

The Symmetry Puzzle:
A Friendly Introduction to Spontaneous Breaking
in Bose-Einstein Condensates

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At a Glance

As children, we were told that there are three states of matter: solid, liquid, and gaseous. The harsh truth is that there is a whole fascinating variety of states of matter. One of them is known as the Bose-Einstein condensate, predicted by an Indian physicist, Satyendra Nath Bose, who, in a letter to Albert Einstein, commented on that theoretical curiosity in which quantum mechanics theory played a leading role in describing such a state. In this text, a pedagogical deduction of a Bose-Einstein condensate is developed.

On the other hand, every time we boil water, a transition in matter occurs: from liquid to gaseous. The physics describing such a process can be generalized to study the transition of a Bose gas to a Bose-Einstein condensate through Landau Theory. This leads to symmetry breaking in the condensate: in principle, it can be described by any equally valid phase (symmetry), but a conservative treatment implies that it should only *be* in one defined phase (breaks the symmetry). Everything necessary for a first approximation to this effect is included in the text.

An important fact is that not only does a Bose-Einstein condensate undergo spontaneous symmetry breaking, but some cosmological models of the early universe also experience it. This led Sir Thomas Walter Bannerman Kibble to wonder what happens when the state that minimizes energy is chosen in regions of spacetime that are causally disconnected (i.e., outside the light cone). Later, Wojciech Hubert Zurek applied that idea to the disconnected areas to study the topological defects remaining remnants of a phase transition. An introductory discussion is included.

Finally, it reviews how achieving the physical requirements to observe a Bose-Einstein condensate is possible since it is not as simple as evaporating water. Along with an Appendix section sufficient to follow the text, an attractive introductory *review* on quantum gas physics is expected to be presented.

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Chapter 1

Bose-Einstein Condensate

A gas is considered ideal if the particles do not interact with each other. Let us consider a monoatomic ideal gas without internal structure¹ consisting of N particles trapped in a box of size V . The Hamiltonian for each particle will not include a potential $\mathcal{V}(q)$:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \mathcal{V}(\hat{q}) \xrightarrow{\text{No interaction}} \hat{H} = \frac{\hat{p}^2}{2m}$$

The most important function in Statistical Mechanics is the partition function Z . It is given by the sum of all possible states of a quantum system. Classically, the state of a particle is determined by a point in the **phase space**, so the partition function for each particle in the classical gas system is given by:

$$\begin{aligned} Z_1 = \text{Tr } e^{-\beta \hat{H}} &= \frac{1}{h^3} \int d^3 q d^3 p e^{-\beta H(p, q)} \quad \rightarrow \quad Z_1 = \frac{1}{(2\pi\hbar)^3} \int d^3 q d^3 p e^{-\beta \vec{p}^2/2m} \\ &\rightarrow \quad Z_1 = \frac{1}{(2\pi\hbar)^3} V \left[\sqrt{\frac{\pi}{\beta/2m}} \right]^3 \\ &\rightarrow \quad Z_1 = V \left(\frac{mk_B T}{2\pi\hbar^2} \right)^{3/2} \end{aligned}$$

where we use the well-known result of the Gaussian integral and $\beta = \frac{1}{k_B T}$, with the **Boltzmann constant** $k_B \approx 1.381 \times 10^{-23} \text{ J/K}$. Another constant also appears: the **Planck constant**, $\hbar \approx 6.626 \times 10^{-34} \text{ J}\cdot\text{s}$. Why does it appear if we are considering a classical gas? The presence of \hbar is merely a reminder that the classical world originates from the quantum one². Since Z_1 is dimensionless, we can think of Z_1 as the number of times that a region determined by $(\lambda)^3$, called the **thermal de Broglie wavelength**, fits into volume V :

$$\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_B T}} \quad \rightarrow \quad Z_1 = \frac{V}{(\lambda)^3},$$

so the partition function for an ideal gas of N indistinguishable bosonic particles³ in the canonical ensemble (fixed number of particles N) is:

$$Z(N, V, T) = \frac{1}{N!} Z_1^N = \frac{V^N}{N! \lambda^{3N}}. \quad (1.1)$$

From this partition function, we can derive the ideal gas law. Indeed, writing the Helmholtz free energy F and its relationship with pressure p :

$$F = -k_B T \log Z \Rightarrow p = -\frac{\partial F}{\partial V} = k_B T \frac{\partial(\log Z)}{\partial V}$$

¹That is, without rotational or vibrational degrees of freedom.

²A brief discussion can be found in "Statistical Physics", David Tong, page 32.

³The difference between bosonic and fermionic particles is detailed in the Appendix section.

$$\begin{aligned}
&= k_B T N! (\lambda^{3N}) / V^N (N V^{N-1}) / (N! (\lambda^{3N})) \\
&= N k_B T / V,
\end{aligned}$$

which is an appropriate equation of state for low-density gases, i.e., when interactions between atoms are not yet relevant for calculations.

However, the classical treatment of a monoatomic ideal gas breaks down as the temperature decreases since $\lambda \propto T^{-1/2}$. Eventually, this thermal wavelength will become comparable to the separation between particles:

$$\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_B T}} \xrightarrow{T \ll 0} \lambda \sim \left(\frac{V}{N}\right)^{\frac{1}{3}}$$

In other words, quantum effects will become noticeable at low temperatures. Since we are still working with non-interacting particles, there will only be one significant effect to consider: quantum statistics.

This text will focus exclusively on monoatomic bosonic particles at low energies. In our day-to-day experience, this refers to atoms composed of an even number of fermions that behave as bosons, provided the **bound state** ensures the atom's stability remains intact. This stability can break down if the temperature rises significantly, potentially dissociating the constituent fermions and preventing a bosonic description. The stability of the bound state will not be an issue in what follows, as we will focus on low temperatures.

How can we specify the state of a non-interacting bosonic system? One might think that for N particles, we would need to specify the state of each particle. However, since bosons can share states, it is only necessary to indicate **how many** particles are in each state. As we are interested in macroscopic observables, we must pay attention only to the average number of particles in a given state labeled by $|r\rangle$. The Bose-Einstein distribution gives this quantity.

1.1 Bose-Einstein Distribution

Finding how particles are distributed (the average number of particles per state) is simpler within the framework of the **Grand Canonical Ensemble**, where a chemical potential μ is introduced, allowing the number of particles N to fluctuate. The chemical potential μ can be thought of as a way to measure how much energy is required to add a particle to the system without changing entropy S or volume V , or how the free energy varies at constant temperature and volume:

$$\mu = \left. \frac{\partial E}{\partial N} \right|_{S,V} = \left. \frac{\partial F}{\partial N} \right|_{T,V}$$

It is important to emphasize that the grand canonical ensemble is used only for mathematical convenience, as in most experiments N remains fixed. Thus, in this ensemble, μ is determined by changes in N or T , i.e., $\mu = \mu(N, T)$. Later, to return to work in the canonical ensemble, we will fix N , which will also cause μ to change.

The partition function of the grand canonical ensemble is

$$\mathcal{Z}(T, \mu, V) = \sum_n e^{-\beta(E_n - \mu N_n)}$$

where the sum spans all possible **states** of the system. When dealing with bosons, it is simpler to work with a label $|r\rangle$ that determines the state of each particle but can be shared by many particles. This allows summing over the number of particles in a given state instead of summing over all states for each particle. Since the energy of the entire state depends on how many particles occupy a particular energy level, the partition function for particles in state $|r\rangle$ is given by:

$$\mathcal{Z}_r = \sum_{n_r} e^{-\beta n_r (E_r - \mu)} = \frac{1}{1 - e^{-\beta(E_r - \mu)}}. \quad (1.2)$$

At this step, we assume that $E_r > \mu$; otherwise, the summation diverges. We can shift the energy levels such that the ground state is at $E_0 = 0$, ensuring that $\mu < 0$.

As we are in the grand canonical ensemble, the occupation of a given state $|r\rangle$ is independent of another state $|r+1\rangle$.

Therefore, the total partition function for a monoatomic non-interacting gas is:

$$\mathcal{Z} = \prod_r \mathcal{Z}_r = \prod_r \frac{1}{1 - e^{-\beta(E_r - \mu)}}, \quad (1.3)$$

from which it follows that the average number of particles is:

$$N = \frac{1}{\beta} \frac{\partial}{\partial \mu} \log \mathcal{Z} = \sum_r \frac{1}{e^{\beta(E_r - \mu)} - 1}.$$

Naturally, the total number of particles is simply the sum of the average number of particles in each state $|r\rangle$:

$$N \equiv \sum_r \langle N_r \rangle,$$

which makes clear the **Bose-Einstein distribution**:

$$\langle N_r \rangle = \frac{1}{e^{\beta(E_r - \mu)} - 1}. \quad (1.4)$$

In practical terms, what interests us is the thermodynamic limit (when it no longer makes sense to count the total number of particles, i.e., $N \rightarrow \infty$). Since the relative fluctuation of any of the three ensembles coincides in the thermodynamic limit (i.e., $\Delta N/\langle N \rangle \sim 1/\sqrt{\langle N \rangle}$), we can write N_r instead of $\langle N_r \rangle$, as fluctuations around the average are negligible.

1.2 Condensate as a Statistical Phenomenon

The condensation of a boson gas can be summarized as an overwhelming occupation of the ground state. To derive this, we define the **fugacity**:

$$z = e^{\beta\mu} \quad (1.5)$$

which is constrained between $0 < z < 1$ since $\mu < 0$. In the laboratory, we know the number of particles we are working with, N . However, as we are working in the grand canonical ensemble, we must calculate it as $N = N(\mu, T)$. It is straightforward to deduce that the number of particles is given by:

$$N = \int dE \underbrace{g(E)}_{\text{State distribution}} \underbrace{\frac{1}{z^{-1} e^{\beta E} - 1}}_{N^\circ \text{ particles per state}},$$

where we use the Bose-Einstein distribution 1.4 in terms of fugacity z . Thus, we need the **density of states** $g(E)$. But this is just another way of thinking about the partition function since it sums over all states compatible with a given energy configuration E . On the other hand, we know that quantum mechanically, energy becomes discrete when confined within a box of volume $V = L^3$. The energy of a particle is:

$$E_{\vec{n}} = \frac{4\pi^2 \hbar^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2).$$

Notably, this energy scaled by the factor β depends on the thermal wavelength λ :

$$\frac{E_n}{k_B T} = \frac{2\pi^2 \hbar^2}{m} \frac{n^2}{L^2} \frac{1}{k_B T} \approx \frac{2\pi \hbar^2}{mk_B T} \frac{n^2}{L^2} = \lambda^2 \frac{n^2}{L^2}.$$

Since λ is much smaller than the length of any box, then $E_n < k_B T$. Therefore, many states will contribute to the sum in the partition function:

$$Z_1 = \sum_{\vec{n}} e^{-\beta E_{\vec{n}}}.$$

Thus, we can approximate it with an integral:

$$\sum_{\vec{n}} \approx \int d^3 n \underbrace{\rightarrow}_{k=\frac{2\pi n}{L}} \frac{V}{(2\pi)^3} \int d^3 k = \frac{4\pi V}{(2\pi)^3} \int_0^\infty dk k^2,$$

where in the last integral we use spherical coordinates (the factor 4π comes from angular directions and a Jacobian). Moreover, for a free particle:

$$E = \frac{\hbar^2 k^2}{2m} \rightarrow dE = \frac{\hbar^2 k}{m} dk \rightarrow \frac{4\pi V}{(2\pi)^3} \int dk k^2 = \frac{V}{2\pi^2} \int dE \sqrt{\frac{2mE}{\hbar^2}} \frac{m}{\hbar^2} \equiv \int dE g(E),$$

where the **density of states** is:

$$g(E) = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2}. \quad (1.6)$$

Now we can calculate how many particles $N(\mu, T)$ we should expect given μ and T . Previously, it was mentioned that the thermodynamic limit involves taking $N \rightarrow \infty$, but additionally, we must take $V \rightarrow \infty$. Thus, N/V approaches a constant in the thermodynamic limit, and we work with this quantity.

$$\begin{aligned} \frac{N}{V} &= \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty dE \frac{E^{1/2}}{z^{-1} e^{\beta E} - 1} \\ &= \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty dE \frac{ze^{-\beta E} E^{1/2}}{1 - ze^{-\beta E}} \\ &= \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} z \int_0^\infty dE \frac{\sqrt{\beta E}}{\sqrt{\beta}} e^{-\beta E} \frac{1}{1 - ze^{-\beta E}} \quad x = \beta E \rightarrow dE = \frac{dx}{\beta} \\ &= \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \frac{z}{\beta^{3/2}} \int_0^\infty dx \sqrt{x} e^{-x} (1 + ze^{-x} + \dots) \end{aligned} \quad (1.7)$$

These integrals transform into a series of Gaussian integrals if we set $x = u^2$. Several factors will emerge from these that contribute to forming the thermal wavelengths λ . Finally, we can write the particle density as:

$$\frac{N}{V} = \frac{z}{\lambda^3} \left(1 + \frac{z}{2\sqrt{2}} + \dots \right) \quad (1.8)$$

Three comments are necessary at this point:

- Recall that we worked in the grand canonical ensemble purely for mathematical convenience, and now we must adhere to experiments by keeping **N fixed**.
- Not much has been said about fugacity yet. When it was defined in 1.5, we only mentioned that its value is bounded. Now we can elaborate:

What happens to z as $T \rightarrow 0$? At first glance, one might think that $\beta\mu \rightarrow \infty$ as $T \rightarrow 0$, thus $z \rightarrow 0$. However, since N/V must remain constant, from 1.8 it is necessary for fugacity z to scale as $T^{-3/2}$:

$$\frac{N}{V} \Big|_{T_1} = \frac{N}{V} \Big|_{T_2} \rightarrow \frac{z}{\lambda^3} \sim \text{const.} \rightarrow z \sim T^{-3/2},$$

and therefore $z \rightarrow 1$ as $T \rightarrow 0$. As a corollary, the decrease of $\mu < 0$ is greater than that of $1/T$ at low temperatures.

- While equation 1.8 is valid, it is not entirely correct. This is because in the density of states (1.6), the ground state does not contribute anything since $E_0 = 0$. However, this unfortunate situation can be remedied by manually adding the number of particles with $E_0 = 0$ using the Bose-Einstein distribution:

$$N_0 = \frac{1}{e^{-\beta\mu} - 1} = \frac{z}{1 - z}. \quad (1.9)$$

For most systems, it would make little difference whether or not we include this last term, as ultra-cold temperatures are uncommon in nature. However, as $T \rightarrow 0$, more and more particles will occupy the ground state. By rewriting

equation (1.7) while taking the upper integral and adding the new term, we obtain:

$$\begin{aligned} \frac{N}{V} &= \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty dE \frac{E^{1/2}}{z^{-1} e^{\beta E} - 1} + \frac{z}{1-z} \\ &= \frac{1}{4\pi^2} \left(\frac{2mk_B T}{\hbar^2} \right)^{3/2} \int_0^\infty dx \frac{x^{1/2}}{z^{-1} e^x - 1} + \frac{z}{1-z} \\ &= \frac{V}{\lambda^3} g_{3/2}(z) + \frac{z}{1-z}, \end{aligned} \quad (1.10)$$

where $g_n(z) = \sum_{m=1}^{\infty} \frac{z^m}{m^n}$. For values of z close to 1, $g_n(1) = \zeta(n)$ (the Riemann zeta function). This shows that as temperature decreases, the first term becomes less relevant (since it scales as $T^{-3/2}$), while the second term becomes significant. However, it cannot diverge because finite and constant N prevents it. Thus, z cannot reach the value $z = 1$, but rather approaches $z \approx 1 - 1/N$ as $T \rightarrow 0$.

Nevertheless, it is convenient to define a temperature for when $z = 1$. If we have a sufficiently large sample to accept $N \rightarrow \infty$, we can set $g_{3/2}(1) = \zeta(3/2) \approx 2.61$ to obtain the **critical temperature**:

$$T_c = \left(\frac{2\pi\hbar^2}{k_B m} \right) \left(\frac{1}{\zeta(3/2)} \frac{N}{V} \right)^{2/3} = 3.3125 \frac{\hbar^2}{mk_B} \left(\frac{N}{V} \right)^{2/3}, \quad (1.11)$$

which is extremely close to absolute zero.

For temperatures $T < T_c$, we approximate $g_{3/2}(z) = \zeta(3/2)$, and we can derive:

$$\begin{aligned} N &= \frac{V}{\lambda^3} \zeta(3/2) + \frac{z}{1-z}, & T_c &= \lambda T \left(\frac{1}{\zeta(3/2)} \frac{N}{V} \right)^{2/3} \rightarrow \frac{1}{\zeta(3/2)} \frac{N}{V} = \left(\frac{T_c}{\lambda T} \right)^{-3/2} \\ \Rightarrow 1 &= \frac{V}{\lambda^3 N} \zeta(3/2) + \frac{N_0}{N}. \end{aligned}$$

Thus, the occupation ratio of the ground state for temperatures $T < T_c$ is given by:

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c} \right)^{3/2}. \quad (1.12)$$

This equation is enlightening. As the temperature decreases, a significant fraction of the available particles will occupy the lowest energy state, losing their individuality and emerging as a collective of atoms that can be described by just *one* wave function. This macroscopic object, governed by the laws of quantum mechanics and large enough to potentially be seen with the naked eye, is known as a **Bose-Einstein condensate**.

1.3 Heat Capacity near the Critical Temperature

Heat capacity is a great ally in thermodynamics. It is an easy-to-understand concept with significant physical richness. If you add a known amount of energy to a system and measure how much its temperature increases, you will obtain the value of C^{-1} . Heat capacity is defined as

$$C = \frac{\partial E}{\partial T},$$

so we first need an expression for the energy.

Given the density of states $g(E)$ detailed in 1.6, we can not only calculate the number of particles N , but it also allows us to study the average energy in a Bose gas:

$$\langle E \rangle = \int dE \underbrace{E}_{\text{Energy of the state}} \underbrace{\widehat{g(E)}}_{\text{State distribution}} \underbrace{\frac{1}{z^{-1} e^{\beta E} - 1}}_{N^{\circ} \text{ particles per state}}$$

On the other hand, since the **grand canonical potential** Φ ⁴ can be written in two ways:

$$\Phi = -p_{(T,\mu)} V = -k_B T \log \mathcal{Z},$$

where \mathcal{Z} is the partition function 1.3, then we have

$$pV = \frac{1}{\beta} \log \mathcal{Z} = \frac{1}{\beta} \log \left(\prod_r \frac{1}{1 - ze^{-\beta E_r}} \right) = -\frac{1}{\beta} \int dE g(E) \log(1 - ze^{-\beta E}).$$

This integral can be simplified. By integrating by parts⁵, one contribution cancels out due to $g(E) \sim \sqrt{E}$:

$$\int dE \underbrace{g(E) \log(1 - ze^{-\beta E})}_{f'} \underbrace{- \int dE f(h')}_{h} + \int dE (fh)'.$$

Note that since we assigned f' to $g(E)$, to perform integration by parts, we need f :

$$f' = g(E) = \# E^{1/2} \quad \rightarrow \quad f = \frac{2}{3} \# E^{\frac{3}{2}} = \frac{2}{3} g(E) E,$$

where $\#$ indicates the proportionality constants of $g(E)$. After performing integration by parts, we have:

$$pV = \frac{2}{3} \int dE \frac{Eg(E)}{1 - ze^{-\beta E}} \frac{z^{-1} e^{\beta E}}{z^{-1} e^{\beta E}} = \frac{2}{3} \int dE \frac{Eg(E)}{z^{-1} e^{\beta E} - 1} = \frac{2}{3} E. \quad (1.13)$$

As we are interested in the behavior near the critical temperature T_c , we can use an expression for the pressure p for such temperatures. To do this, note that the function $g_{3/2}(z)$, which we already encountered in 1.10, is just a particular function of a class of polylogarithmic functions:

$$\begin{aligned} g_n(z) &= \frac{1}{\Gamma(n)} \int dx \frac{zx^{n-1}e^{-x}}{1 - ze^{-x}} \\ &= \frac{1}{\Gamma(n)} z \int dx x^{n-1} e^{-x} \sum_{m=0}^{\infty} z^m e^{-mx} \\ &= \frac{1}{\Gamma(n)} \sum_{m=1}^{\infty} z^m \int dx x^{n-1} e^{-mx} \\ &= \frac{1}{\Gamma(n)} \sum_{m=1}^{\infty} \frac{z^m}{m^n} \underbrace{\int du u^{n-1} e^{-u}}_{\Gamma(n)} \\ &= \sum_{m=1}^{\infty} \frac{z^m}{m^n} \end{aligned}$$

Thus, if we are interested in the pressure p at low temperatures, we will be interested in the behavior of this function when $z \rightarrow 1$:

$$g_n(1) = \sum_{m=1}^{\infty} \frac{1}{m^n} = \zeta(n),$$

where $\zeta(n)$ is the Riemann zeta function. Noting that 1.13 has the form $g_n(z)$ with $n = 5/2$, then for low temperatures, the pressure behaves as follows:⁶

$$p = \frac{k_B T}{\lambda^3} \zeta(5/2).$$

⁴Which can be understood as the Legendre transform of the free energy $F = \langle E \rangle - TS$.

⁵Derived from $d(f)h = -fd(h) + d(fh)$

⁶See, for example, equation 2.70 in *Bose-Einstein Condensation in Dilute Gases*, C. J. Pethick and H. Smith (2008).

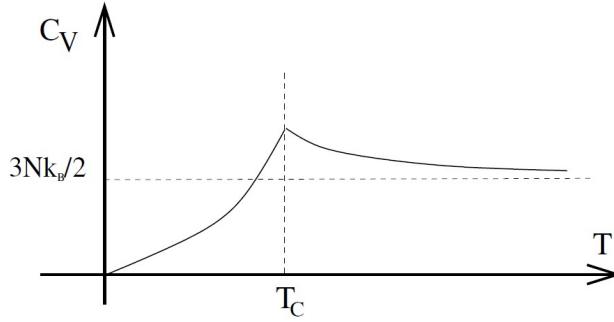


Figure 1.1: Heat capacity for a Bose-Einstein condensate.

Replacing this, we can express the energy in terms of the function $g_{5/2}(z)$, which will be discussed further later:

$$\frac{E}{V} = \frac{3}{2} \frac{k_B T}{\lambda^3} g_{5/2}(z).$$

All this calculation allows us to write the volumetric heat capacity in an interesting form:

$$\frac{C_V}{V} = \frac{1}{V} \frac{dE}{dT} = \frac{15k_B}{4\lambda^3} g_{5/2}(z) + \frac{3}{2} \frac{k_B T}{\lambda^3} \frac{dg_{5/2}}{dz} \frac{dz}{dT}. \quad (1.14)$$

Why is it interesting? As shown in figure 1.1, the heat capacity has a point that we will see is problematic: the derivative of C_V is not continuous at T_c . We will later explore what this fact means. For now, let us examine how both terms of equation 1.14 and their derivatives behave. For this, we need $g_{5/2}(z)$ and its derivatives. Recall that:

$$g_n(z) = \sum_{m=1}^{\infty} \frac{z^m}{m^n} \rightarrow \frac{d}{dz} g_n(z) = \frac{1}{z} g_{n-1}(z),$$

so there will be no issues with discontinuity. Let us study whether the term dz/dT behaves appropriately. For now, this term contributes little to the heat capacity for temperatures $T < T_c$, since $z \approx 1$ and therefore its derivative is nearly zero. But what happens when $T > T_c$ and we approach T_c from above? It is possible to derive the behavior of fugacity z for this case:⁷

$$z \approx 1 - a \left(\frac{T - T_c}{T_c} \right)^2, \rightarrow \frac{dz}{dT} \approx b \left(\frac{T - T_c}{T_c} \right),$$

where a and b are constants that at present do not influence the discussion. Thus, we obtain a heat capacity that can well be defined piecewise:

$$C_V = \begin{cases} \frac{15V k_B}{4\lambda^3} g_{5/2}(z) & \text{si } T < T_c \\ \frac{15V k_B}{4\lambda^3} g_{5/2}(z) - c \left(\frac{T - T_c}{T_c} \right) & \text{si } T > T_c \end{cases} \quad (1.15)$$

where again c is a constant without influence on the discussion. However, there is a subtlety: all along, we have been working in the thermodynamic limit $N \rightarrow \infty$. What happens for finite systems? For this, we need to revisit the fugacity z one last time. Will it contribute to finite systems when $T < T_c$? We already know that most of the particles will be in the ground state, so if we look at equations 1.9 and 1.12, we can write:

$$N_0 = \frac{z}{1-z} \rightarrow z = \frac{N_0}{1+N_0} = \frac{1}{1+N_0^{-1}} = \frac{1}{1+N \left[1 - (T/T_c)^{3/2} \right]}. \quad (1.16)$$

Thus, fugacity is a non-constant function below the critical temperature when the system is finite, and therefore a non-zero contribution to the heat capacity is expected. In some way, the discontinuity only occurs when dealing with non-finite systems in the thermodynamic limit.

⁷Derived in *Statistical Physics*, David Tong, page 88.

Since it is uncommon to encounter theories with discontinuous behavior that aim to faithfully describe nature, it may be worth studying in depth the peculiar figure 1.1. The heat capacity across the critical temperature is an example of a phenomenon known as a **phase transition**.

Chapter 2

Phase Transitions and Spontaneous Symmetry Breaking

A phase transition is a discontinuous change in the properties of a system. At first glance, a phase change is not particularly exotic: when water boils, there is a phase transition¹. However, it is possible to provide a perspective on systems that are not as familiar in everyday life. But what should we observe? A discontinuous change in what? Fortunately, there are scalar quantities that help represent the thermodynamic state of a system: the so-called **thermodynamic potentials**. Therefore, if there is an abrupt change in the properties of a system, it implies an abrupt change in these potentials.

The thermodynamic potentials are the quantities E (energy), F (Helmholtz free energy), G (Gibbs free energy), and H (enthalpy); they are well-defined only in states of thermodynamic equilibrium and are related to each other through **Legendre transformations**².

$$\begin{aligned} dU &= TdS - pdV + \mu dN \\ dF &= -SdT - pdV + \mu dN \\ dH &= TdS + Vdp + \mu dN \\ dG &= -SdT + Vdp + \mu dN \end{aligned} \tag{2.1}$$

We will say that we have a **phase transition of n -th order** when the n -th derivative of a thermodynamic potential is discontinuous. Thus, we can classify the case of the heat capacity of the Bose-Einstein condensate as a second-order phase transition since the derivative of the heat capacity is discontinuous, and this quantity is the derivative of energy E with respect to temperature.

But under what framework should phase transitions be studied? The famous example of boiling water is constructed by examining the van der Waals equation, which describes an interacting gas. Another example, where a sudden change in the magnetization of spins is observed, is built using the mean-field approximation of the Ising model³. However, both examples share the concept of **critical exponents**, which are the exponents that indicate how specific properties scale before and after the phase transition. For instance, the change in specific volume during the liquid-gas transition scales as $v_{\text{gas}} - v_{\text{liquid}} \sim (T_c - T)^\beta$. Additionally, the difference in pressure with respect to a critical value p_c corresponding to the phase transition behaves as $p - p_c \sim (v - v_c)^\delta$, and compressibility scales as $\kappa \sim (T - T_c)^{-\gamma}$.

The key point is that for both examples, the exponents are similar ($\beta \approx 0.32$, $\delta \approx 4.8$, $\gamma \approx 1.2$), which suggests the existence of a general framework for studying phase transitions. This unified way of studying phase transitions is known as Landau Theory.

¹In fact, this is a first-order phase transition. It involves a discontinuous change in volume V . Written in relation to a thermodynamic potential, the volume is $\frac{\partial G}{\partial p} \Big|_{N,T} = V$, and therefore it is of first order.

²The intuitive meaning of a Legendre transformation can be found in the Appendix section.

³This example is highly relevant to the following discussion and is developed in detail in the Appendix section.

2.1 Landau Theory

Landau theory is based on the free energy $F = F(T, V; m)$ and a parameter m called the **order parameter**. If the system lacks a certain degree of order, m will have a value close to zero (for example, a system of spins with random directions). If $m \approx 1$, there will be spontaneous symmetry breaking⁴. Although thermodynamic potentials are only well-defined in a state of equilibrium, it is possible to extend this perspective to systems where the average value of the order parameter m remains constant.

To gain some intuitive understanding of the parameter m , let us return to familiar cases of phase transitions such as water freezing and ferromagnetism. Liquid water enjoys continuous symmetry under translations (i.e., if I have an infinite volume of water and it is translated while my microscope is off, I would not notice its displacement when I turn it on). When it freezes, it undergoes a phase transition and thus breaks this symmetry. To avoid seeing a displacement when turning on the microscope, it must have been shifted by an amount $n \in \mathbb{Z}$ times the lattice parameter. In this case, the order parameter is pressure p , closely linked with volume in everyday systems like our boiling kettle. In ferromagnetism, before the transition, the system was invariant under rotations. After the transition, all spins align in the same direction, breaking this symmetry. In ferromagnetism, the order parameter m represents the magnetization of the system.

For each system of interest, Landau theory begins by choosing an appropriate order parameter m . In the case of a Bose-Einstein condensate, the order parameter is related to the 'off-diagonal long-range order' in the single-particle density matrix⁵ (that is, it traces over all particles in the system except one). Once the order parameter is identified, the next step is to write the free energy in terms of it. This can be complicated. However, a common trick is to assume that expanding the free energy into an analytic power series in m is possible. Logically, such a series will only make sense for values of m close to zero. However, near the critical temperature, this does not pose a problem.

Finally, it should be noted that we are only interested in a second-order phase transition⁶, so the theory will have a parity symmetry $m \rightarrow -m$, and therefore⁷, at fixed volume, we can write the free energy as:

$$F(T; m) = F_0(T) + a(T)m^2 + b(T)m^4 + \dots \quad (2.2)$$

Since we are interested in studying the change in F as m varies, the term $F_0(T)$ is unimportant for this discussion. We seek the equilibrium solutions of F , whether stable or unstable. Thus, we calculate the first derivative and set it equal to zero:

$$\frac{\partial F}{\partial m} \approx 2a(T)m + 4b(T)m^3 = 0 \rightarrow a(T) + 2b(T)m^2 = 0 \quad (2.3)$$

We will assume $b(T) > 0$ for all T . If we relax this condition, we would need to add higher-order terms in m , which give rise to phenomena such as the triple critical point. Later, we will see that a quartic order in m is sufficient, so we maintain $b(T) > 0$. However, $a(T)$ can change its sign as T varies. This is the essence of phase transitions.

⁴Its meaning will be detailed later.

⁵Although it is commonly simplified as the population level in the ground state $|\psi_0|^2$.

⁶This discussion can be found below equations 2.1.

⁷This can be directly seen from the Gross-Pitaevskii equation.

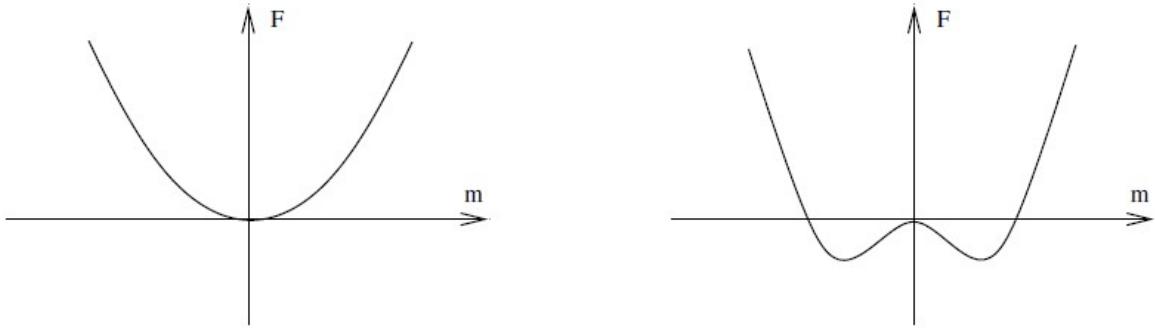


Figure 2.1: For F up to order $\mathcal{O}(m^4)$, the graph depends on the behavior of the first term $a(T)$. On the left, $a(T) > 0$. On the right, $a(T) < 0$.

When we have $a(T) > 0$, there is only one stable minimum of F at $m = 0$. But when $a(T) < 0$, there are three solutions for $\frac{\partial F}{\partial m} = 0$ (as seen in the graph on the right in Figure 2.1). The solution $m = 0$ is unstable, while the stable solutions are characterized by $m = \pm m_0$, where:

$$m_0 = \sqrt{\frac{-a}{2b}} \quad T < T_c.$$

If the function $a(T)$ is continuous, then the minimum value of m changes continuously from $m = 0$ (when $a(T) > 0$) to $m \neq 0$ (when $a(T) < 0$). This describes a second-order phase transition at a temperature T_c such that $a(T_c) = 0$.

Once we know the equilibrium value of m , we can substitute it into

$$F(T; m) \approx F_0(T) + a(T)m^2 \quad \rightarrow \quad F(T; m) = F_0(T) + a\left(\frac{-a}{2b}\right), \quad T < T_c$$

to obtain the free energy of an equilibrium system, which is given by

$$F(T) = \begin{cases} F_0(T) & T > T_c \\ F_0(T) - a^2/2b & T < T_c \end{cases}.$$

It is important to highlight that $F(T)$ is continuous at $T = T_c$, and the entropy

$$S = -\frac{\partial F}{\partial T} = \begin{cases} -F'_0(T) & T > T_c \\ -F'_0(T) + \frac{aa'}{b} - \frac{a^2}{2} \frac{b'}{b} & T < T_c \end{cases}$$

is also continuous, since all terms contain $a(T)$, which is zero at $T = T_c$. However, the heat capacity $C = T\partial S/\partial T$ contains a term a'^2/b that does not vanish at $T = T_c$, so the transition from $C(T > T_c)$ to $C(T < T_c)$ is not continuous, as calculated in the previous chapter.

2.2 Free Energy F in the Context of Landau Theory

As we saw in the previous section, Landau theory for phase transitions involves finding an appropriate order parameter (which for a Bose-Einstein condensate is $|\psi_0|$, see the Appendix) and rewriting the Helmholtz free energy F in terms of that order parameter m . However, since F is given by

$$F = \langle H \rangle - TS,$$

we must first find the average value of the system's Hamiltonian in terms of the order parameter.

The Hamiltonian for a gas of interacting particles can be written as

$$H = \sum_{\vec{k}} E_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{1}{2V} \sum_{\vec{p}, \vec{q}, \vec{k}} U(k) a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_{\vec{q}+\vec{k}} a_{\vec{p}-\vec{k}}, \quad (2.4)$$

where this Hamiltonian has two parts: $H = H_0 + H_I$, where:

- $\sum_{\vec{k}} E_k \hat{a}_k^\dagger \hat{a}_{\vec{k}}$ describes free particles with the dispersion relation $E(k) = \frac{k^2}{2m}$. Additionally, the operators satisfy the canonical commutation relations $[\hat{a}_{\vec{p}}, \hat{a}_{\vec{q}}^\dagger] = \delta(\vec{p} - \vec{q})$, $[\hat{a}_{\vec{p}}, \hat{a}_{\vec{q}}] = 0 = [\hat{a}_{\vec{p}}^\dagger, \hat{a}_{\vec{q}}^\dagger]$.
- $H_I = \frac{1}{2V} \sum_{\vec{p}, \vec{q}, \vec{k}} U(k) \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}+\vec{k}} \hat{a}_{\vec{p}-\vec{k}}$ describes the interaction between particles via the potential $U(k)$ in a volume V .

This can be interpreted as two particles initially having momenta $\vec{q} + \vec{k}$ and $\vec{p} - \vec{k}$, which, after interacting, end up with momenta \vec{p} and \vec{q} .

While the original argument for the Bose-Einstein condensate phenomenon does not account for interactions, it is necessary to include them for a more realistic treatment of the system. However, it is possible to attenuate interactions in a gas by externally tuning the scattering length of the gas using external magnetic fields, thereby creating a bosonic gas closer to what Einstein and Bose initially envisioned. It is crucial to keep in mind that there will always be minimal interaction between particles; otherwise, it would not be possible to thermalize the gas and obtain thermodynamic potentials, which are defined for systems in thermodynamic equilibrium.

Calculating the average energy for the Hamiltonian 2.4 is not straightforward. Still, if we assume that the potential is constant $U(k) = U$, then the average energy of the interaction term in 2.4 becomes:

$$\frac{U}{2V} \sum_{\vec{p}, \vec{q}, \vec{k}} \langle \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}+\vec{k}} \hat{a}_{\vec{p}-\vec{k}} \rangle.$$

However, not all terms in the summation contribute equally. Recall that we are working at low energies, where the occupation of the ground state is significant. We can write the total number of particles according to Bogoliubov's approximation⁸ as:

$$\begin{aligned} N &= \hat{a}_0^\dagger \hat{a}_0 + \sum_{\vec{p} \neq 0} \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{p}} \\ &= N_0 + \sum_{\vec{p} \neq 0} \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{p}} \end{aligned}$$

This helps rewrite the interaction term. Considering low energies, the momentum differences between particles are negligible, motivating us to set $\vec{k} = 0$. In this way:

$$\begin{aligned} \sum_{\vec{p}, \vec{q}} \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}} \hat{a}_{\vec{p}} &= \sum_{\vec{p}} \hat{a}_{\vec{p}}^\dagger \left(N_0 + \sum_{\vec{q} \neq 0} \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}} \right) \hat{a}_{\vec{p}} \\ &= N_0 \sum_{\vec{p}} \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{p}} + \sum_{\vec{p}, \vec{q} \neq 0} \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}} \hat{a}_{\vec{p}} \\ &= N_0 \left(N_0 + \sum_{\vec{p} \neq 0} \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{p}} \right) + \sum_{\vec{p}=0, \vec{q} \neq 0} \hat{a}_0^\dagger \hat{a}_0 \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}} + \sum_{\vec{p} \neq 0, \vec{q} \neq 0} \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}} \hat{a}_{\vec{p}}, \end{aligned}$$

where we can neglect the case $\vec{p} = \vec{q}$, allowing $\hat{a}_{\vec{p}}^\dagger$ to commute with $\hat{a}_{\vec{q}}$. We define the number of excited particles as those not in the ground state, i.e., $N_{ex} = \sum_{\vec{p} \neq 0} \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{p}}$. On the other hand, we must consider the symmetry $\mathbf{p} \rightarrow -\mathbf{q}$, $\mathbf{q} \rightarrow -\mathbf{p}$, meaning that the number of excited particles will have double weight in the count. Finally, the average value of the interaction Hamiltonian becomes:

$$\sum_{\vec{p}, \vec{q}, \vec{k}} \langle \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}+\vec{k}} \hat{a}_{\vec{p}-\vec{k}} \rangle = N_0^2 + N_0 N_{ex} + N_0 N_{ex} + 2N_{ex}^2$$

⁸See the construction of the BEC order parameter in the Appendix.

If the gas is cold enough to neglect the kinetic energy from the free Hamiltonian, then the average energy of the total Hamiltonian will be:

$$\langle H \rangle = \frac{U}{2V} N_0^2 + \frac{U}{V} N_0 N_{\text{ex}} + \frac{U}{V} N_{\text{ex}}^2 \quad (2.5)$$

$$= \frac{U}{V} \left(N^2 - NN_0 + \frac{1}{2} N_0^2 \right). \quad (2.6)$$

Now, we need the entropy S . Entropy is defined as:

$$S(E) = k_B \log \Omega(E),$$

where $\Omega(E)$ is the number of possible microstates compatible with the macroscopic energy E . In this case, the energy will be dominated by the number of excited particles $N_{\text{ex}} = \sum_{\vec{p} \neq 0} N_{\vec{p}}$. To heuristically obtain the entropy, we need to ask how many configurations the gas can have. There will be particles with $\vec{p} = 2\hat{p}$, $\vec{p} = 7\hat{p}$, etc. For each fixed value of \vec{p} , we must place the remaining particles with different momenta such that:

$$\Omega(|H\rangle) \approx \prod_{\vec{p}} N_{\vec{p}}.$$

Thus, the entropy S of the system is approximately⁹:

$$S \approx k_B \sum_{\vec{p}} \ln N_{\vec{p}}. \quad (2.7)$$

Now suppose that in a certain region of momentum space \vec{p} there are N_s particles and that the momenta of these particles do not differ significantly. Therefore, the value of $N_{\vec{p}}$ does not deviate much from the average $\bar{N}_{\vec{p}} = N_{\text{ex}}/N_s$. With this assumption, we can consider each term in equation 2.7 to have an equal value. Finally, the entropy can be written as:

$$\begin{aligned} S &\approx k_B N_s \ln(\bar{N}_{\vec{p}}) = k_B N_s \ln(N_{\text{ex}}/N_s) \\ &= k_B N_s [\ln(N - N_0) - \ln N_s]. \end{aligned}$$

We now have $\langle E \rangle$ and S . We can write the Helmholtz free energy as:

$$F = \frac{UN^2}{V} - UN \frac{N_0}{V} + \frac{1}{2} U \frac{N_0^2}{V} - k_B T N_s [\ln(N - N_0) - \ln N_s].$$

Recall that the goal was to express F in a form similar to 2.2, that is, as a power series of the system's order parameter $|\psi_0|$. To achieve this, we divide the condensed fraction N_0 by the volume V :

$$|\psi_0|^2 = \frac{N_0}{V},$$

and thus obtain:

$$\frac{F}{V} = \frac{F_0}{V} - U \frac{N}{V} |\psi_0|^2 + \frac{1}{2} U |\psi_0|^4 - k_B T \frac{N_s}{V} \left[\ln \left(N/V - |\psi_0|^2 \right) - \ln N_s/V \right], \quad (2.8)$$

which is the desired expression for F . If we create a 2D plot, it becomes clear that $\psi_0 = 0$ is an unstable equilibrium point. As the number of particles increases, the interaction energy decreases, making it no longer the true minimum (see Figure 2.2).

⁹See *An Introduction to Quantum Statistics*, William Band, page 162, where a rigorous derivation of:

$$S = -k_B \sum_{\vec{p}} \left(N_{\vec{p}} \ln N_{\vec{p}} - (1 + N_{\vec{p}}) \ln(1 + N_{\vec{p}}) \right)$$

is presented. From there, it is possible to derive the same entropy as in equation 2.7.

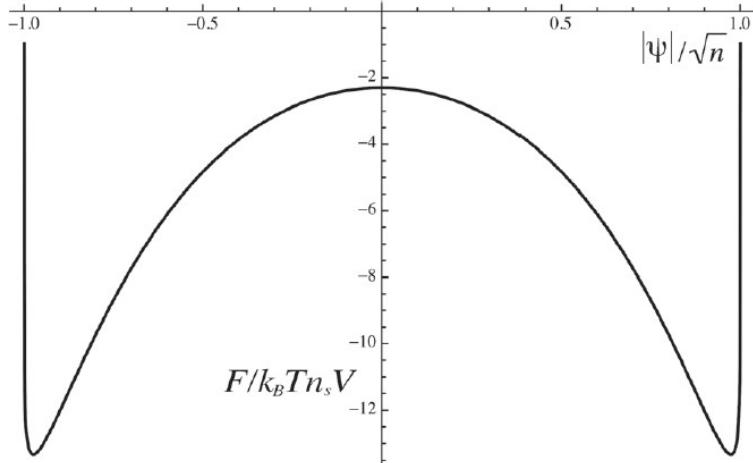


Figure 2.2: Free energy for an interacting BEC with $Un/k_B T = 1$ and $N/N_s = 10$.

This plot can have either the real or imaginary part of $\psi_0 = \sqrt{n_0} e^{i\theta}$ as the x -axis (where $n_0 = N_0/V$ and θ is the phase angle). A more detailed figure would show the continuum of possible values for θ , resembling Figure 2.3.

The shape of the graph for F is typical for systems that transition from a symmetric minimum at $m = 0$ to an off-center minimum at $m = pmm_0$. This represents spontaneous symmetry breaking.

2.3 Spontaneous Symmetry Breaking

To minimize the Helmholtz free energy $F(T)$ for temperatures $T < T_c$ in a ferromagnetic system, it is necessary to choose one of the minima $m = \pm m_0$. This breaks the \mathbf{Z}_2 symmetry, and thus, it is said that the ground state *spontaneously* breaks the symmetry by choosing either the right or left minimum in Figure 2.1.

However, for a Bose-Einstein condensate, we can only consider¹⁰ $m = |\psi_0| > 0$. The broken symmetry will not be \mathbf{Z}_2 ; instead, there is now a continuum of ground states that minimize $F(T)$, and the system will select only one value among them. This is equivalent to choosing the phase of ψ_0 , which until now remained completely undetermined.

¹⁰See Appendix 4, where the order parameter for a BEC is studied.

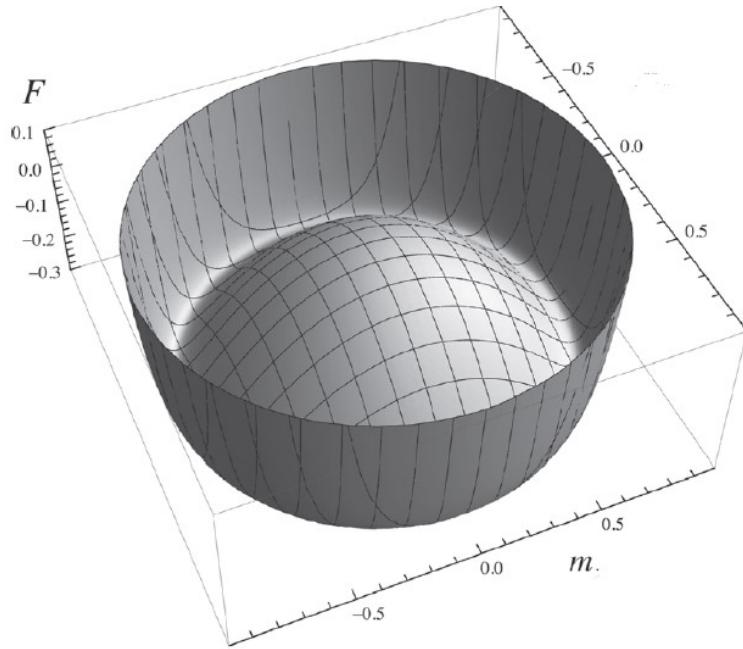


Figure 2.3: For values $m > 0$, there is a continuum of phase values that lead to a minimum of F .

A stable minimum value of F is found on a ring with fixed amplitude. That is, we can treat the order parameter as:

$$m = |\psi_0(r)|^2 = |e^{i\theta} \psi_0(r)|^2 \quad \rightarrow \quad \vec{m} = m(\hat{x} \cos \theta + \hat{y} \sin \theta),$$

where θ is arbitrary. When a specific value of θ is chosen, it is said that the system has spontaneously broken the continuous symmetry $U_{(1)}$. It is worth mentioning that variations in θ are known as **Goldstone modes**, while oscillations of m in the radial direction of the so-called Mexican hat potential in Figure 2.3 are known as **Higgs modes**.

Let us return for a moment to the ferromagnetic case. What causes the system to favor a minimum at $m = m_0$ or $m = -m_0$? Recall that, in this case, the order parameter is magnetization, so any external electromagnetic field would suffice to create a preferred direction toward which the spins tend to align. The system amplifies this slight asymmetry until it reaches a macroscopic value for the average value of m .

So, what external fluctuation triggers the spontaneous breaking of $U_{(1)}$ symmetry in a BEC? This is an open question in the field. Since the nature of the order parameter is entirely different, it is not known with certainty what causes it—or even if there *is* an external fluctuation that causes it. Whether all spontaneous symmetry breakings correspond to analogs of the ferromagnetic case is also an open question. One factor to consider is the measurement process, but without a complete understanding of the phenomenon, this cannot be accepted or dismissed as an answer.

This presents a scenario similar to early-universe cosmology, where spontaneous symmetry breaking is also observed—for example, in the Higgs mechanism that gives mass to fundamental particles. It is difficult to answer whether such symmetry breakings are due to external fluctuations (external to the universe?) or the measurement phenomenon (by whom?). In any case, if one region at some edge of the universe broke symmetry before a causally disconnected region, it is expected that their minimum values would not necessarily match.

2.4 Landau-Ginzburg Theory

The issue with Landau's theory is that it assumes the same order parameter regardless of where it is observed: $m \neq m(\vec{r})$. If the system's fluctuations cannot be ignored, then treating the order parameter as an average is insufficient; instead, it must be generalized as a quantity that varies in space: $m = m(\vec{r})$. For a second-order phase transition, we move from

the expression for the free energy

$$F(T; m) = F_0(T) + a(T)m^2 + b(T)m^4 + \dots$$

to now considering the free energy as a functional (i.e., a function of a function $m(\vec{r})$), meaning its value involves integrating over the entire space encompassed by \vec{r} :

$$F[m(\vec{r})] = \int d^3r [a(T)m^2 + b(T)m^4 + c(T)(\nabla m)^2], \quad (2.9)$$

where, for simplicity, we write $m(\vec{r}) = m$, omit the constant $F_0(T)$, and add the gradient squared term ∇m as a reminder of a system with some 'rigidity.' In other words, an energetic cost is associated with varying the order parameter from one point to another.

We must use the same variational methods as in Lagrangian mechanics to find the minimum free energy. We set the variation to zero and obtain the analog of the Euler-Lagrange equation for the free energy:

$$\begin{aligned} \delta F &= \int d^3r [2am\delta m + 4bm^3\delta m + 2c\nabla m \cdot \nabla \delta m] \\ &= \int d^3r \left[2am\delta m + 4bm^3\delta m - 2c\nabla^2 m \underbrace{\delta m}_{\text{boundary term}} + 2c\nabla \cdot (\nabla m \delta m) \right] \\ &= \int d^3r [2am + 4bm^3 - 2c\nabla^2 m] \delta m \\ &= 0, \end{aligned}$$

which implies that

$$c\nabla^2 m = am + 2bm^3 \quad (2.10)$$

Considering $m = \text{constant}$, we recover equation 2.3 from Landau's theory. On the other hand, if $m = m(\vec{r})$, we can find more interesting solutions. The first observation is that we cannot expect an abrupt change in the parameter $m(\vec{r})$, as this would lead to an infinite contribution to the free energy F . Therefore, if two regions have different order parameters, they will be separated by domain walls with a nonzero width.

Let us now suppose that we have a very localized region with a fluctuation of $m(\vec{r})$ that stands out from the surrounding average. How can we characterize such a fluctuation? Imagine the system is in its ground state with an average order parameter $m = m_0$. We can write a fluctuation around it as

$$m(\vec{r}) = m_0 + \delta m(\vec{r}).$$

By substituting this into 2.10, we obtain

$$\begin{aligned} c\nabla^2(m_0 + \delta m) &= a(m_0 + \delta m) + 2b(m_0 + \delta m)^3 \\ \rightarrow c\nabla^2\delta m &= am_0 + a\delta m + 2b(m_0^3 + 3m_0^2\delta m + 3m_0\delta m^2 + \delta m^3). \end{aligned}$$

We retain only the linear terms in δm ,

$$\begin{aligned} c\nabla^2\delta m &= am_0 + a\delta m + 2bm_0^2 + 6bm_0^2\delta m \quad m_0^2 = \frac{-a}{2b} \\ &= a\delta m - 3a\delta m \\ \Rightarrow \left(\nabla^2 + \frac{2a}{c} \right) \delta m &= 4\pi\delta^3(0), \end{aligned}$$

where we introduced the delta function since it is a localized fluctuation. The solution to this type of equation (up to some factor) is given by

$$\delta m \sim \frac{e^{-r/\xi}}{r},$$

so the fluctuation of the order parameter follows a Yukawa-like potential decay. In this potential, it is common to say that the range of influence is limited by the denominator of the exponent in e . In this case, the correlation of the order

parameter is constrained by what is called the **correlation length** ξ , given by

$$\xi = \sqrt{\frac{-c}{2a}}. \quad (2.11)$$

That length determines the spatial extent of an individual fluctuation. In the context of Landau theory, near the critical temperature T_c , the factors a and b behave as

$$b(T) \approx b_0 \quad , \quad a(T) \approx a_0(T - T_c),$$

since $a(T)$ must change sign during a second-order phase transition. In general, the behavior near T_c is studied in the context of **Critical Phenomena**, requiring tools from the **Renormalization Group**. The correlation length in 2.11 is a specific case of the equilibrium correlation length with $\nu = 1/2$:

$$\xi(\varepsilon) = \frac{\xi_0}{|\varepsilon|^\nu},$$

where $\varepsilon \sim T - T_c$ is known as the reduced temperature of the system. Here, ξ_0 depends on the physics of the system under study, unlike ν , which is common to many physical systems that, in principle, do not need to share this characteristic. Further discussion can be found in the section on the *Kibble-Zurek Mechanism*, which makes universal scaling predictions for the dynamics of out-of-equilibrium systems using known results from the critical behavior of systems in equilibrium.

Chapter 3

Coherence in Condensates and the Kibble-Zurek Mechanism

So far, we have discovered two things: (1) the phase transition to a Bose-Einstein condensate involves a spontaneous symmetry breaking, and (2) the minimum that the system *chooses* can differ between different regions of the system.

Each aspect raises questions of various kinds: (1) Does a gas with $T < T_c$ *have* a defined phase? Is the phase fixed upon observation? (2) How are the regions with a certain *choice* of minimum distributed? Is this distribution characteristic only of a Bose-Einstein condensate? The following sections address these questions.

3.1 The Question of Coherence

In 1997, a team of physicists prepared two Bose-Einstein condensates and released them one right next to the other¹. Given the momentum distribution of the gas, they expand during their time of flight². When launched with a small separation, part of them overlap. This fact is significant because if each condensate acquires a phase upon symmetry breaking, their overlap is expected to manifest as interference on the sensors. This is what was observed in 1997, as shown in Figure 3.1.

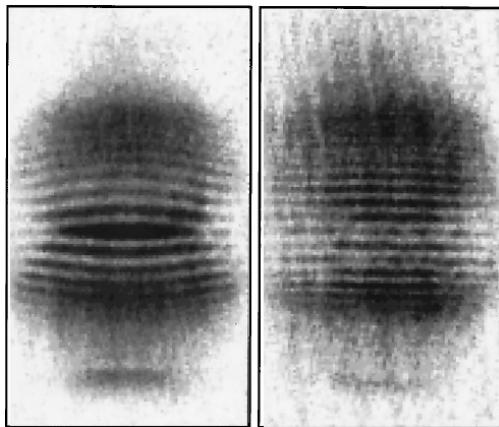


Figure 3.1: Patrón de interferencia dos condensados luego de 40 ms de *time-of-flight*. La absorción máxima es del 90% para la imagen izquierda y 50% para la derecha.

¹ Andrews, M. R., Townsend, C. G., Miesner, H.-J., Durfee, D. S., Kurn, D. M., and Ketterle, W. 1997. *Observation of interference between two Bose condensates*. Science, 275(5300), 637–641.

²In fact, the technique used is called *time-of-flight*.

An interference pattern between two condensates would seem to imply a defined relationship between the phases of both condensates. However, a standard definition of a coherent state $|\alpha\rangle$ in quantum optics is written as a constructive interference of infinite Fock states, which helps establish a well-defined phase:

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad \rightarrow \quad P(n) = |\langle n | \alpha \rangle|^2 = e^{-\langle n \rangle} \frac{\langle n \rangle^n}{n!},$$

but it also carries with it a Poissonian distribution of Fock states³, and therefore, it has an undefined photon number. While the mean photon number $\langle n \rangle$ can be established, the fluctuation will also be on the order of $\langle n \rangle$.

If we assume that the condensate has a defined phase, then it should be well represented by a coherent state. However, at $T \approx 0$, a condensate has a fixed number of particles and therefore cannot be seriously treated as a coherent state. From an experimental perspective, it is impossible to determine whether condensates have a well-defined phase before measurement or if they acquire it afterward. The spontaneous symmetry-breaking framework assumes that the condensate spontaneously adopts a specific defined phase, but experiments do not strictly require this assumption. In fact, it is possible to obtain the interference pattern from an approach that respects particle number conservation for both condensates and scenarios with two condensates with a fixed number of particles each.

The symmetry-breaking framework makes it clear that it is possible to write the initial state of a non-interacting condensate as a product of coherent states, where there are M sites to distribute N atoms homogeneously:

$$|BEC_{SB}\rangle = \prod_l^M e^{-\frac{|\beta_l|^2}{2}} e^{\beta_l b_l^\dagger} |\text{vac}\rangle,$$

where $|\beta_l|^2$ is the average number of particles at the site labeled by l , and the subscript SB refers to the *symmetry-breaking* scenario. On the other hand, if we require conservation of N particles in a homogeneous system with M sites, we can write the initial state as

$$|BEC_N\rangle = \frac{1}{\sqrt{N!N^N}} \left(\sum_i^M \beta \hat{b}_i^\dagger \right)^N |\text{vac}\rangle,$$

since $\beta_l = \beta$ in a homogeneous system. It is possible to show⁴ that both scenarios lead to the same time-dependent correlation function:

$$|BEC_{SB}\rangle \quad \rightarrow \quad \langle b_i^\dagger b_j \rangle(t) = |\beta|^2 e^{|\beta|^2(2\cos(Ut)-2)}, \quad (3.1)$$

$$|BEC_N\rangle \quad \rightarrow \quad \langle b_i^\dagger b_j \rangle(t) = |\beta|^2 e^{|\beta|^2(2\cos(Ut)-2)}. \quad (3.2)$$

Thus, they produce the same interference pattern observed in Figure 3.1, as long as the number of particles is sufficiently large, as shown in Figure 3.2.

So, why is a coherent treatment almost ubiquitous in the literature? Conceptually and mathematically, it is simpler and predicts the correct experimental results. Thus, we will always see $\hat{\Psi}(r) \approx \psi_0(r) = \sqrt{N_0} \varphi_0(r) = \sqrt{N_0} e^{i\theta(r)}$ as the state describing a Bose-Einstein condensate.

To summarize, in the spontaneous symmetry-breaking formalism (also called the coherent state formalism), each BEC chooses a random phase $\theta_1(r)$ and $\theta_2(r)$. These phases are not observable, but through the interference of both BECs, it is possible to measure interference patterns related to the phase difference $\theta_1(r) - \theta_2(r)$. This phase will be different for each repetition of the experiment since each phase is random. However, this state cannot describe a condensate because, as $T \rightarrow 0$, there are no fluctuations in the number of atoms in the condensate.

On the other hand, in the Fock state formalism, the condensate is described by the number state $|N_0\rangle$ with a flat phase distribution, meaning it is entirely indeterminate. In the article *Relative phase of two Bose-Einstein condensates*⁵, it is

³These are states with a well-defined photon number.

⁴See Nick P. Proukakis, David W. Snoke, Peter B. Littlewood, *Universal Themes of Bose-Einstein Condensation*, Cambridge University Press (2017), pages 90–93.

⁵*Relative phase of two Bose-Einstein condensates*, Yvan Castin, Jean Dalibard, Phys. Rev. A 55, 4330 – June 1, 1997.

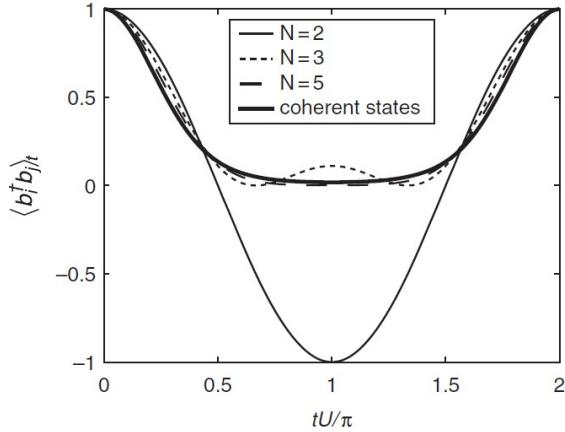


Figure 3.2: Time evolution of the off-diagonal elements of the density matrix for a single particle (i.e., the order parameter). For $N = 5$, the prediction for a Fock state closely matches that of the coherent state (thick solid line).

shown (through a thought experiment) that it is still possible to observe an interference pattern between two BECs even when each BEC is in a Fock state with particle number conservation.

3.2 Kibble-Zurek Mechanism

Within the Landau-Ginzburg theoretical framework, when considering spatially dependent parameters $m = m(\vec{r})$, it becomes evident that causally disconnected regions cannot guarantee alignment in their selection of minima within the Mexican hat potential. Different spatial domains may independently choose distinct phases (minima positions) with equal validity, as no external symmetry-breaking field exists to preferentially select a specific direction - unlike ferromagnetic systems where even weak external fields establish directional preference. This naturally leads to the emergence of domains with random phase orientations.

As previously noted, Bose-Einstein condensation constitutes a continuous phase transition. The theory of **critical phenomena** dictates that near criticality, correlation functions exhibit universal scaling behavior governed by critical exponents that remain independent of microscopic system details. For *homogeneous* systems approaching the critical point, the correlation length ξ follows scaling relations characterized by the critical exponent ν , generalizing the result in 2.11 from Landau-Ginzburg theory. This scaling behavior is expressed as:

$$\xi = \frac{\xi_0}{|\epsilon|^\nu}, \quad \text{where } \epsilon = \frac{T - T_c}{T_c}$$

where ϵ denotes the reduced temperature, and ξ_0 represents a system-dependent constant determined by the gas's microscopic parameters - in contrast to ν , which remains universal across diverse physical systems. Specifically, Bose gases belong to the XY universality class, sharing critical exponents with superfluid systems such as helium-4. For this class, $\nu \approx 1/2$, though this value depends on the theoretical framework employed (whether derived through Landau-Ginzburg theory or Renormalization Group approaches).

Similarly to how ξ governs the spatial extent of individual fluctuations, one can define a corresponding parameter for their temporal duration. The equilibrium relaxation time τ is expressed as:

$$\tau = \frac{\tau_0}{|\epsilon|^{\nu z}},$$

where z denotes the dynamic critical exponent, which crucially *does not* depend on the system's intrinsic parameters but rather on its universality class. For this specific case, $z \approx 2$. Both correlation measures, ξ and τ , originate from equilibrium system analyses.

While fundamentally important in its own right, the principal significance of equilibrium critical fluctuation theory

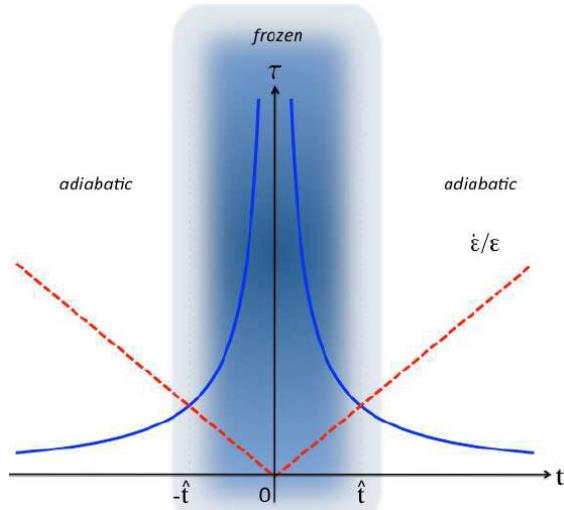


Figure 3.3: Schematic representation of Kibble-Zurek mechanism stages. In the $t > 0$ region, phase symmetry becomes compromised due to divergence of relaxation time τ near $\epsilon = 0$. Red lines compare equilibrium relaxation time with elapsed time post-critical point crossing at $t = 0$, following $\tau(\hat{t}) \approx |\dot{\epsilon}/\epsilon| = |t\tau_Q^{-1}/\tau_Q^{-1}| = t$.

lies in its extension to non-equilibrium physics - particularly regarding critical exponent scaling and universality class behavior. A prominent example of such extension is the **Kibble-Zurek mechanism** (KZM), which utilizes equilibrium relationships to predict non-equilibrium dynamics during second-order phase transitions.

The physical scenario can be conceptualized as follows: A system initially in equilibrium undergoes linear temperature reduction through the critical temperature towards a new equilibrium state. During this temperature variation, the system traverses a phase transition. For sufficiently slow cooling rates (large τ_Q), one might reasonably expect the system to maintain global phase coherence - analogous to a uniform white sheet. Conversely, rapid cooling prevents global phase selection, resulting in spatially fragmented domains characterized by local rather than global minima. These domains containing distinct phase orientations (topological defects) retain crucial information about the non-equilibrium transition process.

The mechanism aims to quantify the spontaneous defect density distribution. KZM postulates linear temporal evolution of the reduced temperature parameter:

$$\epsilon = \frac{T - T_c}{T_c} = \frac{t}{\tau_Q}$$

where τ_Q represents the cooling (quench) duration, with $t \in [-\tau_Q, \tau_Q]$ and critical point crossing occurring at $t = 0$. At this juncture, system dynamics effectively freeze due to divergence of τ . KZM partitions the process into three distinct regimes: initial adiabatic evolution, frozen dynamics near criticality, and subsequent adiabatic evolution as $\epsilon(t)$ changes sign. Figure 3.3 provides schematic representation of these stages.

This dynamic arrest **does not** imply complete cessation of system evolution or order parameter development: microscopic states continue evolving according to the governing Hamiltonian. However, the order parameter ceases pursuing global equilibrium values, potentially achieving local equilibrium post-critical crossing after delay \hat{t} - constrained by topological defects. This delay marks the frozen regime boundary, characterized by relaxation time τ surpassing remaining system evolution time to critical point.

$$\begin{aligned}\hat{t} &= \tau(\hat{t}) \\ \rightarrow \hat{t} &= \tau_0 \tau_Q^{\nu z} \frac{1}{\hat{t}^{\nu z}} \\ \rightarrow \hat{t}^{1+\nu z} &= \tau_0 \tau_Q^{\nu z}\end{aligned}$$

$$\longrightarrow \hat{t} = (\tau_0 \tau_Q^{\nu z})^{\frac{1}{1+\nu z}}$$

where \hat{t} denotes the unfreezing time. Spontaneous symmetry breaking induces ground state degeneracy. In extended systems, causally disconnected regions make independent phase choices. KZM proposes average domain sizes through correlation length ξ at temperature $\hat{\epsilon} = |\epsilon(\hat{t})|$:

$$\hat{\epsilon} = (\tau_0 \tau_Q^{\nu z})^{\frac{1}{1+\nu z}} \tau_Q^{-1} = \tau_0^{\frac{1}{1+\nu z}} \tau_Q^{\frac{\nu z}{1+\nu z}-1} = \left(\frac{\tau_0}{\tau_Q} \right)^{\frac{1}{1+z\nu}}$$

yielding correlation length at this temperature:

$$\hat{\xi} = \xi(\hat{\epsilon}) = \xi_0 \left(\frac{\tau_Q}{\tau_0} \right)^{\frac{\nu}{1+z\nu}}$$

constituting KZM's central prediction. This result is often reformulated as topological defect density estimation from spontaneous symmetry breaking:

$$n \sim \frac{\hat{\xi}^d}{\hat{\xi}_0^D} = \frac{1}{\xi_0^{D-d}} \left(\frac{\tau_0}{\tau_Q} \right)^{(D-d)\frac{\nu}{1+z\nu}}, \quad (3.3)$$

where D and d represent spatial and defect dimensions respectively. Since non-equilibrium duration spans $2\tau_Q$, rapid cooling ($\tau_Q \ll 1$) produces abundant transition defects, while slow near-adiabatic cooling ($\tau_Q \gg 1$) minimizes defect formation.

This estimation provides order-of-magnitude guidance, typically overestimating actual defect densities. However, verification of power law 3.3 suggests universal non-equilibrium phase transition dynamics through KZM.

As Bose-Einstein condensates share critical exponents with helium-based superfluids, they exhibit $\nu \approx 0.67 \pm 0.13$ and $z \approx 1.4 \pm 0.2$ ⁶. For example, 3D superfluid vortex lines would involve $D = 3$ and $d = 1$.

⁶Navon, N., Gaunt, A. L., Smith, R. P., and Hadzibabic, Z. 2015. *Critical dynamics of spontaneous symmetry breaking in a homogeneous Bose gas*. Science, 347, 167.

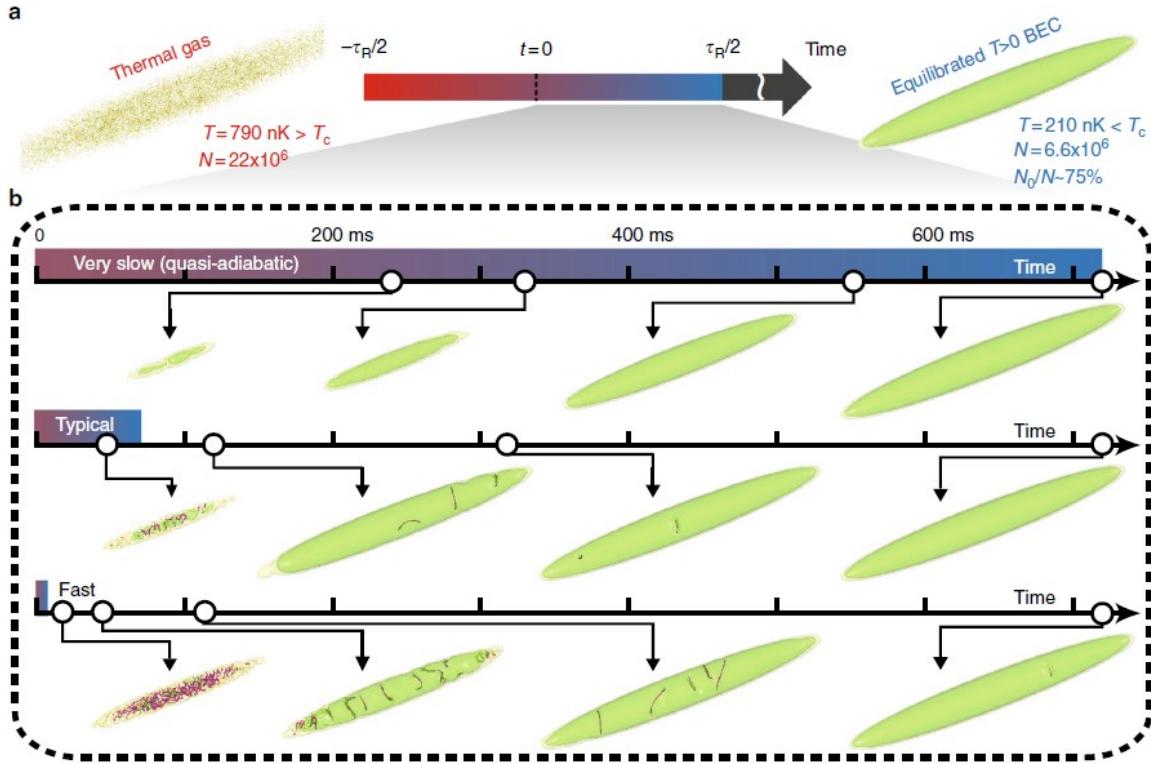


Figure 3.4: Dynamic response of thermal equilibrium gas under three cooling regimes with $\tau_R = 1440, 144, 18\text{ms}$ (where $\tau_R = \tau_Q$). Taken from Wojciech H. Zurek and A. del Campo, *Universality of Phase Transition Dynamics: Topological Defects from Symmetry Breaking*, with the authors' authorization. Available on arXiv (arXiv:1310.1600, 2013, <https://arxiv.org/abs/1310.1600>).

This scenario was recently investigated⁷, simulating thermal bosonic gas ($T > T_c$) cooling under three regimes (slow, typical, rapid) to achieve 75% Bose-Einstein condensation. Figure 3.4 demonstrates that near-instantaneous cooling produces dense random vortex tangles with phase discontinuities, while near-adiabatic processing yields uniform phase distribution - consistent with equation 3.3 predictions.

⁷I. Liu, S. Donadello, G. Lamporesi, G. Ferrari, S. Gou, F. Dalfovo and N. P. Proukakis, *Dynamical equilibration across a quenched phase transition in a trapped quantum gas*, Nature Communications Physics volume 1, Article number: 24 (2018).

Chapter 4

Atomic Cooling

When we talk about low temperatures, how low are these temperatures? Suppose we have 1 million Rubidium atoms in a cube of 0.1 square millimeters. Thanks to 1.11 we can actually calculate the critical temperature in this scenario:

$$\begin{aligned} m \approx 85.46 u &= 1.42 \times 10^{-25} [\text{kg}] & \frac{N}{V} &= \frac{10^6}{10^{-12}} = 10^{18} & \frac{\hbar^2}{k_B} &\approx 8 \times 10^{-46} [\text{kg m}^2 \text{ K}] \\ \Rightarrow T_c &= 3.3125 \left(\frac{\hbar^2}{k_B} \right) \frac{1}{m} \left(\frac{N}{V} \right)^{2/3} & & & & \\ &= 3.3125 \times 8 \times 1.42 \times (10^{-46+25+12}) [\text{K}] & & & & \\ &= 37.63 \times 10^{-9} [\text{K}]. & & & & \end{aligned}$$

This gives us the idea that to create a BEC we need temperatures on the order of nano-Kelvin, quite close to absolute zero. How is it possible to achieve temperatures low enough to observe a Bose-Einstein condensate? In simple terms, we need three sets of techniques to meet the theoretical requirements of BEC:

- We need to control a gas of atoms, using a magnetic trap (*Magnetic trapping*).
- The gas of atoms must be cooled as much as possible using laser cooling (*Laser cooling*). A limiting temperature for this technique will be reached, called the recoil temperature.
- Because the gas is not yet cold enough, we need to remove the most energetic atoms through evaporative cooling (*Evaporative cooling*).

4.1 Laser Cooling

The classical **equipartition of energy** principle relates the temperature of a gas to the average speed of its constituents. From equation 1.1, we can obtain the average energy of a monoatomic bosonic gas

$$E = -\frac{\partial}{\partial \beta} \log Z = \frac{3}{2} N k_B T,$$

and therefore each particle that only has three translational degrees of freedom contributes an energy $E = 3k_B T/2$. The equipartition of energy principle states that each degree of freedom contributes $Nk_B T/2$ to the thermal energy of each particle. Since we are interested in non-interacting (or weakly interacting) gases, we can correspond this energy to the

kinetic energy of a free particle: $mv_x^2/2$. For three translational degrees of freedom, we have¹

$$\frac{1}{2}mv^2 = \frac{3}{2}k_B T \rightarrow v^{\text{rms}} = \sqrt{\frac{3k_B T}{m}}.$$

Therefore, a relationship can be established between the temperature (which we are interested in decreasing) and the velocity of each particle. Laser cooling helps to reduce this velocity.

The idea of using a **laser** to cool a gas seems strange, as this would intuitively add energy to the gas and thus increase the temperature. The key to cooling is to tune the laser to a frequency close to resonance with the atomic transition of the gas.

For this purpose, let's consider an atom (with transition frequency ν_0) moving in the $+x$ direction with velocity v_x . We assume it will interact with a laser in the opposite direction with wavelength λ_L and frequency ν_L . This frequency is adjusted to a value close to the resonance frequency of the atom ν_0 . We can write the laser frequency as

$$\nu_L = \nu_0 + \delta = c/\lambda_L,$$

where $\delta \ll \nu_0$. In the atom's frame of reference, the laser source is approaching the atom, and due to the **Doppler effect**, its frequency changes as

$$\nu'_L = \nu_L \left(1 + \frac{v_x}{c}\right) = (\nu_0 + \delta) \left(1 + \frac{v_x}{c}\right) \approx \nu_0 + \delta + \frac{v_x}{c} \nu_0,$$

where $v_x \ll c$. The key to laser cooling consists of appropriately choosing the laser frequency such that

$$\delta = -\nu_0 \frac{v_x}{c} = -\frac{v_x}{\lambda_L}$$

and thus we'll have $\nu'_L = \nu_0$. In other words, if the atom is moving in the direction opposite to the laser, it will come into resonance and absorb photons. The atom will then emit a photon in an arbitrary direction due to spontaneous emission. Note that this effect only affects those atoms moving in the direction opposite to the laser. To cool the gas, the emission-absorption cycle must be repeated several times since the atom absorbs a photon with momentum $p = h/\lambda_L$ and then emits in a random direction, so on average, the change in momentum due to emission is zero, unlike in absorption, which is always in the direction opposite to the laser. Finally, the cycle results in a change of the momentum of the atom

$$\Delta p_x = -\frac{h}{\lambda_L}.$$

The main difficulty lies in gradually changing the value of δ (and therefore changing λ_L) as the atoms decrease their velocity. Even so, in general terms, if we consider a laser with sufficient intensity to re-excite the atom immediately after emission, we will obtain a deceleration of the atom given by

$$F_x = \frac{dp_x}{dt} \approx \frac{\Delta p_x}{2\tau} = -\frac{h}{2\lambda_L \tau} \rightarrow \dot{v}_x = \frac{F_x}{m} \approx -\frac{h}{2m\lambda_L \tau}$$

where F_x is a friction force and τ is the mean lifetime of the excited atom before emitting the photon by spontaneous emission. The factor of two in the denominator is explained because, for high-intensity lasers, a gas of N atoms will have a population level in the excited state equal to $N/2$. Thus, only half of the gas can absorb photons from the laser, while the other half will be emitting. More precisely, the friction force is equal to the change in momentum experienced in each emission-absorption cycle multiplied by the net rate of such cycles

$$F_x = -\frac{h}{\lambda_L} \times R(I, \Delta) = -\hbar k_L \times R(I, \Delta),$$

¹The acronym **rms** indicates the *root mean square* velocity, and is defined as the square root of the mean of the squares of the velocities of the molecules in a gas. The reason for using **rms** velocity instead of average velocity is that the latter is zero, as the particles are moving randomly in all directions.

where the net absorption rate $R(I, \Delta)$ is given by the absorption rate minus the emission rate that is stimulated by the laser (and therefore will depend on the laser intensity), and is given by

$$R(I, \Delta) = \frac{\gamma}{2} \left(\frac{I/I_s}{1 + I/I_s + [2(\Delta + k_L v_x)/\gamma]^2} \right),$$

where $\gamma = 1/\tau$ is the natural linewidth in frequency units, and I_s is the saturation intensity of the transition. It should be noted that for very high intensities $R(I, \Delta) \sim \gamma/2 = 1/(2\tau)$, and for low intensities we can ignore the term I/I_s in the denominator, so the net absorption rate grows linearly with I .

Naturally, this cooling process will not be useful when a velocity v_x is reached such that $v_0 v_x/c$ is too small to adjust the laser. Under these conditions, the thermal energy of the atom will be practically equal to $h\nu_0$, and therefore the order of the minimum temperature provided by this Doppler cooling technique is given by

$$k_B T_{\min} \sim h\nu_0$$

If we continue bombarding the gas with $v_L \sim v_0$, eventually the atoms moving in the $+x$ direction will experience an opposite acceleration, reaching velocities in the $+x$ direction. Therefore, to achieve low temperatures, it is necessary to have two lasers, as shown in the image:

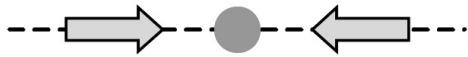


Figure 4.1: Two opposing lasers are used for greater cooling.

For a three-dimensional gas, six lasers are needed to carry out the cooling². Through this process, the changing velocity of the gas is damped, which is why this technique is called **optical molasses**³, capable of reaching minimum temperatures⁴

$$T_{\min} = \frac{\hbar\gamma}{2k_B} \equiv \frac{\hbar}{2k_B\tau}.$$

This shows that the minimum temperature that can be achieved with Doppler cooling is limited by the mean lifetime τ of the transition. Finally, associated with this temperature is a limit velocity that is minimal for this technique

$$\frac{1}{2}mv_x^2 = \frac{1}{2}k_B T \quad \rightarrow \quad v_x^{\min} = \sqrt{\hbar/2m\tau}$$

4.1.1 Sisyphus Cooling

Fortunately, Doppler cooling is one of the few examples where the experiment works better than predicted by theory. The discrepancy is explained by taking into account the opposite direction of the lasers. They can generate a fortunate interference effect.

Consider an alkali atom⁵ in the ground state ${}^2S_{1/2}$ moving in the $+x$ direction and transitioning to an excited state ${}^2P_{3/2}$ under the influence of laser resonance. As long as the atom remains in the same magnetic sublevel, it will continuously convert kinetic energy to potential energy in a cyclic manner.

²Typically two per translational degree of freedom, although if the angles are chosen appropriately, it is possible to use only four lasers to cool a three-dimensional gas.

³Molasses is a kind of thick syrup that results from refining sugar.

⁴A rigorous treatment can be found in section 11.2.2 of *Quantum Optics, An Introduction*, Mark Fox (2006).

⁵That is, its outermost electron is in an s-orbital.

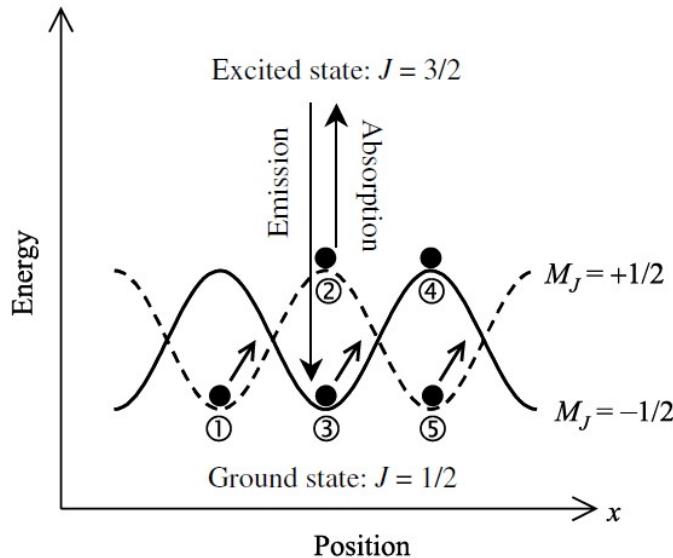


Figure 4.2: Sisyphus cooling showing a cyclic transition $J = 1/2 \rightarrow J = 3/2$ for an alkali atom. The atom moves in the $+x$ direction and interacts with two opposing lasers.

The energies for the sublevels $M_J = \pm 1/2$ of the ground state $J = 1/2$ vary sinusoidally with respect to the position x in the interference pattern of the lasers. The frequency is adjusted such that the atom can only make a transition to the excited state at the top of one of the potential hills (positions 2 and 4). From $M_J = +1/2$, the atom can emit and land in $M_J = +1/2$ or $M_J = -1/2$ (positions 3 and 5). If an atom follows the path $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5 \rightarrow \dots$, the energy difference between the absorbed and emitted photon is borrowed from the total energy of the atom, cooling it. In this case, the atom constantly loses energy as it must constantly climb the potential hill, only to return to a different M_J . However, if the atom returns to the same level, there is no energy difference and, therefore, no cooling. The similarity to the myth of Sisyphus gave the effect its name.

As the atom recoils each time photons with wavelength λ are emitted in random directions, the limiting temperature corresponds precisely to when recoiling no longer means losing temperature. This is the **recoil limit** and is given by the minimum amount of momentum h/λ :

$$\frac{1}{2}k_B T_{\text{recoil}} = \frac{(h/\lambda)^2}{2m} \quad \rightarrow \quad T_{\text{recoil}} = \frac{h^2}{mk_B \lambda^2}$$

4.2 Magnetic Traps

In 1922, Otto Stern and Walter Gerlach observed that part of an atomic beam bent upwards (and the other part downwards) after passing through an inhomogeneous magnetic field. This experiment helped lay the foundations for the role of spin in quantum theory. What was the force that bent the beam? From electrodynamics, it is known that a magnetic dipole $\vec{\mu}$ in an external magnetic field \vec{B} has an energy

$$V = -\vec{\mu} \cdot \vec{B}.$$

Since in an atom the direction of $\vec{\mu}$ is dominated by the external field \vec{B} , the energy does not vary with the direction of \vec{B} as the dipole moves adiabatically to align with the field. In other words, the energy only depends on the magnitude of the field $B = |\vec{B}|$. Thus, the magnitude of the magnetic force along the z-axis will be

$$F = -\mu \frac{dB}{dz}.$$

This explains the Stern-Gerlach experiment and is the basis for magnetic traps, as it is possible to bend the trajectories of atoms through magnetic fields.

4.2.1 Radial Confinement

We can use the magnetic force to confine the gas of atoms in the radial direction by positioning four wires in a configuration as shown in the following figure:

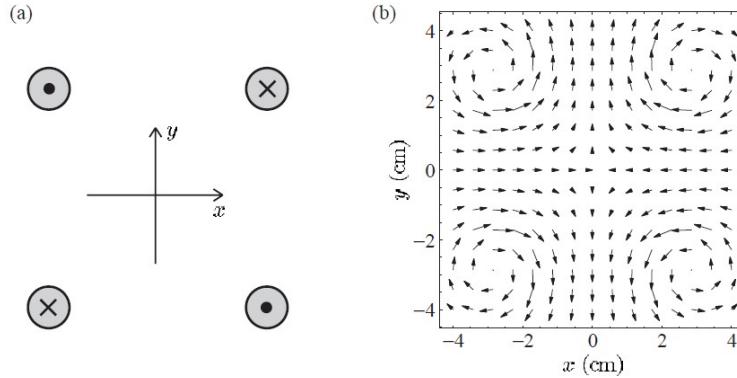


Figure 4.3: (a) A cross-section of the four wires. Two have current direction into the plane and the other two out of the plane. (b) The direction of the magnetic field \vec{B} around the wires.

This arrangement shows a magnetic quadrupole without field gradient in the z direction. Therefore, according to Maxwell's equation

$$\nabla \cdot \vec{B} = 0 \quad \rightarrow \frac{dB_x}{dx} = -\frac{dB_y}{dy} = b',$$

that is, the gradients have the same magnitude but opposite sign. Then, the magnetic field must be

$$\vec{B} = b' (x\hat{e}_x - y\hat{e}_y)$$

with a magnitude linear in the radial coordinate $r = \sqrt{x^2 + y^2}$

$$|\vec{B}| = b' (x^2 + y^2)^{1/2} = b'r,$$

and whose graph corresponds to the following figure on the left:

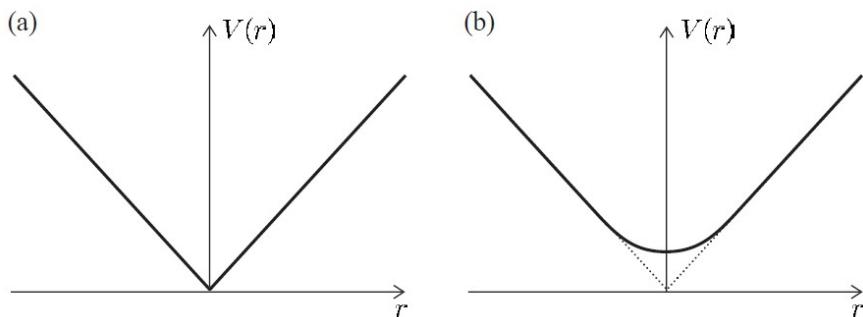


Figure 4.4: (a) Magnetic potential in the radial direction. The peak at the base allows non-adiabatic transitions of trapped atoms. (b) The additional field along the z direction gives us a harmonic potential near the axis.

This field produces a force in the radial direction

$$\vec{F} = -\nabla V = -\mu b' \hat{e}_r$$

which, considering the Zeeman sublevels, can be written as

$$\vec{F} = -g_F \mu_B M_F b' \hat{e}_r.$$

From here, a fundamental problem with this quadrupole field can be observed. Near the center, the magnitude of the field is minimal, so the Zeeman sublevels will have a very small energy separation. In this region, atoms with different magnetic numbers mix and transfer angular momentum M_F to each other (where F is the total spin of the atom). This non-adiabatic transition allows atoms to escape from the trap. This is like having a pool with a hole in its base. Somehow we'll have to patch it. This patch cannot be a field in the x direction or in the y direction, as this will only shift the hole through which they escape. The solution is to add a field in the z direction:

$$\vec{B} = b' (x \hat{e}_x - y \hat{e}_y) + B_0 \hat{e}_z,$$

whose magnitude is approximately

$$|\vec{B}| = \left\{ B_0^2 + (b'r)^2 \right\}^{1/2} \simeq B_0 + \frac{b'^2 r^2}{2B_0}$$

when the radial distance is such that $b'r \ll B_0$. The graph of such a field is shown on the right of figure 4.4. This potential can be seen as a harmonic potential with radial oscillation frequency for an atom of mass M

$$\omega_r = \sqrt{\frac{g_F \mu_B M_F}{MB_0}} b'$$

since

$$\begin{aligned} V(r) &= V_0 + g_F \mu_B M_F \left(\frac{b'^2 r^2}{2B_0} \right) \\ &= V_0 + \frac{1}{2} M \frac{g_F \mu_B M_F}{MB_0} b'^2 r^2 \\ &= V_0 + \frac{1}{2} M \omega_r^2 r^2. \end{aligned}$$

Great, we have controlled the gas in two of its translational degrees of freedom. We just need to trap it in its remaining degree.

4.2.2 Axial Confinement

To confine in the axial direction, another pair of coaxial coils is needed with current flowing in the same direction to produce a field in the z direction with a minimum between the coils (i.e., where $dB_z/dz = 0$), which produces a harmonic potential as shown in the following figure.

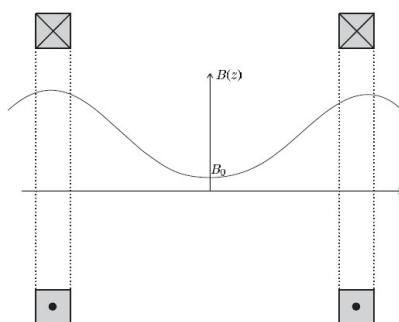


Figure 4.5: The coils have current in the same direction and create a magnetic field along the z -axis with a minimum between them, at $z=0$.

The coils that generate this field are called *pinch* coils (as they seek to pinch the tube containing the atoms) and,

schematically, produce a magnetic field of the form

$$B_{\text{pinch}}(z) = B_{\text{pinch}}(0) + \frac{d^2 B_z}{dz^2} \frac{z^2}{2}.$$

Commonly, the axial oscillation frequency ω_z is an order of magnitude smaller than the radial frequency ω_r , so the atoms concentrate in a region similar to the shape of a cigar.

However, in the radial confinement 4.2.1, it was shown that a field contribution in the z -axis was necessary to prevent atom leakage. Now we place these coils for axial confinement, so the external field $B_0 \hat{e}_z$ is altered. To fix this problem, an additional pair of compensation coils is introduced to create a uniform field in the axial direction. A sketch of the final arrangement to create a magnetic trap is shown in the following figure:

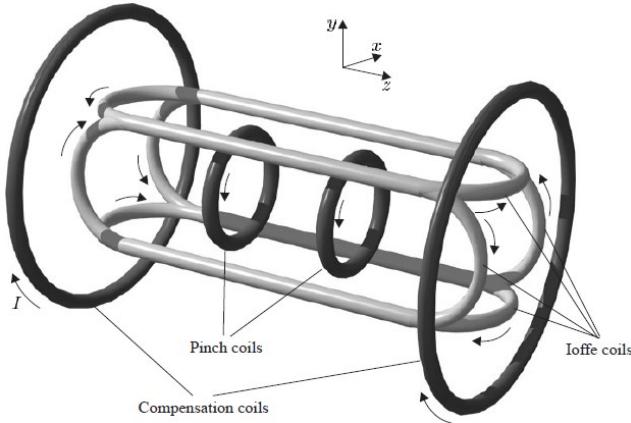
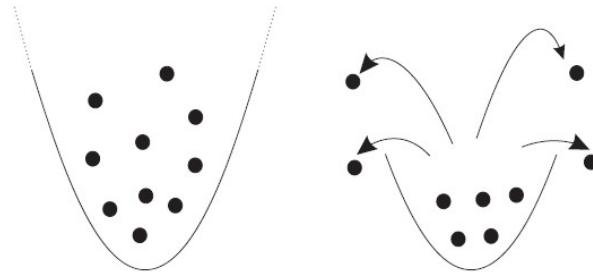


Figure 4.6: From the center to the periphery: the *Pinch coils* generate a harmonic potential for axial confinement, the *Ioffe coils* produce radial confinement, and the *Compensation coils* counteract the field in the z direction so that it is uniform. This arrangement is known as the *Ioffe-Pritchard* magnetic trap.

4.3 Evaporative Cooling

The gas adopts a cigar-like shape inside the magnetic trap as $\omega_r > \omega_z$. What happens if we increase the current to generate an even higher radial frequency? This translates to having the atoms even more confined in the radial direction and an even more pronounced cigar shape. How is this useful?

Having the atoms in an extremely confined region means having a higher density of atoms. Suppose we adjust the trap potential so that the most energetic atoms can escape the confined region. In that case, we will be left with only the atoms with lower kinetic energy (and therefore lower temperature).



The mechanism is similar to how a cup of coffee cools: the most energetic atoms escape from the cup through evaporation and leave the sad consumer with colder coffee.

A simple model to understand the process involves considering evaporation as a sequence of steps. At the beginning,

the atoms have an energy distribution given by a Boltzmann distribution

$$N(E) = N e^{-\frac{E}{k_B T_1}}$$

characteristic for a temperature T_1 (and therefore we assume that the system is in thermal equilibrium, only in that case is the temperature well defined). Atoms with energy greater than a certain value E_{cut} will escape from the trap, and after thermalization, the gas will be at a temperature $T_2 < T_1$. The process continues similarly, extracting the most energetic atoms from the distribution $f(E) = e^{-E/k_B T_2}$, waiting for their thermalization to continue removing the most energetic ones, etc.

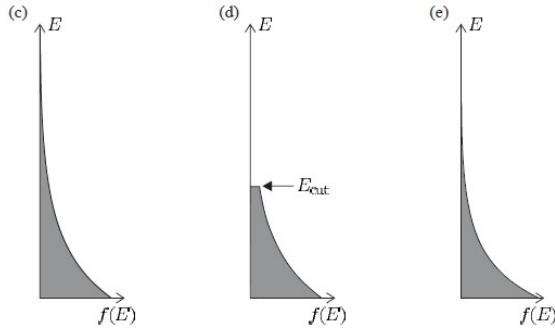


Figure 4.7: The initial distribution $f(E) = e^{-\frac{E}{k_B T_1}}$ in (c) is cut up to an energy E_{cut} in (d), which after thermalizing leaves a distribution $f(E) = e^{-\frac{E}{k_B T_2}}$ in (e), with $T_2 < T_1$.

The density increases as evaporative cooling is performed, to such an extent that quantum statistics begin to be relevant (the thermal de Broglie wavelength is no longer negligible), and therefore, it is possible to achieve a Bose-Einstein condensate with this setup.

For a trapped gas previously cooled with Doppler techniques, evaporative cooling allows temperatures on the order of nano-Kelvin, precisely the necessary temperature calculated in this chapter's introductory example.

Chapter 5

Appendices

5.1 Appendix 1: Differences between bosonic and fermionic particles

At first glance, it might seem that equation 1.1 should rather be:

$$Z(N, V, T) = Z_1^N = \frac{V^N}{\lambda^{3N}} \quad (5.1)$$

Since the partition function for a composite system is simply the product of the partition functions of its constituents. Writing the total function as it is written above does not really modify the values of pressure or energy (since both go as the derivative of $\log Z$, so any constant will disappear when having $\frac{1}{Z}Z'$). However, $\log Z$ will be present in one of the terms of the entropy

$$S = k_B \frac{\partial}{\partial T} (T \log Z) = k_B \left[\frac{\partial T}{\partial T} \log Z + T \frac{\partial \log Z}{\partial T} \right].$$

Therefore, the presence of $1/N!$ is relevant. In fact, equation 5.1 gives rise to a non-extensive entropy. That is, $S \propto V$ was expected, but equation 5.1 allows to derive $S \propto V \ln NV \neq V$. This made Gibbs suspect about the indistinguishability of bosonic particles¹. A bosonic particle will be defined as one where, if we have a pair of them and swap their positions, the overall state of the system remains unchanged:

$$\varphi_b(\vec{r}_1, \vec{r}_2) = \varphi_b(\vec{r}_2, \vec{r}_1) \quad (5.2)$$

They are particles with integer spin, unlike fermionic particles, which have half-integer spin, and when permuted, the system remains the same, except for a change of sign:

$$\varphi_f(\vec{r}_1, \vec{r}_2) = -\varphi_f(\vec{r}_2, \vec{r}_1). \quad (5.3)$$

An important fact is that fermions obey the **Pauli exclusion principle** and bosons do not. Therefore, an arbitrary number of particles can occupy the ground state. But what is spin? It is an amount of angular momentum intrinsic to a fundamental particle. Does this mean that the notion of Boson and Fermion is only reserved for fundamental particles? No, an atom can also be thought of as a boson or a fermion depending on whether it has an even or odd number of fundamental particles with half-integer spin, as stated by the **Spin-statistics theorem**². Let's see what spin means from the Lagrangian language.

¹This fact is popularly known as Gibbs' Paradox: if I have two boxes with the same gas and I join them, I should expect that the total entropy would not change ($\Delta S_{\text{Indistinguishable}} = 0$), but calculations using 5.1 indicated that there was a change in entropy before and after joining the boxes ($\Delta S_{\text{Distinguishable}} = N \ln 2$).

²P. Ehrenfest and J. R. Oppenheimer, *Note on the Statistics of Nuclei* Phys. Rev. 37, 333 (1931)

5.1.1 Conserved angular momentum and spin

Through **Noether's Theorem**, it is known that every continuous symmetry of the Lagrangian leads to a conserved quantity. A symmetry means:

$$\begin{aligned} \mathcal{L}(\Phi(x_\mu), \partial_\mu \Phi(x_\mu), x_\mu) &= \mathcal{L}(\Phi'(x'_\mu), \partial_\mu \Phi'(x'_\mu), x'_\mu). \\ \rightarrow \quad \delta \mathcal{L} &= 0 \end{aligned}$$

A total change of a function of functions, when the independent functions and the points at which it is evaluated change, is given by

$$df(g(x), h(x), \dots) = \frac{\partial f}{\partial g} \delta g + \frac{\partial f}{\partial h} \delta h + \dots + \frac{\partial f}{\partial x} \delta x,$$

therefore, when applied to the Lagrangian, we get

$$\delta \mathcal{L} = \frac{\partial \mathcal{L}}{\partial \Phi} \delta \Phi + \frac{\partial \mathcal{L}}{\partial (\partial_\mu \Phi)} \delta (\partial_\mu \Phi) + \frac{\partial \mathcal{L}}{\partial x_\mu} \delta x_\mu,$$

which can be rewritten using the **Euler-Lagrange** equations

$$\begin{aligned} \delta \mathcal{L} &= \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\mu \Phi)} \right) \delta \Phi + \underbrace{\frac{\partial \mathcal{L}}{\partial (\partial_\mu \Phi)} \delta (\partial_\mu \Phi)}_{= \partial_\mu \delta \Phi} + \frac{\partial \mathcal{L}}{\partial x_\mu} \delta x_\mu \\ &= \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\mu \Phi)} \delta \Phi \right) + \frac{\partial \mathcal{L}}{\partial x_\mu} \delta x_\mu. \end{aligned} \tag{5.4}$$

The key point in understanding spin as a conserved quantity given a symmetry of rotations (or boost) is to note that the variation $\delta \Phi$ consists of two parts

$$\delta \Phi = \epsilon_{\mu\nu} S^{\mu\nu} \Phi(x) - \frac{\partial \Phi(x)}{\partial x_\mu} \delta x_\mu. \tag{5.5}$$

Before delving into the details, it's important to understand that a variation in the field Φ arises from two sources. First, there's the change in each component when the point x is altered, which accounts for the second term. Second, there's the **mixing between the components**, which is represented by the first term. This mixing is characterized by the transformation operator $S_{\mu\nu}$ acting on a finite-dimensional basis, with $\epsilon_{\mu\nu}$ as the transformation parameters. This term will later add a portion of intrinsic angular momentum to some particles. It is important to emphasize that it is not possible to mix components if Φ has only one component, so scalar fields do not have spin. On the other hand, spinors have more than one component so that they will have half-integer spin (hence their name). As a field will have finite components, a matrix that mixes them will have to be finite-dimensional, so we will call the matrix of the first term of 5.5 as $S_{\mu\nu} = M_{\mu\nu}^{\text{fin}}$.

Returning to the second term, it can also be considered an operator acting on x_μ . But how many components do x_μ have? Also, this operator will incorporate the generators of rotations and boosts, as in the previous case. Thus, we can rewrite 5.5 as the first term already explained, together with an infinite-dimensional operator that we will call $M_{\mu\nu}^{\text{inf}}$

$$\delta \Phi = \epsilon^{\mu\nu} M_{\mu\nu}^{\text{fin}} \Phi(x) - \frac{\partial \Phi(x)}{\partial x_\mu} (M^{\text{inf}})_\mu^\sigma x_\sigma \tag{5.6}$$

It is possible to show³ that each $M_{\mu\nu}$ is related to the rotation generators by $J_i = \frac{1}{2} \epsilon_{ijk} M_{jk}$ and to the boost generators by $K_i = M_{0i}$, so $M_{\mu\nu}$ allows us to work with rotation and boost generators at the same time. It is not surprising that $M_{\mu\nu}^{\text{fin}}$ is the finite-dimensional representation of the Lorentz group and that $M_{\mu\nu}^{\text{inf}}$ is the infinite-dimensional representation of the Lorentz group, given by the differential operator

$$M_{\mu\nu}^{\text{inf}} = i(x^\mu \partial^\nu - x^\nu \partial^\mu).$$

³See Jakob Schwichtenberg, *Physics from Symmetry*, Springer (2018).

Therefore, a complete transformation of the field Φ is given by a combination of both the transformation generated by the finite-dimensional representation and that generated by the infinite-dimensional one

$$\Phi_a(x) \rightarrow \left(e^{-i \frac{\omega^{\mu\nu}}{2} M_{\mu\nu}^{\text{fin}}} \right)_a^b e^{-i \frac{\omega^{\mu\nu}}{2} M_{\mu\nu}^{\text{inf}}} \Phi_b(x)$$

Moreover, by defining $M_{\mu\nu} = M_{\mu\nu}^{\text{inf}} + M_{\mu\nu}^{\text{fin}}$, we can write the total transformation of the field as

$$\Phi_a(x) \rightarrow \left(e^{-i \frac{\omega^{\mu\nu}}{2} M_{\mu\nu}} \right)_a^b \Phi_b(x)$$

Lastly, mention that each $M_{\mu\nu}$ (finite or infinite dimensional) satisfies the Lorentz algebra

$$[M_{\mu\nu}, M_{\rho\sigma}] = i(\eta_{\mu\rho} M_{\nu\sigma} - \eta_{\mu\sigma} M_{\nu\rho} - \eta_{\nu\rho} M_{\mu\sigma} + \eta_{\nu\sigma} M_{\mu\rho}).$$

Let's return to the discussion about spin.

With the variation 5.6, we can rewrite the general variation of the Lagrangian shown in 5.4 as

$$\delta \mathcal{L} = \partial_\nu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\nu \Phi)} \epsilon^{\alpha\beta} M_{\alpha\beta}^{\text{fin}} \Phi(x) - \left[\frac{\partial \mathcal{L}}{\partial (\partial_\nu \Phi)} \frac{\partial \Phi(x)}{\partial x_\mu} - \delta_\mu^\nu \mathcal{L} \right] (M^{\text{inf}})^{\mu\sigma} x_\sigma \right) = 0, \quad (5.7)$$

where the variation is equal to zero because we are talking about symmetries of the Lagrangian. Defining the symmetric tensor

$$T_\mu^\nu = \frac{\partial \mathcal{L}}{\partial (\partial_\nu \Phi)} \frac{\partial \Phi(x)}{\partial x_\mu} - \delta_\mu^\nu \mathcal{L}$$

then, since $M^{\nu\sigma}$ is antisymmetric, we have

$$\delta \mathcal{L} = \partial_\nu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\nu \Phi)} \epsilon^{\alpha\beta} M_{\alpha\beta}^{\text{fin}} \Phi(x) - \frac{1}{2} (T^{\mu\nu} x^\sigma - T^{\sigma\nu} x^\mu) M_{\mu\sigma}^{\text{inf}} \right)$$

with $(J^\nu)^{\sigma\mu} \equiv T^{\mu\nu} x^\sigma - T^{\sigma\nu} x^\mu$ the Noether current, which for scalar fields determines the total conserved charge $\partial_\nu (J^\nu)^{\sigma\mu} = 0$. For such fields, the quantity conserved in time corresponds to having $\nu = 0$. Therefore, a quantity J^0 will be conserved for each index σ, μ in $M_{\mu\sigma}$. The case for a general field can be constructed based on this analogy, and we conclude that the quantities conserved in time will be given by

$$Q^{jk} = \int d^3x \left(\frac{\partial \mathcal{L}}{\partial (\partial_0 \Phi)} S^{jk} \Phi(x) + (T^{j0} x^k - T^{k0} x^j) \right),$$

with which we will have the quantities conserved in time for a general field with more than one component

$$\begin{aligned} L^i &= \frac{1}{2} \epsilon^{ijk} Q^{jk} = \frac{1}{2} \epsilon^{ijk} \int d^3x \left(\frac{\partial \mathcal{L}}{\partial (\partial_0 \Phi)} S^{jk} \Phi(x) + (T^{j0} x^k - T^{k0} x^j) \right) \\ &= L_{\text{spin}}^i + L_{\text{orbit}}^i, \end{aligned} \quad (5.8)$$

this is because the variation of the Lagrangian for symmetry transformations is zero

$$\partial_0 L^i = \frac{1}{2} \epsilon^{ijk} \int d^3x \partial_0 \left(\frac{\partial \mathcal{L}}{\partial (\partial_0 \Phi)} S^{jk} \Phi(x) + (T^{j0} x^k - T^{k0} x^j) \right) = \frac{1}{2} \epsilon^{ijk} \int d^3x 0 = 0.$$

Thus, as equation 5.8 demonstrates, it is the total angular momentum—comprising both the spin contribution and the orbital component—that remains conserved.

Specifically, a spinor field is a representation $\left(\frac{1}{2}, 0\right)$ of the Lorentz group⁴, where each number indicates the dimension

⁴Although it can also be a representation $\left(0, \frac{1}{2}\right)$ or $\left(\frac{1}{2}, 0\right) \otimes \left(0, \frac{1}{2}\right)$.

of each $SU(2)$ group that composes the Lorentz group⁵, so this representation will have a 2-dimensional representation of $SU(2)$, i.e., $N_i^+ = \frac{\sigma_i}{2}$, and a 1-dimensional representation of $SU(2)$, i.e., $N_i^- = 0$. Therefore, to mix the components of the spinor under a rotation we can use the same Pauli matrices, obtaining the spin operator that determines the first contribution of 5.8,

$$\hat{S}_i = \frac{\hbar}{2} \epsilon_{ijk} S_{jk} = \frac{\hbar}{2} \sigma_i,$$

where \hbar has units of angular momentum.

⁵Remember that the Lorentz group is constructed as two copies of the $SU(2)$ group, since the Lorentz algebra can be written

$$\begin{aligned} [N_i^+, N_j^+] &= i\epsilon_{ijk} N_k^+ \\ [N_i^-, N_j^-] &= i\epsilon_{ijk} N_k^- \\ [N_i^+, N_j^-] &= 0, \end{aligned}$$

where $N_i^\pm = \frac{1}{2}(J_i \pm iK_i)$, so technically the algebra of the group is $\mathfrak{so}(1, 3)_{\mathbb{C}} \cong \mathfrak{sl}(2, \mathbb{C}) \oplus \mathfrak{sl}(2, \mathbb{C})$, where $\mathfrak{so}(1, 3)_{\mathbb{C}}$ is the complexification of the Lie algebra of the Lorentz group.

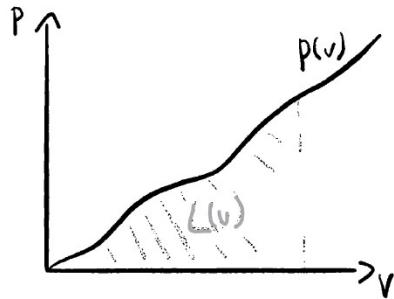
5.2 Appendix 2: Legendre Transform

A mathematical transformation is a method that allows expressing the information contained in a function in a more convenient way. For example, the Fourier transform $F(k)$ of a function $f(x)$ allows expressing the information in terms of how much each building block e^{ikx} labeled by k contributes. Another known transformation is the inverse $f^{-1}(x)$ of a function $f(x)$, which can be thought of as the mirror version of f and therefore contains the same information. Similarly, a Legendre transformation is a more convenient way of showing the information of any function. Thus, if, for any specific reason, it is easier to work with enthalpy H instead of working with Gibbs free energy G , it will be better to apply the Legendre transform between the thermodynamic potentials to obtain H , as shown in 2.1.

This appendix attempts to give an intuitive view of the Legendre transform, for which we will work with a function $L = L(v)$ of only one variable v . A well-behaved function $L(v)$ can be written in terms of its slope:

$$p(v) = \frac{\partial L(v)}{\partial v} \Rightarrow L(v) = \int_0^v p(v') dv'.$$

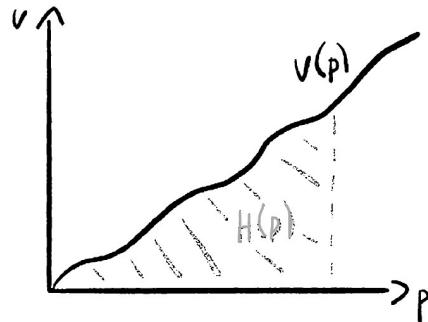
So what is under this function $p(v)$ will tell us the precise value of $L(v)$ at the value v . Graphically



Nothing very exciting. But, just as we think of $p = p(v)$ as a function of v , we can reasonably think of $v = v(p)$ as a function of p . This is taking the inverse function of $p(v)$; that is, it is enough to take the mirror version of figure 5.2 to have the graph of $v(p)$.

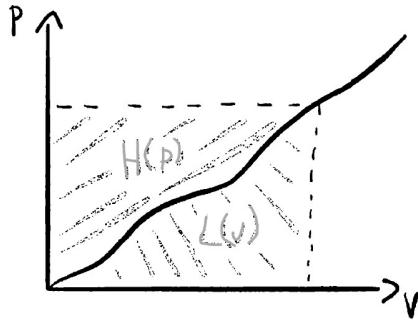
Now comes the key idea: we can define the quantity that is below the graph $v(p)$ as a new function, which we will call the **Legendre transform** $H(p)$ of the function $L(v)$,

$$H(p) \equiv \int_0^p v(p') dp'$$



We can now ask ourselves if it has an interesting relationship with the original function $L(v)$. The answer is yes, as it is easy to see that if we include the areas of both functions, we obtain a rectangle of area vp ; that is, mathematically we have

$$L(v) + H(p) = vp,$$



and therefore rearranging, we obtain a famous expression:

$$H(p) = pv - L(v).$$

As we anticipated, the information contained in the Legendre transform $H(p)$ is the same as the original function $L(v)$ only from another perspective. This is true for any function $L(v)$ whose first derivative is monotonic; that is, if one connects two points of the graph of the function $L(v)$, it never passes below the function. Another known expression relates $H(p)$ and $L(v)$ with the variables p and v :

$$\begin{aligned}\frac{\partial L}{\partial v} &= p \\ \frac{\partial H}{\partial p} &= v\end{aligned}$$

With the intuition already built, we can extend it to functions L that depend on more than one variable, for example, $L = L(q, v)$. All the previous discussion was based on the transformation concerning the variable v , but we can proceed similarly with q . In this case, we will have the slope function

$$f = \frac{\partial L}{\partial q}$$

and therefore we will obtain the Legendre transform in a completely analogous way to the previous case:

$$G(f, v) = fq - L(q(f), v).$$

Moreover, we can transform the function $G(f, v)$, now with respect to the variable v to obtain

$$K(f, p) = pv - (fq - L(q(f), v)) = pv - G(f, v).$$

This is the transformed function with respect to v and q . Rearranging, we can express this 'double' transform in terms of the transform of $L(q, v)$ with respect to v :

$$K(f, p) = pv - (fq - L(q(f), v)) = (-f)q - ((-pv) - L(q(f), v)) = (-f)q - H(q, -p, t).$$

These transformations in Classical Mechanics are known as the Hamiltonian H , the 'Gamiltonian' G and the 'Kamiltonian' K of the original function called Lagrangian L , although generally the functions G and K are not so used.

In Statistical Mechanics, they represent the thermodynamic potentials seen in 2.1, where generally all possible transformations are used, that is, all potentials. The key observation is a bijective relationship between the variables that represent the area of the rectangle (pv , fq , etc.). For example, the bijective relationship between position q and momentum p (related to velocity v) is well known in Classical Mechanics.

5.3 Appendix 3: Ferromagnetism

Throughout the text, comparisons have been made between a Bose-Einstein condensate and a ferromagnetic system, so it's worth studying the latter more closely.

A model used to carve out the physics of ferromagnetism is the so-called **Ising model**. It consists of N sites in a d -dimensional lattice. At each site, there is a quantum spin that can be *up* (\uparrow) or *down* (\downarrow). We will denote the spin value at the i -th site by $s_i = \pm 1$. As is typical for any system in which we are interested in knowing its thermodynamics, we want to find its partition function, which in the canonical ensemble will be the sum of all possible ways to arrange the spin system:

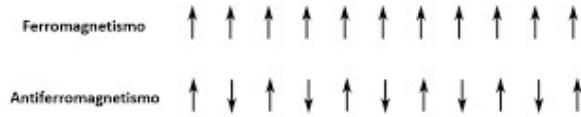
$$Z = \sum_{\{s_i\}} e^{-\beta E[s_i]},$$

so we must figure out what the system's energy contributions are.

In the Ising model, there will be two contributions: (1) one from the interaction of the spins with an external magnetic field and (2) another from the interaction between neighboring spins. Specifically for the first contribution, we will consider that the magnetic field is such that the more *up* spins there are, the more energy the lattice will have. On the other hand, spins that interact with their immediate neighbors (which we will denote by $\langle ij \rangle$) will tend to be aligned in a ferromagnetic system and to be anti-aligned in an anti-ferromagnetic. The total energy of the system will be given by

$$E = -J \sum_{\langle ij \rangle} s_i s_j - B \sum_i s_i, \quad (5.9)$$

with J the interaction energy. If $J > 0$, the least energetic configuration explains that the spins will prefer to be aligned ($\uparrow\uparrow$ or $\downarrow\downarrow$), that is, it will be ferromagnetic. On the contrary, if $J < 0$, it's an anti-ferromagnetic system with anti-aligned spins ($\uparrow\downarrow$).



So we already have an expression for the partition function. The problem is that solving it is extremely complicated,

$$Z = \sum_{\{s_i\}} \exp \left(\beta J \sum_{\langle ij \rangle} s_i s_j + \beta B \sum_i s_i \right),$$

so a method that provides an approximation of Z known as **mean field theory** is used, which consists of ignoring those terms that are very far from the average magnetization of the system, given by

$$m = \frac{1}{N} \sum_i \langle s_i \rangle = \frac{1}{N\beta} \frac{\partial \log Z}{\partial B},$$

therefore, the first term of 5.9 can be approximated as

$$\begin{aligned} s_i s_j &= [(s_i - m) + m][(s_j - m) + m] \\ &= \cancel{(s_i - m)}(\cancel{s_j - m}) + m(s_j - m) + m(s_i - m) + m^2 \\ &= m(s_i + s_j) - m^2 \\ \Rightarrow -J \sum_{\langle ij \rangle} s_i s_j &= -J \sum_{\langle ij \rangle} m(s_i + s_j) - m^2 \end{aligned}$$

If we write the number of pairs of close neighbors as $\sum_{\langle ij \rangle} \rightarrow Nq/2$ (since a d -dimensional lattice has $q = 2d$ neighbors),

then the total energy under the mean field approximation is

$$E = \frac{1}{2}JNqm^2 - (Jqm + B) \sum_i s_i$$

so the interaction between spins has been removed. Instead, the interaction is now considered as a contribution to an effective magnetic field

$$B_{\text{ef}} = B + Jqm \quad \rightarrow \quad E = \frac{1}{2}JNqm^2 - B_{\text{ef}} \sum_i s_i$$

which encourages each spin to be aligned with the average m . As each spin acts independently, and there are N of them, then Z will be the product of each partition function of each particle, which can have spin *up* or spin *down*. Therefore,

$$Z = e^{-\frac{1}{2}\beta JNqm^2} (e^{-\beta B_{\text{eff}}} + e^{\beta B_{\text{eff}}})^N = e^{-\frac{1}{2}\beta JNqm^2} 2^N \cosh^N \beta B_{\text{eff}}$$

Finally, we can obtain a new expression for the average magnetization through

$$m = \frac{1}{N\beta} \frac{\partial \log Z}{\partial B} \quad \rightarrow \quad m = \tanh(\beta B + \beta Jqm)$$

If we turn off the magnetic field, $B = 0$, we can graph the magnetization of a ferromagnetic system according to temperature. If the temperature is high, then

$$\beta Jqm = \frac{Jqm}{k_B T} < 1,$$

on the contrary, $\beta Jqm > 1$ for low temperatures. Suppose we graph the magnetization of the system according to this consideration. In that case, we will see that for low temperatures, two possible values represent a minimum, so, with $B = 0$, a ferromagnetic system would undergo a spontaneous symmetry breaking.

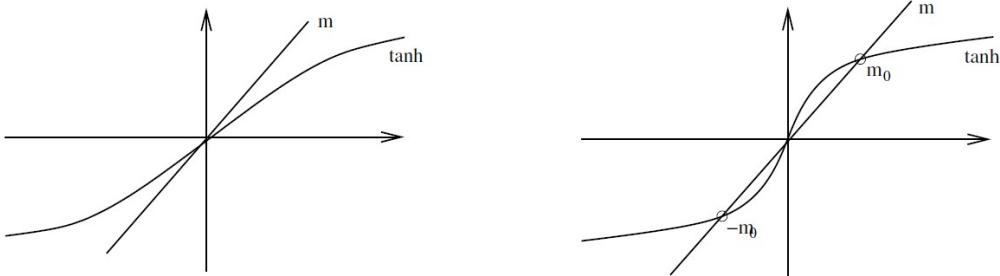


Figure 5.1: Average magnetization of a ferromagnetic system for high temperatures (left side, $\beta Jqm < 1$) and for low temperatures (right side $\beta Jqm > 1$). The line $m = m$ was drawn over the function $\tanh(\beta B + \beta Jqm)$, so the intersections will be the solutions of $m = \tanh(\beta B + \beta Jqm)$.

Naturally, m represents the order parameter, as $m \approx 0$ above a specific critical temperature T_c , and below it $m = \pm 1$ in some units. Finally, we must distinguish this spontaneous symmetry breaking from that seen for a Bose-Einstein condensate, as one can always blame some imperceptible (but present) magnetic field B that is responsible for the system choosing a magnetization $m = +m_0$ or $m = -m_0$, unlike a BEC, where it is unknown if there is any external field that encourages it to take a particular phase.

5.4 Appendix 4: Order parameter in Bose-Einstein condensate

As mentioned in the text, the order parameter of a Bose-Einstein condensate is related to the so-called *off-diagonal long-range order*. Although it will be detailed later, there is a more direct way to find the order parameter.

A condensate is made of many bosonic particles. From a second quantization point of view⁶, the field operator $\hat{\Psi}(r)$ ($\hat{\Psi}^\dagger(r)$) that annihilates (creates) a particle at position r can be written as a sum of bosonic destruction (creation) operators \hat{a} (\hat{a}^\dagger) in a particular state $\varphi(r)$, that is

$$\hat{\Psi}(r) = \sum_i \varphi_i(r) \hat{a}_i. \quad (5.10)$$

As we are dealing with bosons, the commutation rules of \hat{a} and \hat{a}^\dagger are the typical ones found in the quantum harmonic oscillator problem

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}, \quad [\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0.$$

Moreover, as the field modes are independent,

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

then we have the commutation rules for a bosonic field

$$\begin{aligned} [\hat{\Psi}(r), \hat{\Psi}^\dagger(r')] &= \left[\sum_i \varphi_i(r) \hat{a}_i, \sum_j \varphi_j^*(r') \hat{a}_j^\dagger \right] \\ &= \sum_i \sum_j \varphi_i(r) \varphi_j^*(r') \underbrace{[\hat{a}_i, \hat{a}_j^\dagger]}_{\delta_{ij}} \\ &= \sum_i \varphi_i(r) \varphi_i^*(r') \\ &= \sum_i \langle r | i \rangle \langle i | r' \rangle \\ &= \langle r | r' \rangle \\ &= \delta(r - r') \end{aligned}$$

where we used the completeness relation for a particle $\sum_i |i\rangle\langle i| = \hat{I}$. If we work near the critical point, that is, at temperatures close to T_c , we expect a macroscopic number of particles in the ground state, so we can decompose the operator 5.10 into two terms: those of the condensate, that is, those with $i = 0$ (less energetic terms) and those that do not correspond to the condensate ($i \neq 0$, excited states):

$$\hat{\Psi}(r) = \varphi_0(r) \hat{a}_0 + \sum_{i \neq 0} \varphi_i(r) \hat{a}_i \quad (5.11)$$

One way to approximate 5.11 is to consider that the macroscopic occupation of the lowest energy state is so large that one can forget about quantum fluctuations and treat the operator \hat{a}_0 as a number: $\hat{a}_0 = \sqrt{N_0}$. In this way, the occupation number of the lowest energy state $\langle \hat{a}_0^\dagger \hat{a}_0 \rangle = N_0$ is satisfied trivially and allows rewriting 5.11 conveniently by clarifying that the main contribution of the field operator will be $\sqrt{N_0}$ times the function $\varphi_0(r)$ (which will give the state of the particle in the ground state)

$$\varphi_0(r) \hat{a}_0 = \varphi_0(r) \sqrt{N_0} = \psi_0(r)$$

⁶The name second quantization has a historical character: the first quantization consisted of noting that physical objects that were previously considered continuous (energy, light, etc.) could be thought of through non-continuous fundamental units (quantized energy, photon, etc.). Then these units were thought of as a 'quantum' of a quantized field (which was originally continuous). For the case of light: field → photon → quantized field.

plus the term of the excited states $\delta\hat{\psi}(r) = \sum_{i \neq 0} \varphi_i(r)\hat{a}_i$. With these observations on the table, we can rewrite 5.11 as

$$\hat{\Psi}(r) = \psi_0(r) + \delta\hat{\psi}(r) \quad (5.12)$$

recognized as the **Bogoliubov approximation**, describing the field operator $\hat{\Psi}(r)$ in a mean-field way, that is, as a classical field ψ_0 and small fluctuations $\delta\hat{\psi}$ around the average, as long as the occupation level is considerable (that is, at low temperatures, according to 1.12). Let's focus on the classical field ψ_0 . If we are below the critical temperature T_c , the fluctuations of $\delta\hat{\psi}$ can be neglected, and the entire system will be in the ground state. Therefore, above T_c we will have $0 < \psi_0 \ll 1$ and below T_c a significant fraction will be characterized by the same field, $\psi_0 \approx 1$ in some units. We have found the **order parameter** we were looking for: ψ_0 .

But why is it called ODLRO (*Off-diagonal long-range order*)? Let's consider a system formed by a large number N of bosons characterized by the coordinates $r_i (i = 1, 2, \dots, N)$. Any state of several particles s of the system can be written in the form

$$\Psi_N^s \equiv \Psi_s(r_1, r_2, \dots, r_N).$$

where the function Ψ_s is symmetric under an exchange of any pair i, j (this defines the boson!). However, a definition can also come from a density matrix, writing a mixture of different pure states Ψ_s (mutually orthogonal), each with a statistical weight p_s . We will define the single-particle density matrix $\rho_1(r, r')$ as

$$\begin{aligned} \rho_1(r, r') &\equiv N \sum_s p_s \int dr_2 dr_3 \dots dr_N \Psi_s^*(r, r_2, \dots, r_N) \Psi_s(r' r_2, \dots, r_N) \\ &\equiv \langle \hat{\Psi}^\dagger(r) \hat{\Psi}(r') \rangle \quad (r \equiv r_1, r' \equiv r'_1) \end{aligned} \quad (5.13)$$

It is important to note that the definition does not contemplate an integration over r_1 . Thus, the physical meaning of ρ_1 is, intuitively, the probability amplitude of finding a particle in r multiplied by the amplitude of seeing it in r' , averaged by the behavior of all $N - 1$ particles. In what way is it a matrix? ρ_1 can be seen as a matrix with respect to its spatial index r .

It is clear from the definition 5.13 that it is a Hermitian matrix $\rho_1(r, r') \equiv \rho_1^\dagger(r', r)$, so it can be diagonalized

$$\rho_1(r, r') = \sum_i n_i \varphi_i^*(r) \varphi_i(r'),$$

where $\varphi_i(r)$ are the columns of a unitary matrix U . How does all this relate to the order parameter? If we focus on the behavior of ρ_1 in the limit $|r - r'| \rightarrow \infty$, we can postulate that ρ_1 can be written as

$$\lim_{|r - r'| \rightarrow \infty} \rho_1(r, r') = \underbrace{\psi_0^*(r) \psi_0(r')}_{\rightarrow \neq 0} + \underbrace{\tilde{\rho}_1(r, r')}_{\rightarrow 0},$$

that is, we identify the order parameter as that contribution that does not vanish in the limit $|r - r'| \rightarrow \infty$. Obviously, this way of conceiving the order parameter cannot be applied in the case of a trapped gas when the limit $|r - r'| \rightarrow \infty$ does not make sense. In such a case, it is convenient to think of the order parameter simply as shown in 5.12. To see more directly the similarity of both definitions, we write ρ_1 separating between the least energetic term and the others

$$\rho_1(r, r') = \psi_0^*(r) \psi_0(r') + \sum_{i \neq 0} n_i \varphi_i^*(r) \varphi_i(r')$$

making clear the similarity with 5.11. It is enlightening to highlight that the order parameter is called *off-diagonal* since it does not vanish when $r \neq r'$, that is, off the diagonal. If we establish $r = r'$ (the diagonal terms), we obtain the probability density of finding the particle in that region of space: $\langle \hat{\Psi}^\dagger(r) \hat{\Psi}(r) \rangle = |\Psi(r)|^2$.

An important point of ψ_0 , also called the condensate wave function, is that its direction in the complex plane is determined by a particular phase $S = S(r)$, which in principle is arbitrary

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

but, as with any *c-number* whose physical meaning arises with its squared modulus, it is invariant under a global phase $e^{i\alpha}$. In this particular case, ψ_0 is such that $\psi_0^*(r)\psi_0(r) = |\psi_0(r)|^2 = n_0(r)$, where $n_0(r)$ is the particle density in the ground state. For this reason, we say that the order parameter $m = |\psi_0|^2$ of the condensate is invariant under a $U(1)$ **gauge symmetry**

$$n_0(r) = |\psi_0(r)|^2 \stackrel{!}{=} |e^{i\alpha} \psi_0(r)|^2.$$

Chapter 6

References

For the theoretical derivation of the Bose-Einstein condensate in **Chapter 1**, it's sufficient to consult any canonical Statistical Physics book. For this purpose, the main reference was:

- **Statistical Physics, David Tong, University of Cambridge Part II Mathematical Tripos (2012).**

which also provides an illuminating discussion of Landau Theory and Landau-Ginzburg Theory. The rest of **Chapter 2** was mainly constructed following the exposition in chapter 5 of the following book:

- **Universal Themes of Bose-Einstein Condensation, Edited by Nick P. Proukakis, David W. Snoke and Peter B. Littlewood, Cambridge University Press (2017).**

That chapter, along with chapter 7 of the same book, provided support for **Chapter 3** of these notes, together with the following works related to the Kibble-Zurek mechanism:

- **Cosmological experiments in superfluid helium?, Wojciech H. Zurek, Nature volume 317, pages505–508 (1985).**
- **Universality of Phase Transition Dynamics: Topological Defects from Symmetry Breaking, Adolfo del Campo and Wojciech H. Zurek, available on arXiv, arXiv:1310.1600 (2013).**

Chapter 4, which shows only schematically the atomic cooling, is based on:

- **Atomic Physics, Christopher J. Foot, Oxford Master Series in Physics (2005).**
- **Quantum Optics: An Introduction, Mark Fox, Oxford Master Series in Physics (2006).**

where each mechanism can be developed more deeply. On the other hand, we can suggest several references for each appendix in **Chapter 5**. Appendix 1 concisely summarizes developments shown in:

- **Physics from Symmetry, Jakob Schwichtenberg, Springer Undergraduate Lecture Notes in Physics (2018).**

For the section on the Legendre transform, the following was followed:

- **No-Nonsense Classical Mechanics: A Student-Friendly Introduction, Jakob Schwichtenberg, No-Nonsense Books (2019).**

Finally, for the derivation of the order parameter, it was useful to consult:

- **Bose-Einstein Condensation and Matter-Wave Lasers, Yoshihisa Yamamoto, QIS 385 Quantum Information Processing Summer School (2012),**
- **Quantum Liquids: Bose condensation and Cooper pairing in condensed-matter systems, Anthony James Leggett, Oxford Graduate Texts (2006).**