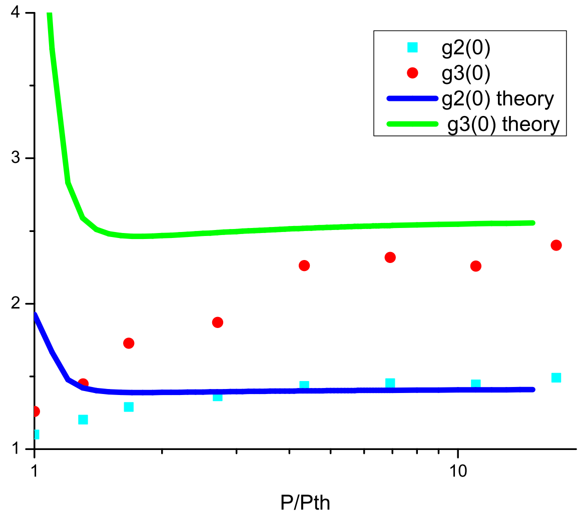

Figure 2.6: The measured $g^{(2)}(\tau = 0)$ and $g^{(3)}(\tau = 0)$ for an exciton-polariton condensate for varying pump rates [17].

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