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Thermal expansion coefficient for a trapped Bose gas during the phase transition

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Thermal expansion coefficient for a trapped Bose gas during the phase transition

Dissertation presented to Graduate Program in Physics at the Instituto de Física de São Carlos, Universidade de São Paulo to obtain the degree of Master of Science.

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A Shirly Lara, mi novia. Y a mi madre, Noris

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Una de las personas a quien más tengo que agradecer es mi madre, Noris Gutiérrez, todo lo bueno que tengo y he podido alcanzar es gracias a la formación que me dio. Ha sido mi mayor motivación para poder salir adelante y demostrarle que todo lo que me enseño valió la pena. Agradecer también a mis hermanos por todas sus locuras. y a todas las personas en Colombia que me apoyaron para que pudiera venir a Brasil, personas como Jorge Mercado, Gloria Grillo y Francisco Racedo quien fue mi orientador en el pregrado y me dio la motivación necesaria para poder llegar hasta aquí. Debo agradecer también a las personas que me acogieron cuando llegue a Brasil como lo fue Eliseo Gomes, Rubén Fonseca, y Edwin Pedrozo. Este último, desde el último año ha sabido ser mi amigo y compañero de historias en el laboratorio, una persona que sabe mucho lo que hace, es muy inteligente y divertido, además de ser una gran persona. Andrés Rodríguez también merece un lugar en estos agradecimientos, a pesar de que a veces pueda ser desesperante, tiene un gran corazón y que a pesar de todo lo considero como un gran amigo.

Patricia Castilho ha sido también una persona que se ha ganado algunas letras aquí, es una persona muy trabajadora y responsable, que con trabajo me ha enseñado el significado del esfuerzo y la dedicación. A veces es una persona difícil y complicada, todos somos diferentes y todos tenemos nuestras virtudes y fraquezas. También quiero agradecer a todas las personas que me ayudaron a revisar esta disertación, como lo fue Alexandre Novikov, André Cidrin y Pedro Tavares, quienes junto a Patricia hicieron un gran esfuerzo para poder entender este trabajo :). Agradecer muy especialmente a Amilison Fritsch e a Pedro Tavares durante mi paso fugaz por el BEC I, gracias a ellos pude mejorar mi portugués y mis piadas, además de ser excelentes compañeros.

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Abstract

MERCADO-GUTIÉRREZ, E. D. Thermal expansion coefficient for a trapped Bose gas during phase transition. 2016. 79p. Dissertation (Master in Science) - Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, 2016.

Ultra cold quantum gas is a convenient system to study fundamental questions of modern physics, such as phase transitions and critical phenomena. This master thesis is devoted to experimental investigation of the thermodynamics susceptibilities, such as the isothermal compressibility and the thermal expansion coefficient of a trapped Bose-Einstein condensate (BEC) of ⁸⁷Rb atoms. The critical phenomena and the critical exponents across the transition can explain the behavior of the isothermal compressibility and the thermal expansion coefficient near the critical temperature T_C . By employing the developed formalism of global thermodynamics variables, we carry out a statistical treatment of Bose gas in a 3D harmonic potential. After that, comparison of obtained results reveals the most appropriate state variables describing the system, namely volume and pressure parameter \mathcal{V} and Π respectively. The both are related with the confining frequencies and BEC density distribution. We apply this approach to define the set of new thermodynamic variables of BEC, and also to construct the isobaric phase diagram $\mathcal{V} - T$. Its allows us to extract the compressibility κ_T and the thermal expansion coefficient β_{Π} . The behavior of the isothermal compressibility corresponds to the second-order phase transition, while the thermal expansion coefficient around the critical point behaves as $\beta \sim t_r^{-\alpha}$, where t_r is reduced temperature of the system and α is the critical exponent on the basic of these. Results we have obtained the critical exponent $\alpha = 0.15 \pm 0.09$, which allows us to determine the system dimensionality by means of the scaling theory, relating the critical exponents with the dimensionality. As a result, we found out that the dimensionality of the system to be $d \sim 3$, one is in agreement with the real dimension of the system.

Keywords: Bose-Einstein condensates. Global thermodynamics variables. Critical exponents. Isothermal compressibility. Thermal expansion coefficient.

Resumo

MERCADO-GUTIÉRREZ, E. D. Coeficiente de expansão térmica de um gas de Bose durante a sua transição de fase. 2016. 79p. Dissertação (Mestrado em Ciências) -Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, 2016.

Amostras atômicas ultrafrias de um gás de Bose são convenientes para estudar questões fundamentais da física moderna, como as transições de fase e fenômenos críticos em condensados de Bose-Einstein (BEC). A minha dissertação dedica se à investigação das susceptibilidades termodinâmicas como a compressibilidade isotérmica e o coeficiente de expansão térmica de a traves da transição de um BEC de ⁸⁷Rb. Os fenômenos críticos e os exponentes críticos a traves da transição podem explicar o comportamento da compressibilidade isotérmica e do coeficiente de expansão térmica perto da temperatura crítica T_C . Ao empregar o desenvolvido formalismo das variáveis termodinâmicas globais, levamos a cabo o tratamento estatístico de um gás de Bose num potencial harmônico 3D. Depois da comparação dos resultados obtidos, revelam as mais apropriadas variáveis de estado descrevendo o sistema, chamadas parâmetro de volume e pressão, $\mathcal{V} \in \Pi$ respectivamente. As duas estão relacionadas com as frequências de confinamento e a distribuição de densidade do BEC. Nós aplicamos esta abordagem para definir um conjunto de novas variáveis termodinâmicas do BEC, e também para construir o diagrama de fase isobárico $\mathcal{V}-T$. O anterior nós permite extrair a compressibilidade κ_T e o coeficiente de expansão termina β_{Π} . O comportamento da compressibilidade isotérmica corresponde a uma transição de fase de segunda ordem enquanto que o coeficiente de expansão térmica ao redor do ponto crítico comporta se como $\beta \sim t_r^{-\alpha}$, onde t_r é a temperatura reduzida do sistema, e α o exponente crítico. Deste resultado nós obtemos um exponente crítico, $\alpha = 0.15 \pm 0.09$, que permite determinar a dimensionalidade do sistema a traves da teoria de escala, relacionando os exponentes críticos com a dimensionalidade. Como resultado, encontramos que a dimensionalidade do sistema é $d \sim 3$ que está de acordo como a dimensão real do sistema.

Palavras-chave: Condensados de Bose-Einstein. Variáveis termodinâmicas globais. Exponentes críticos. Compressibilidade isotérmica. Coeficiente de expansão térmica

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Chapter 1

Introduction

The fundamental works of A. Einstein and S. Bose, devoted to a quantum statistics of ideal bosons, established a basis for one of the most interesting branches of a modern physics. the most important result of the proposed statistic is prediction of a phase transition at extremely low temperature leading to macroscopic population of the lowest energy state of a system, while the other states are populated negligibly. this effect has been called the Bose-Einstein condensation, where the macroscopic population of the state is Bose-Einstein condensate (BEC). a Theoretical formalism of BEC description has been finally formulated at the middle of 1960, while its experimental observation took place only 1995, initially in the gas of rubidium and a bit latter in the gas of sodium. In general, such a trapped BEC has two peculiar features: (i) weak interatomic interaction and (ii) strong spatial inhomogenity. Also it is worth to mention that one is a good example of quantum system with precise controllability all the key parameters, such as number of particles, temperature, density and dimensionality. Altogether it opens door for variety of theoretical and experimental investigations One of them is study of phase transition and relevant critical phenomena.

In generally, all phase transition manifest an abrupt change in some specific physical property of a system. For instance, in thermodynamics and statistical mechanics, BEC represents a quantum phase transition where a macroscopic number of particles occupying one single-particle state leads to an abrupt change in the system's density.(2) The phase transitions are classified in discontinuous and continuous phase transitions, the first one are related with a singularity in the first derivative of the free energy respect to someone state variable, such as, temperature, pressure or volume. Generally, this kind of transitions involve a latent heat. The second one, continuous phase transitions, has discontinuities in higher order of the free energy derivative respect with the state variables.(3) They are related to critical phenomena which refer to the thermodynamic properties near the critical temperature.

Landau's theory of critical phenomena(4) attempts to explain continuous phase transitions in general, however it fails in prediction of system's behavior near the critical point. A more rigorous description of the critical phenomena, is known as the renormalization group theory which can include all the fluctuations of the system on all the length scales.(5) This theory successfully explains the universality of critical exponents in critical phenomena for variety of systems.(5, 6) These exponents are related to divergence of some thermodynamic quantity which can be expressed as a function of the reduced temperature $t_r = |T - T_C/T_C|$, as t_r^{-c} , where c is the critical exponent typically labeled with Greek letters, depending on the thermodynamic quantity.(7)

Phase transitions and critical phenomena signatures are present in the thermodynamic susceptibilities when we study them in a quantum system such as a BEC. For this reason, our aim in this work is to investigate behavior of two of these thermodynamic susceptibilities, namely the isothermal compressibility and thermal expansion coefficient, around temperature of, the phase transition followed by its associating with a critical phenomena through finding the critical exponents.(8) For this purpose, we employ the formalism of thermodynamic global variables approach developed by Romero-Rochín and Vanderlei S. Bagnato.(9)The idea of this approach is to take the most favorable variables to macroscopically describe the quantum system. One has been used before in our group to explore the behavior of the thermodynamic susceptibilities such as heat capacity(10), isothermal compressibility(11) and the behavior of quantum pressure at zero temperature.(12)

This Dissertation consist of four section: introduction, chapters, conclusions and references list. In the first one, the introductions, we introduce the concept of phase transitions and BEC showing the critical phenomena as an important topic to describe the thermodynamic susceptibilities.

In Chapter 2, we introduce the history of the Bose-Einstein condensation and consider the statistical description of Bose gas. Furthermore, some theoretical formalism of BEC description to be present.

In Chapter 3, we discuss the evolution and classification of phase transitions. Also a description of the systems near the critical point, by mean critical exponents, showing that behavior of certain thermodynamic quantities can be considered as universals, to be presented. Our experimental setup and technology of BEC creation are described in Chapter 4. In Chapter 5 we define the appropriate global thermodynamic variables and show how they have been used for study the thermodynamics of quantum systems.

Finally, in Chapter 6, we present the experimental results on the behavior of the isothermal compressibility and the thermal expansion coefficient near the critical temperature as a function of the critical exponents. Conclusions summarizes the main result of the work. At the end, the references list is presented.

Statistical Description of Trapped BEC

2.1 History

In 1924 S. Bose sent an article to A. Einstein about the way in which he reaches the Planck's formula for black body radiation, considering the electromagnetic radiation as a gas of photons (massless bosonic particles).(13) With this consideration, Bose deduced the Planck's formula for the black body radiations without considering any classical approximation. Einstein extend Bose's results to non-interacting bosonic massive particles and produced a serie of three articles in this context. (14, 15) Furthermore, Einstein predicted that below a certain critical temperature all particles of the system would be in its minimal state of energy. This phenomenon was called Bose-Einstein condensation (BEC), which has become a new and interesting macroscopic quantum degenerate system. The race to prove the existence of the BEC begun right after its prediction and was strongly motivated by the observation of the superfluidity phenomenon in liquid helium cooled below 2.18K. This was first observed in 1938 by P. Kapitiza, and J F. Allen. (16, 17) F. London indicated that the phenomena of superfluidity would be a consequence of achieving the BEC on liquid helium. A long time was spent on the development of new techniques in the way of cooling and trapping neutral atoms and just in 1982 W. D. Phillips and H. Metcalf observed for the first time the deceleration and velocity bunching of Na atoms in an atomic beam caused by the absorption of photons of the resonant laser beam. (18) The great success of laser cooling and other techniques awarded the Nobel Prize in physics in 1977 to Steven Chu, Cohen-Tannoudji and William Phillips.(19–22) Fundamental particles are divided into bosons and fermions depending on their internal angular momentum, or 'spin'. If the total spin is an integer multiple of Planck's constant, \hbar , the particle is a boson. An ultracold ensemble of these particles can condense into the lowest possible quantum energy state, where it forms a BEC.

The building blocks of matter such as electrons, protons, and neutrons are, how-

Chapter 2

ever, particles with half-integer spin (fermions). Fermions obey Pauli's exclusion principle, which forbids two or more particles to occupy the same quantum state. The formation of an ultracold condensate similar to a BEC is thus not allowed for a system of single fermions.(23) From this point, a large number of papers has been development exploring in more detail quantum phenomena such as superfluidity (23, 24), quantum information(References), the high precision system of metrology and others.(References) today, different atomic species have been brought to quantum degeneracy, alkaline species as ⁸⁷Rb(2), ²³Na(25), ⁷Li(26), ¹H(27), ⁸⁵Rb(28), ³⁹K(29), ⁴He(30, 31), ⁴¹K(32), and ⁸⁷Cs.(33) Those help us to understand how works the systems when the temperature its order to nano-kelvin. The vast interest in Bose-Einstein condensation arises partly from the fact that this phenomenon touches several physical disciplines thus creating a link between them: In thermodynamics BEC occurs as a phase transition from gas to a new state of matter, quantum mechanics view BEC as a matter-wave coherence arising from overlapping de Broglie waves of the atoms and draw an analogy between conventional and "atom lasers", quantum statistics explain BEC as more than one atom sharing a phase space cell, in the quantum theory of atomic traps many atoms condense to the ground state of the trap, in quantum field theory BEC is closely related to the phenomenon of spontaneous breaking of the gauge symmetry.(34)

2.2 The non-interacting Bose gas

From statistical mechanics, we use the macrocanonical ensemble to study open systems, which are able to exchange matter and energy with the surrounding. If we consider a system of N bosons with mass m at temperature T, the best way to describe the system is through the macrocanonical partition function $\Xi(T, \mathcal{V}, \mu)$ defined by the following expression

$$\Xi(T, \mathcal{V}, \mu) = \sum_{N=1}^{\infty} \exp\left(-\beta(H - \mu N)\right), \qquad (2.2.1)$$

where μ is the chemical potential, \mathcal{V} is the volume parameter, which is an extensive variable that depends on the confinement potential (we discuss this variable in more details later), $\beta = 1/k_BT$, H is the total Hamiltonian of the system which can be written as

$$H = \sum_{i=1}^{N} \left(\frac{P_i^2}{2m} + U(r_i) \right) + \sum_{i < j}^{N} V(r_{ij}).$$
(2.2.2)

In eq. 2.2.2, P_i is the momentum for each particle, $U(r_i)$ is the confinement potential in the position of each particle and $V(r_{ij})$ is the interaction potential between the particles. If we consider that $V(r_{ij})$ goes to zero and the atoms are in a 3D harmonic oscillator with different frequencies $\omega_k = 2\pi f_k$; k = x, y, z, the total hamiltonian of the system can be rewritten as

$$H = \sum_{i=1}^{N} \left\{ \frac{P_i^2}{2m} + \frac{1}{2}m \left[(\omega_x x_i)^2 + (\omega_y y_i)^2 + (\omega_z z_i)^2 \right] \right\},$$
 (2.2.3)

where $U(r_i) = \frac{1}{2}m\left[(\omega_x x_i)^2 + (\omega_y y_i)^2 + (\omega_z z_i)^2\right]$ was used. Is convenient to rewrite the Hamiltonian in terms of the number occupation, so applying second quantization to the Hamiltonian we obtain

$$H_n = \sum_{i=1}^{N} \hbar \left[\omega_x \left(n_x^i + \frac{1}{2} \right) + \left(n_y^i + \frac{1}{2} \right) + \left(n_z^i + \frac{1}{2} \right) \right], \qquad (2.2.4)$$

with $n_k^i k = x, y, z$ the occupations number. Replacing H_n in eq. 2.2.1, we obtain the macrocanonical partition function of the system, which can be written as

$$\Xi(T, \mathcal{V}, \mu) = \prod_{n_k} \left\{ 1 - \exp\left[-\beta \hbar \left(\sum_{k=1}^3 \omega_k n_k\right) - \beta E_0 + \beta \mu\right] \right\}^{-1}.$$
 (2.2.5)

In this expression, $E_0 = \frac{\hbar}{2}(\omega_x + \omega_y + \omega_z)$ is the ground-state energy of the system and $\sum_{k=1}^{3} \omega_k n_k \equiv \omega_x n_x + \omega_y n_y + \omega_z n_z$. We can relate the microscopical states with the macroscopic features of the system, using the thermodynamic potentials. In an open system, the direct connection between the macrocanonical partition function and the state variables is through the macrocanonical potential Ω , defined in (35) as

$$\Omega(T, \mathcal{V}, \mu) = -k_B T \ln \Xi(T, \mathcal{V}, \mu). \tag{2.2.6}$$

In this way the macrocanonical potential for an ideal gas in an anisotropic harmonic oscillator is

$$\Omega(T, \mathcal{V}, \mu) = k_B T \sum_{n_k} \ln\left[1 - z \exp\left(-\beta \epsilon_{n_k}\right)\right], \qquad (2.2.7)$$

where $\epsilon_{n_k} = \hbar \left(\sum_{j=1}^3 \omega_k n_k \right) + E_0$ is the total energy for each set of $\{n_k\}$ and $z = \exp(\mu/k_B T)$ is the fugacity. The state equations such as entropy, pressure parameter $\Pi(T, \mathcal{V}, \mu)$, which is the conjugate variable of the volume parameter \mathcal{V} and the number of atoms, can be obtained following the next relations

$$S(T, \mathcal{V}, \mu) = -\left[\frac{\partial \Omega(T, \mathcal{V}, \mu)}{\partial T}\right]_{\mathcal{V}, \mu},$$

$$\Pi(T, \mathcal{V}, \mu) = -\left[\frac{\partial \Omega(T, \mathcal{V}, \mu)}{\partial \mathcal{V}}\right]_{T, \mu},$$

$$N(T, \mathcal{V}, \mu) = -\left[\frac{\partial \Omega(T, \mathcal{V}, \mu)}{\partial \mu}\right]_{T, \mathcal{V}}.$$
(2.2.8)

Furthermore, through Euler's relation we can relate the macrocanonical potential with the state variables as

$$\Omega = U - TS - \mu N, \qquad (2.2.9)$$

$$U = TS - \Pi \mathcal{V} + \mu N. \tag{2.2.10}$$

Using these relations it is easy to show that

$$\beta \Omega = -\beta \Pi \mathcal{V} = -\sum_{n_k} \ln \left[1 - z \exp\left(-\beta \epsilon_{n_k}\right) \right], \qquad (2.2.11)$$

$$N = \sum_{n_k} \left[\frac{1}{z^{-1} \exp(\beta \epsilon_{n_k}) - 1} \right].$$
 (2.2.12)

The sum of those expression can be replaced by integrals because at higher energies the number of particles can be considered as continuous.(35, 36) Therefore, we replace the sums by the phase-space density for a harmonic oscillator as in

$$\sum_{n_k} \to \frac{1}{h^3} \int d^3r \int d^3p = \int \left[\frac{2\pi}{h^3} (2m)^{2/3} \int d^3r \sqrt{\epsilon - \frac{1}{2}m\bar{\omega}^2 r^2} \right] d\epsilon = \int g(\epsilon)d\epsilon, \quad (2.2.13)$$

where $g(\epsilon)$ is the one particle state density and $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric mean of the trap frequencies. Thus, the state density is given by

$$g(\epsilon) = \frac{1}{2} \frac{\epsilon^2}{(\hbar\bar{\omega})^3}.$$
(2.2.14)

Taking the value for the ground estate $\epsilon = 0$ in equations 2.2.11 and 2.2.12 and replacing the sum by the integral in those equations we will have the integral corresponding to all the values of the energy except $\epsilon = 0$ and the term that take count of the zero energy as follow

$$N = \frac{1}{2(\hbar\bar{\omega})^3} \int \frac{\epsilon^2}{z^{-1} \exp(\beta\epsilon) - 1} d\epsilon + N_0, \qquad (2.2.15)$$

$$\beta\Omega = \frac{\beta}{6(\hbar\bar{\omega})^3} \int \frac{\epsilon^3}{z^{-1}\exp(\beta\epsilon) - 1} d\epsilon - \ln\left[1 - z\right].$$
(2.2.16)

Here $N_0 = z/(1-z)$ is the number of particles for $\epsilon = 0$, the ground state. the same was done $\beta\Omega$, which has been treated by using integral by parts. The integrals in the equations 2.2.15 and 2.2.16 can be solved using the function

$$g_n(z) = \frac{1}{\Gamma(n)} \int \frac{x^{n-1}}{z^{-1} \exp(x) - 1} dx = \sum_{k=1}^{\infty} \frac{z^k}{k^n},$$
(2.2.17)

with the substitution $x = \beta \epsilon$ and n = 3 for eq. 2.2.15 and n = 4 for eq. 2.2.16. This function is called the Bose function, and is related with the Riemann's Zeta function. For $z = 1 (\mu = 0)$, we have

$$g_n(1) = \sum_{k=1}^{\infty} \frac{1}{k^n} = \zeta(n), \qquad n > 1.$$
 (2.2.18)

We are interested in the values when n = 3 and n = 4, which correspond to $\zeta(3) = 1.202$ and $\zeta(4) = 1.082$ respectively. Thus, the expressions for the number of atoms N and Ω are

$$N = N_0 + \frac{k_B^3 T^3}{(\hbar \bar{\omega})^3} g_3(z), \qquad (2.2.19)$$

$$\Omega = \frac{k_B^4 T^4}{(\hbar \bar{\omega})^3} g_4(z) - \frac{1}{\beta} \ln [1-z]. \qquad (2.2.20)$$

The second term in the eq. 2.2.19, $N_{ex} = \frac{k_B^3 T^3}{(\hbar\omega)^3} g_3(z)$, represents the number of particles in excited states, while the first term, N_0 , determines the number of particles in the state $\epsilon = 0$. Since z only can assume values $0 \le z \le 1$, because the chemical potential $\mu \le 0$, the maximum number of particles in the excited estate are limited by the Bose function in $0 \le g_3(z) \le \zeta(3)$. Thus no more than $N_{ex}^{max} = \frac{k_B^3 T^3}{(\hbar\omega)^3} \zeta(3)$ can be in excited states.(35) When the system achieves the critical temperature an interesting behavior occur: z assumes its maximum value (z = 1) and the particles of the system macroscopically occupy its ground-state. If $N < N_{ex}^{max}$, N_0 can be neglected and the critical temperature at this point is given by

$$T_C^3 = \frac{\hbar^3 \bar{\omega}^3}{k_B^3 \zeta(3)} N.$$
 (2.2.21)

This was calculated by first time by Bagnato et al.(36, 37) Dividing eq. 2.2.19 by N and inserting eq. 2.2.21 into eq. 2.2.19, we obtain the condensed fraction of a harmonic trapped Bose gas.

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_C}\right)^3,$$
(2.2.22)

this equations shows the coexistence of the condensed state and excited states, two phases in thermal equilibrium. Where $N \ge N_0$ and $T \le T_C$. Retaking the macrocanonical potential, it is better to rewrite it in terms of the pressure parameter as in eq. 2.2.11

$$\Pi = -\frac{\Omega}{\mathcal{V}} = \Pi_0 + \frac{k_B^4 T^4}{\hbar^3} g_4(z), \qquad (2.2.23)$$

where $\Pi_0 = -k_B T \ln [1-z]$ and $\mathcal{V} = (\bar{\omega})^{-3}$. In the same way for z = 1 we can obtain the critical pressure parameter

$$\Pi_C = \frac{k_B^4 T_C^4}{\hbar^3} \zeta(4). \tag{2.2.24}$$

2.3 The weakly-interacting Bose gas

2.3.1 Mean field approximation

In real gases, the interaction between particles is non zero and we have to preserve the second sum on the hamiltonian of eq. 2.2.2 to completely understand the behavior of such gases. Now the total Hamiltonian, including the interaction is

$$\hat{H} = \sum_{i=1}^{N} \left(\frac{\hat{P}_i^2}{2m} + \hat{U}(r_i) \right) + \sum_{i < j}^{N} \hat{V}(r_{ij}).$$

Considering that a system of N atoms trapped in a harmonic potential as we saw before, the quantum state of the system can be represented by

$$\hat{\psi}^{\dagger}(r,t) = \sum_{n} \psi_{n}^{*}(r,t)\hat{a}_{n}^{\dagger}, \qquad \hat{\psi}(r,t) = \sum_{n} \psi_{n}(r,t)\hat{a}_{n}, \qquad (2.3.1)$$

where \hat{a}_n^{\dagger} and \hat{a}_n are the creation and annihilation operator respectively and $\hat{\psi}^{\dagger}$ and $\hat{\psi}$ are the new operator that represents the system. The quantum states of the system can be decomposed into its condensed and fluctuating parts, as

$$\hat{\psi}(r,t) = \Phi(r,t) + \delta\hat{\psi}(r,t), \qquad \Phi(r,t) = \langle \hat{\psi}(r,t) \rangle, \qquad (2.3.2)$$

where the average part $\Phi(r,t)$ is a complex function, such that its module square corresponds to the density of the condensate $n_0(r,t) = |\Phi(r,t)^2|$. Because the condensaton corresponds to a very large number of atoms $N_0 \gg 1$ in the ground state, the fluctuating part $\delta \hat{\psi}(r,t)$ can be considered negligible. The evolution equation for the condensate wave function $\Phi(r,t)$ can be derived from the Heisenberg equation for the field operator $\hat{\psi}(r,t).(38)$ At this point we will assume that the particles of the gas can be considered as hard spheres of radius a_s , where a_s is known as the scattering length. The information about the interaction between particles is introduced in this parameter a_s . This approximation is valid when collisions are at low energy the scattering is dominated by s-wave collisions.(39) The effective interaction between two atoms at r and r' positions is commonly stated in the form(40)

$$\int d^3r' V_{eff}(r', r) = g \int d^3r' \,\delta(r - r') = g = \frac{4\pi\hbar^2}{m} a_s, \qquad (2.3.3)$$

where V_{eff} is an effective contact potential. Then, the total Hamiltonian of the eq. 2.2.2 can be rewritten as

$$\hat{H} = \int \hat{\psi}^{\dagger}(r,t) \left[\frac{\hat{P}^2}{2m} + \hat{U}(r) \right] \hat{\psi}(r,t) dr + \frac{1}{2} \int dr \int dr' \hat{\psi}^{\dagger}(r,t) \hat{\psi}^{\dagger}(r',t) V_{eff}(r,r') \hat{\psi}(r,t) \hat{\psi}(r',t)$$
(2.3.4)

In the $T \to 0$ limit, that mean, temperatures for below the critical temperature T_C , we can replace the operator $\hat{\psi}(r,t)$ by its average $\Phi(r,t)$, and we get

$$i\hbar\frac{\partial}{\partial t}\Phi(r,t) = H\Phi(r,t), \qquad H \equiv -\frac{\hbar^2}{2m}\nabla^2 + (U(r) - \mu) + g \|\Phi(r,t)\|^2.$$
 (2.3.5)

This is the time dependent Gross-Pitaevskii equation (GPE)(38) This is valid for the case in which the atoms operator is exactly the mean field $\Phi(r, t)$ and a very large number of atoms is in the condensed phase, $N_0 \gg 1$. Here it is important to notice that the scattering length can be positive $a_s > 0$, for repulsive interactions between atoms, which implies that the effective energy increases as a function of the density, and negative $a_s < 0$, for attractive interactions. (26, 38, 40, 41)

2.3.2 Thomas-Fermi approximation

For a large number of condensed atoms, the repulsive interactions lead to a lower density in the cloud, since the atoms are pushed outwards. As a consequence, the quantum pressure has a small influence and only contributes near the boundary surface of the condensate, i.e. the interaction term dominates the dynamics. In this case the GPE gives the solution

$$n_0(r) = \left\|\Phi(r,t)\right\|^2 = \frac{1}{g} \left[\mu - U(r)\right], \qquad (2.3.6)$$

with $n_0(r) = 0$ in the outside region where μ becomes smaller than U(r). This is usually called the *Thomas-Fermi approximation* (TFA).(38) Since our external potential is a 3D harmonic oscillator, we can see that the density profile of the condensate takes the form of an inverted parabola. The size of the condensate is therefore determined by the condition $\mu = U(r)$. For our trap, $U(r) = m\bar{\omega}^2 R^2/2$, and the normalization of the density $N_0 = \int d^3r n_0(r)$. The chemical potential is

$$\mu = \hbar \bar{\omega} \left(\frac{15N_0 a_s}{\bar{a}} \right)^{2/5}, \qquad (2.3.7)$$

which is function of the total number of condensed atoms N_0 . Here, $\bar{a} = \sqrt{\hbar/m\bar{\omega}}$ represents the effective volume of the sample (atoms). From these two relations we can then determine the external radius for each direction of the condensate, as a function of the number of atoms, reading

$$R_k = \bar{a} \frac{\bar{\omega}}{\omega_i} \left(\frac{15Na_s}{\bar{a}}\right)^{1/5}, \qquad k = x, \, y, \, z.$$

$$(2.3.8)$$

The R_k 's are known as the Thomas-Fermi radius.

2.4 Observation of the BEC

The size of the BEC is approximately of 10 μ m, in a ultra-high vacuum system, result difficult to interact directly with him. For this reason, the easiest way to observe it is through light. Tho two most important techniques for observing Bose-Einstein condensates are in-situ and time of flight image.(42) In both cases is necessary the use of the density distributions of the clouds when is trapped or when it is in a ballistic expansion falling due to the gravity. The three physics processes involved in the interaction with the atoms with the light are spontaneous absorption of photos, re-emission of photons and shifting the phase of the transmitted light, these three processes are used to explain different imaging techniques as absorptive, fluorescence and dispersive imaging methods, respectively.(42) Absorption imaging is done by illuminating the atoms with resonant light and the absorption of this light create a shadow of the atoms, taking this image in a CCD camera is possible to extract the information of the density of the atoms and other important parameters as the temperature. In the chapter 5 we discuss a little more this imaging method. In the case of the dispersive methods, using the ability to separate scattered and unscattered components of the probe light and manipulate them independently. Dark-ground imaging and phase-contrast are example of dispersive methods of imaging in which the phase of the electric field is shifted by a change in the phase of the field to separate it.

Chapter 3

Phase Transitions and Critical Phenomena

3.1 History

In 1869 was develop the first experiment to show the critical phenomena, Andrews shows that in the critical point in the liquid - vapor phase of carbon dioxide appears a critical opalescence. (43) Motivated with this experiment van der Waals develop his theory of phase transitions studying the ordering in magnets. (44) In 1937 Landau showed that all the second-order phase transitions have in common that, at the transition point, the degree of symmetry of the system changes, this contribution led to the concept of spontaneous symmetry beak. furthermore, was introduced the concept of the order parameter, which above of the critical temperature the value of this quantity is zero representing that in the system there is not and order defined. Below of the critical temperature, the order parameter has a finite value, indicating that the system is in an ordered state. Landau provided a very successful qualitative theory of the phase transitions, getting predict a set of critical exponents that was able to describe the behavior of many important thermodynamic quantities, as heat capacity, the susceptibilities, the correlations length among others. However, in 1944 Onsager compute the exactly the partition function and thermodynamic properties of the two-dimensional Ising model.(6, 45) He find that the critical exponents predicted by the Landau theory are not the same, showing that not all the systems have the same critical exponents but they are classified depending the kind of the system. An extension of the Landau theory was made by Ginzburg in the Landau-Ginzburg theory which includes all the fluctuations that there are not presents when the system reach the critical temperature. (46) Finally, the last important contributions to provide a complete theory of the phase transitions, Wilson in 1971 presented the group renormalization theory (5), this theoretical framework based on the Landau-Ginzburg theory, made the calculation of the critical exponents and other properties feasible and supports the picture of universality classes: The symmetry of the system and the number of components of the order parameter define the behavior of a system at a phase transition.(6)

3.2 Phase transition and classification

When we hear the words "phase transition", maybe the first idea that coming into our minds, is the fact when the liquid water becomes ice or steam. Whatever the case, we are right, the measurement of the external conditions like temperature, pressure or others, at which the transformation occurs is termed the phase transition. Phase transition is characterized by abrupt changes, discontinuities, and strong fluctuations. It has been known for a long time that such singular behavior is a consequence of a cooperative phenomenon and thus intimately related to the interaction between the particles.(47) The phase transitions can be classified follows the modern classification of the phase transitions, although Ehrenfest was the first that classified the phase transitions based on the behavior of the thermodynamic free energy as a function of others thermodynamic variables.(3) Though useful, Ehrenfest's classifications has been found to be an incomplete method of classifying phase transitions, for it not take into account the case where a derivative of the free energy diverges. We shall go to explain a little bit how are the classification of the phase transitions take into account the modern classification which diverges slightly of the Ehrenfest's classification.

3.2.1 First-order phase transition or discontinuous phase transitions

The name of first-order phase transitions comes to the Ehrenfest's classification, while discontinuous phase transitions comes to the modern classifications. But, whichever is his origin name, it is characterized by a discontinuity in the first derivative of the free energy respect to some thermodynamic variable, or discontinuities on the any extensive variable. but generally, we can say that all the discontinuities phase transitions involve a latent heat. An example of this phase transitions is the entropy in a system in which the the water becomes in steam, which is discontinue in the first derivative of the Helmholtz free energy G and the volume also present the same behavior.(48) These relations are given by

$$S = -\left(\frac{\partial F}{\partial T}\right)_{N,V},\tag{3.2.1}$$

$$V = -\left(\frac{\partial G}{\partial P}\right)_{N.T}.$$
(3.2.2)
In the fig. 3.2.1 we can see discontinuous phase transitions (a) and continuous phase transitions (b), showing that, the volume, the heat capacity, and the compressibility in the system present a discontinuity due to the presence of latent heat in the system. In general, first-order phase transition include solid-liquid transition, the solid-vapour transition, and the liquid-solid transition.(49)



Figure 3.2.1 – a). Discontinuous phase transitions. b). Continuous phase transitions. Source: By the author.

3.2.2 Second-order phase transitions or continuous phase transitions

By Ehrenfest's classification, a second-order phase transition has no latent heat because the entropy does not show a discontinuity (and neither does the volume – both are first differentials of G), but quantities like the heat capacity and compressibility (second differentials of G) do.(49) This is illustrated in fig. 3.2.1(b). The isothermal compressibility, the heat capacity and also the thermal expansion coefficient are examples of second-order phase transitions in system in which the latent heat in not involved. They are defined as

$$C_P = T \left(\frac{\partial S}{\partial T}\right)_{N,V} = -T \frac{\partial^2 F}{\partial T^2}, \qquad (3.2.3)$$

$$k_T = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_{N,T} = -\frac{1}{V} \frac{\partial^2 G}{\partial P^2}, \qquad (3.2.4)$$

$$\beta_P = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_{P,N} = -\frac{1}{K} \frac{\partial^2 F}{\partial T \partial V}, \qquad (3.2.5)$$

where K is the isothermal bulk modulus.(50) That kind of transition was observed in the transition of ⁴He for a superfluid. This behavior is called of λ transition.(51, 52)

3.2.3 Order parameter and broken symmetry

A further classification of phase transition involves the notion of symmetry breaking. An example of this behavior is showed in the fig. 3.2.2, which shows atoms in a liquid and in a solid. As a liquid cools there is a very slight contraction of the system but it retains a very high degree of symmetry. However, below the melting temperature, the liquid become a solid and that symmetry is broken. A phase transition is characterized by a spontaneously broken symmetry. This may at first sight seem surprising because the picture of the solid 'looks' more symmetrical than the liquid. The atoms in the solid are all symmetrically lined up while in the liquid they are all over the place. The crucial observation is that any point in a liquid is, on average, exactly the same as any other. If you average the system over time, each position is visited by atoms as often as any other. There are no unique directions or axes along which atoms line up. In short, the system possesses complete translational and rotational symmetry. In the solid, however, this high degree of symmetry is nearly all lost. (49) A phase transition is characterized by a spontaneous broken symmetry. Symmetry-breaking is conveniently described in terms of an order parameter, $\tilde{\phi}$. It's magnitude measures the degree of long-range order in some way. To the order parameter can be associated a thermodynamic conjugated field, h_{ϕ} , which couples directly to $\vec{\phi}$. The corresponding term in the free energy F is $-h_{\phi}\vec{\phi}$. Consequently, the order parameter is defined by $\vec{\phi} - (\partial F/\partial h_{\phi})_T$. Generally the behavior of the order parameter at the phase transition is usually a key to determine the nature of the phase transition.(47) The susceptibility of the order parameter is an important quantity which is expected to be influenced by critical fluctuations. The isothermal ordering susceptibility, χ , is defined by

$$\chi_{\phi} = \left(\frac{\partial \vec{\phi}}{\partial h_{\phi}}\right)_{T}.$$
(3.2.6)

3.2.4 Critical exponents, universality and scaling theory

Continuous phase transitions can be characterized by parameters knows as critical exponents that obeys to a scaling theory. Widom in 1975 (53) was the first to advance the scaling hypothesis for scaling critical phenomena. The phenomenon of different systems exhibiting the same critical behavior is called the *universality*, an example of universality are the critical exponents, represented by Greek letters and appears in the concepts of



Figure 3.2.2 – Spontaneous symmetry broken. An example when the liquid becomes in solid. Source: By the author.

the specific heat at constant pressure C_P , in the isothermal compressibility k_T and the difference of density in the liquid-gas transitions $\Delta \rho_{L-G}$ near of the critical point, these relations are given by

$$C_{P} = C_{\pm} |t_{r}|^{-\alpha},$$

$$k_{T} = k_{\pm} |t_{r}|^{-\gamma},$$

$$\rho_{L} - \rho_{G} = \rho_{c} (-t_{r})^{\beta}.$$
(3.2.7)

In the eq. 3.2.7 C_{\pm} and k_{\pm} refers to $t_r > 0$ and $t_r < 0$, ρ_c is the density at the critical temperature. $t_r = (T - T_C)/T_C$ is the reduced temperature and measure the relative distance of the critical temperature. For a certain critical temperature T_C exist an critical pressure p_C which led another relations of criticality as a functions of the differences of the densities (in the Liquid-Gas transitions),

$$\frac{p - p_C}{p_C} = \left| \frac{\rho_L - \rho_G}{\rho_c} \right|^{\delta}.$$
(3.2.8)

The critical exponents α , β , γ and δ are universal, that mean, the same for a whole class of various phase transitions. Is interesting to note that close the transition the isobaric heat capacity is given in terms of the isobaric thermal expansion coefficient β_P as

$$C_P = VT(\partial P/\partial T)\beta_P + T(\partial S/\partial T).$$
(3.2.9)

Near the transition point the second term in the eq. 3.2.9 can be neglected, and the thermal expansion coefficient can be expressed as

$$\beta_P = \beta_{\pm} |t_r|^{-\alpha}, \qquad (3.2.10)$$

where β_{\pm} correspond to $t_r > 0$ and $t_r < 0$ respectively. Critical exponents are not the only universal quantities, there are others, like scaling functions and universal amplitude ratios, like C_+/C_- and k_+/k_- . The exponents are, however, often the most directly measurable quantities, and their non-trivial and nearly universal experimental values provided the main motivation for the theory of critical phenomena.(7) Scaling implies that not all critical exponents are independent. Indeed, only two of four critical exponents can be chosen independently.

$$\alpha + 2\beta + \gamma = 2,$$

$$\alpha + \beta(\delta + 1) = 2,$$

$$2 - \alpha = d\nu,$$

$$2\beta + \gamma = d\nu.$$

An experimental fundamental observation (54, 55), that the critical exponent values are rather insensitive to detail within the system displaying the critical phenomena. This observation is embodied in the universal hypothesis which states that continuous phase transitions can be classified in a few universality classes, each class giving rise to a certain set of exponents. These classes are determined by a few very fundamental properties of the systems, such as spatial dimension d, range of interaction which critical exponent is ν and the symmetry and dimensionality n of the order parameter. (6, 47, 53) the physical idea underlying the universal hypothesis is that at a critical point, all details of the microscopic interactions are washed out by the long wavelength fluctuations. (47) In this work, we pretend to show how two different thermodynamic susceptibilities such as, the isothermal compressibility and the thermal expansion coefficient are continuous phase transitions and near of the critical temperature, can behaves like λ -transition and also, we can be to relate this behavior with critical phenomena to find the critical exponents. Before that, in the next chapter we going to describe which is the system of the cold atoms for study the critical phenomena mentioned before.

Chapter 4

Experimental Setup

We are interested in achieve experimentally a BEC of rubidium atoms, for this it was necessary to construct a machine able to do it. In this chapter, we will briefly present all processes and technical information of our experimental system and the ⁸⁷Rb atoms. A detail description of our system can be found in (40, 48, 56) references.

4.1 Rubidium atoms

The rubidium atom (Rb), is a element of the periodic table which belongs to the alkali-metals group, characterized by their outermost electron be in an s-obrital. The atomic number is Z = 37 and natural rubidium is a mix of two isotopes, ⁸⁵Rb the only stable one, constitute approximately 72% of it. We are focusing in the other isotope and its optical properties, ⁸⁷Rb with a 28% of abundance which is slightly radioactive . For this it is necessary to understand how is the energy levels structure of the atoms and how it is possible interact with it. The rubidium atom is a hydrogen-like atom which means that have only one electron in the last energy level (n), in Rb case n = 5, principal quantum number. By consequence, all the possibles values of the orbital angular momentum **L** are delimited by $l \leq n-1$ and as we are considering an electron, the spin angular momentum is equal to $\mathbf{S} = 1/2$. We know of the fine structure of the atoms that the coupling between **L** and **S** result in the total angular momentum of the atom **J** which is defined as $\mathbf{J} = \mathbf{L} + \mathbf{S}$. All the possibles values of **J** are given by

$$|L - S| \le J \le |L + S|. \tag{4.1.1}$$

In this way we can express any energy level using the notation $n^{2S+1}L_j$. In this notation the values for l = 0, 1, 2, 3, 4 they are as the most common form S(l = 0), P(l = 1), Dl = 2), F(l = 3), G(l = 4). Therefore, the ground state for the outermost electron in the rubidium atom can be write as $5^2s_{1/2}$, where l = 0, S = 1/2. If the electron makes a transition from the ground state (l = 0) to the first excited state (l = 1), it

is said that is a D line and the total angular momentum for l = 1 can be J = 1/2 or J = 3/2. The transition is split in two components, the D₁-line $(5^2S_{1/2} \rightarrow 5^2P_{1/2})$ and the D₂-line $(5^2S_{1/2} \rightarrow 5^2P_{3/2})$. In the hyperfine structure we have to consider the total nuclear angular momentum **I**, them the coupling now is between **I** and **J**, giving rise to the total atomic angular momentum $\mathbf{F} = \mathbf{I} + \mathbf{J}$. In the same way, all possibles values for **F** are given by

$$|I - J| \le F \le |I + J|. \tag{4.1.2}$$

For ⁸⁷Rb the ground state, $\mathbf{I} = 3/2$ and $\mathbf{J} = 1/2$, so $\mathbf{F} = 1$ or $\mathbf{F} = 2$. For the excited state of the D₁-line $(5^2 P_{1/2})$, also have $\mathbf{F} = 1$ or $\mathbf{F} = 2$, while for the excited state of the D₂-line \mathbf{F} can take any of the values 0, 1, 2, 3. The Hamiltonian that describe the hyperfine structure is (57)

$$\mathbf{H}_{hfs} = A_{hfs}\mathbf{I} \cdot \mathbf{J} + B_{hfs} \frac{3(\mathbf{I} \cdot \mathbf{J})^2 + \frac{3}{2}\mathbf{I} \cdot \mathbf{J} - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)},$$
(4.1.3)

where A_{hfs} is called the magnetic dipole hyperfine structure constant and B_{hfs} is the electric quadrupole interaction constant which can not be applied to the levels with $\mathbf{J} = 1/2$, the ground state. The constant of the hyperfine structure can be determined experimentally, the values for For ⁸⁷Rb can be find it in (57) reference. Due to this interaction the energy shift of the hyperfine structure is

$$E_{hfs} = \frac{1}{2}A_{hfs}K + B_{hfs}\frac{3K(K+1) - 4I(I+1)J(J+1)}{8I(2I-1)J(2J-1)},$$
(4.1.4)

where K is given by

$$K = F(F+1) - I(I+1) - J(J+1).$$
(4.1.5)

For each hyperfine level F we have 2F + 1 magnetic energy sublevels m_F with $|m_F| \leq F$. Without magnetic field all those sublevels are degenerate but, if we place a weak external magnetic field in a given direction for instance B_z along of the atomic quantization axis, the magnetic sublevels will be split linearly according to (57)

$$\Delta E_{F,m_F} = \mu_B g_F m_F B_z, \tag{4.1.6}$$

where μ_B is the Bohr magneton and g_F is the hyperfine landé g-factor which is a function of the spin, orbital and nuclear angular momentum. The hyperfine structure for the ⁸⁷Rb are illustrated in the fig. 4.1.1 and the splitting of the energy sublevels for each m_F are graphed in the fig. 4.1.2



Figure 4.1.1 – Hyperfine structure of ⁸⁷Rb atoms. a). In the graph we can see the D1 line $(5^2s_{1/2} \rightarrow 5^2p_{1/2})$, b). D2 line $(5^2s_{1/2} \rightarrow 5^2p_{3/2})$. The separations of the hyperfine energy levels in units of frequency. Source: By the author.



Figure 4.1.2 – Anomalous zeeman effect for 87Rb. In the graph we can see the splitting of the two first hyperfine energy levels of the ground state $5^2S_{1/2}$, F = 1 and F = 2. Source: By the author.

4.2 Vacuum system



Figure 4.2.1 – Scheme of the double-MOT configuration for the machine of BEC2. Source: By the author.

The vacuum system have two chambers, the first one (MOT1) is made of common glass and the second one (MOT2) is a quartz cell with a high optical quality. They are connected through a thin glass transfer tube with a length of 50 cm, with an inner diameter of 4mm in a configuration known as double-MOT. The first chamber is pumped by an ion pump of 55 L/s achieving a pressure into the cell around of 10^{-9} Torr. The second ion pump can be pumping with a rate of 300 L/s, getting a pressure into the chamber lower than 10^{-11} Torr. In the figure 4.2.1 we can see the double-MOT configuration of our system.

4.3 Laser system and MOT processes

Laser deceleration occurs when a gas with a velocity \vec{v} is counter-propagating to a laser beam with circular polarization. Each photon it is absorbed by atoms which are slowed by $v_{rec} = \hbar k/m$ ($k = 2\pi/\lambda$ where λ is the wave length of the light). In order to absorb again, the atom must return to the ground state by emitting a photon. Photons are emitted in random directions, but with a symmetric average distribution, so their contribution to the atom's momentum averages to zero.(21) With two pairs of coils (quadrupole coils), a weak magnetic field is generated separating the energy sublevels m_F of rubidium atoms, this is known as anomalous Zeeman effect. The current of the coils current are in opposite directions (anti-Helmholtz configuration) supplying the quadrupole magnetic field on the MOT1 (first chamber) and MOT2 (second chamber), this creates a spatial dependence of the light detuning frequency respect to the magnetic field.(22) At the point in the middle of the coils the magnetic fields produced by the coils cancel out, so that B = 0. The value of the magnetic field gradient used in the Magneto-Optical trap (MOT) stage it is approximately of 12 G/cm.(40) All this leads to trap the atoms in the MOT. The MOT is generated in the following way. The Zeeman effect causes that the energy of the three sublevels with $m_F = 0, \pm 1$ of the $5^2 s_{1/2}$ (F = 1). The energy sublevels vary linearly with the atoms position, as show for the z-axis in Fig 4.3.1. For a component of the magnetic field in z-direction B_z and $\Delta m_F = -1$ for z > 0, transition moves closer to resonance with the frequency of the laser beam. Making use of the selection rules the absorption of the photon excites the σ^{-} transition and this gives a scattering force that pushes the atom back, towards the trap center. A similar process occurs for a displacement in the opposite direction z < 0 and σ^+ because $\Delta m_F = +1.(22)$

After the MOT process, it is necessary decrease more the temperature of the atoms. The optical molasses and the optical pumping are processes that reduce the temperature of the atoms after the MOT. The first one, the optical molasses is when the magnetic field of the MOT is switch off quickly and the cooling frequencies detuning goes to red 60 MHz (in our case). In the optical molasses the light exerts a frictional, or damping, force on the atoms just like that on a particle in a viscous fluid.(22) So the force produced by each counter-propagating beam decelerates atoms. The second one, the optical pumping process in which all atoms on the ground state $5^2S_{1/2}$ (F = 1) and $5^2S_{1/2}$ (F = 2) are transferred to the excited state $5^2P_{3/2}$ ($F' = 2 m_F = 2$) when we turn on an additional pair of coils called "optical pumping coils" providing an uniform weak magnetic field of 1 G. With this processes the temperature of the atoms is lower than 40 μ K. The reason why we do this is because the atoms must be magnetically catch able as we shall later.



Figure 4.3.1 – The blue and red balls represent the atoms that can interact with the circular polarized light. When the atom is moving to the right direction (red) it take a kick from the photon in the opposite direction and make that the atom come back to the center of the trap. Occurs the same for atoms moving on the another direction (blue). Source: By the author.

In the first and second chamber the rubidium atoms are confined in by the MOT using three orthogonal pairs of counter-propagating laser beams intercepted at the center of the trap. They are supplied by three diode laser of the company TOPTICA Photonics DLX 110-L with a wave length of 780 nm and linewidth of 1 MHz. During the BEC production occurs different processes with the light, two of the three lasers are locked with a red detuning of 20Mhz (cooling frequency). The corresponding transitions is $5^2 S_{1/2}$ (F = 2) to $5^2 P_{3/2}$ (F' = 3), in which the atoms are pumped to the ground state with F = 2 to F' = 3 of the excited state. With this transition will be possible generate the optical trapping of the MOT1 and MOT2, they are called "Cooling 1" and "Cooling 2" respectively.(40) As the source of atoms is in the MOT1, is necessary to transfer them to the MOT2 where they will be trapped again. For this reason, we add another laser beam called "Push" with the same characteristics of the cooling beams. When the atoms are in the excited state can decay not only the state $5^2 S_{1/2}$ (F = 2) but can also decay into the state $5^2 S_{1/2}$ (F = 1). In this case the third laser is used to pump the atoms into cooling transition with the frequency necessary for the transition from $5^{2}S_{1/2}$ (F = 1) to $5^{2}P_{3/2}$ (F' = 2) of the excited state. Before of begin the BEC another beam is introduced on the atoms. it is called "Optical Pumping". its function is to put all the atoms, $5^2 S_{1/2}$ (F = 1) as $5^2 s_{1/2}$ (F = 2) in the excited state $5^2 P_{3/2}$ ($F' = 2, m_F = 2$). Finally, when the BEC is achieved, one of the way to characterize it is through image absorption. A beam pass across of the BEC, absorbing the light and leaving a hole on the laser beam. It is the "Image Beam" which is completely resonant with the transition $5^2 S_{1/2} (F = 2) \rightarrow 5^2 P_{3/2} (F' = 3).(40)$ The state transitions of the atom and the laser system are illustrated in the figure 4.3.2.



Figure 4.3.2 – On the left side we can see the light scheme of the system in the hyperfine structure of the atom. There are four important frequencies in the system, necessaries to achieve all the stages of the BEC. In the right side we show the optical design of the laser beams in the table work. Source: By the author.

4.4 Magnetic and dipole trap

4.4.1 Magnetic trap

When the MOT, the optical molasses and the optical pumping processes has been achieved, the next step is transfer the atoms cloud in a pure magnetic trap (MT), where all the light are turn off ad the magnetic field is abruptly increased to a gradient of 150 G/cm. Them, the magnetic field is ramped linearly during 500 ms from 60 G/cm to 160 G/cm. The profile of the quadrupole magnetic field can be calculated using the expression given by

$$U_{MT} = \mu_B g_F m_F B'_x \sqrt{x^2 + \frac{y^2}{4} + \frac{z^2}{4}}, \qquad (4.4.1)$$

where $\mu = \mu_B g_F m_F$, the Landé g-factor g_F is for F = 2 and B'_x is the gradient of the magnetic field along the strong direction. After of the confinement of the atoms in the MT, the next step is to do the evaporating cooling technique, which consist to induce a transition of the hyperfine sublevels for a completely repulsive state $(F = 0, m_F = -1, -2)$ by radio frequency (RF), that leaves the atoms feel the potential as repulsive and escapes from the trap. It is necessary to avoid the point in which the magnetic field vanish (the center of the trap). When the atoms are near of the this point, exist a probability to change the spin of the atom, atoms with energy F = 2, $m_F = 1$, 2 which are magnetically catchable, that mean, they feel an attractive magnetic potential. By another way, atoms with energy F = 2, $m_F = 0$, -1, -2 feel a repulsive magnetic potential, doing them escape of the trap. This hole on the magnetic field, and the fact that atoms get away of the trap because the change in the spin state, is known as Majorana Flips.(58) The RF evaporation technique induce selectively the transitions of the atoms, so, its possible to remove remove the most energetic atoms, such a way that the atoms thermalize at lower temperature due to collisions between them.(59)

4.4.2 Optical dipole trap

The optical dipole trap of our system is provided by a Ytterbium fiber laser with a 1064 nm wavelength of the company IPG Photonics. The frequency of the light has to be far-detuned of any resonance frequency of the atom. The model that describes the interaction between the atoms and light field is known as dressed atom model.(60) Follow this model, the potential energy generated by the dipole trap is given by

$$U_{OT} = -\frac{U_0}{(1+y^2/y_R^2)} \exp\left[-\frac{2(x^2+z^2)}{\omega_0^2(1+y^2/y_R^2)}\right],$$
(4.4.2)

with,

$$U_0 = \frac{3c^2 P}{(\omega_{5^2 s_{1/2} \to 5^2 p_{3/2}})^3 \omega_0^2} \left(\frac{\Gamma}{\Delta}\right)^2$$
(4.4.3)

where U_0 is the potential depth, $\omega_{5^2s_{1/2}\to 5^2p_{3/2}}$ and Γ are the resonant frequency and decay rate in the transition $5^2s_{1/2} \to 5^2p_{3/2}$ respectively. Δ is the detuning of the laser frequency, y is the direction of propagation, y_R is called Rayleigh range, P is the laser power and ω_0 is the beam waist.

To avoid the Majorana's hole, the optical dipole trap (ODT) modify the potential profile of the magnetic trap, removing the null point of the magnetic field. Superposing the two traps (MT and ODT), the resulting trap is called "Hybrid Trap" and its expression for the potential energy will be the total sum of the magnetic trap potential U_{MT} , optical

- 100

- 50

0

x(µm)

trap potential U_{OT} and the contribution of the gravitational potential on the atoms. The expression for the hybrid potential is

$$U_{HT} = \mu B'_x \sqrt{x^2 + \frac{y^2}{4} + \frac{z^2}{4}} - \frac{U_0}{(1+y^2/y_R^2)} \exp\left[-\frac{2x^2 + 2(z-z_0)^2}{\omega_0^2(1+y^2/y_R^2)}\right] + mg(z-z_0) + E_0.$$
(4.4.4)

Figure 4.4.1 – Hybrid trap potential in the strong x and weak z direction. A). show the hybrid potential in x direction with four different gradients of magnetic field 150 G/cm (yellow line), 100 G/cm (Green line), 60 G/cm (red line) and 30.6 G/cm (purple line). The dash line is the magnetic quadrupole potential for 150 G/cm. B). is the profile of the hybrid trap in z direction, the color lines are the same that A and the laser power is 6 W. In C) and D) the gradient of the magnetic field is around 30.6 G/cm the plots are for four different power laser, 200 mW (yellow line), 100 mW (green line), 60 mW (red line) and 45 mW (purple line). Source: By the author.

100

50

- 200

- 150

- 100

z(µm)

- 50

In this expression z_0 is the offset between the dipole beam trap depth and the zerofield of quadrupole trap. On the fig. 4.4.1 is showed the profile of the hybrid trap in two situations, when we have a strong magnetic potential and dipole potencial as in fig. 4.4.1(A) and 4.4.1(B), in which we can see the profile of the hybrid trap as we decrease the gradient of the magnetic field from 150 G/cm to 30 G/cm with a laser power of 6 W one in x direction and other in z direction. The waist of the beam used was 75 μK and the offset position $z_0 = 100 \ \mu m$. The another situations happen when we have a weak magnetic potential and dipole potential as in fig. 4.4.1(C) and 4.4.1(D). The gradient of the magnetic field do not compensate anymore the gravity, the atoms "fall" into the depth of the optical dipole trap. In this point, we start the optical evaporation process in which the power laser decrease from 6 W to 45 mW. After this procedure the Bose-Einstein condensation can be observed.

4.5 Bose-Einstein condensation of ⁸⁷Rb

4.5.1 Image system

Finally, when the BEC is reached, all the potentials in the trap are switch off and the ultra-cold cloud is released in time of flight (TOF). This stage is when the image beam take place, a completely resonant beam laser with the transition $5^2s_{1/2}$ (F = 2) $\rightarrow 5^2p_{3/2}$ (F' = 3) go through the BEC, them, the light is absorbed by the cloud leaving a "shadow" on the beam laser, after that, the image is captured by a CCD camera pco.imaging model 270XS which contains a chip with dimensions 1384 × 1024 pixels with 6.45 × 6.45 μ m² by pixel. This method of obtain imaging is known as absorption image (42) which is show in the fig. 4.5.1.



Figure 4.5.1 – Absorption image system. The resonant light of the laser its absorbed by the atoms, creating "shadow". This shadow its collected by an optical arraignment and focused into a CCD camera. Source: By the author.

The resulting image, normalized image, is generated by calculations of another three images captured in TOF. The first one is the image with atoms, the second one is the image without atoms, this image is obtained after of the image with atoms because we need to subtracts the region where there are atoms and not. Finally the third we take an image is the background, for be sure that there is not a offset of the light intensity coming into the camera. The calculation of the normalized image can be obtained through the equation

$$NormalizedImg = \frac{ImgWithAtoms - BackgroundImg}{ImgWithoutAtoms - BackgroundImg}.$$
 (4.5.1)

From the normalized image we obtain the 2D density profile that can help us to determinate the parameter of the atomic cloud as temperature, atoms number and the size of the atomic cloud. since, we collect the cloud image on a CCD camera, the profile is in a 2D we lose information because the density profile come to us in a 3D. Integrating this we obtain information of the density of the cloud, in this way

$$n(z, y) = \int dx \, n(x, y, z) = -\frac{1}{\sigma_0} \left[\frac{I(y, z) - I_b(y, z)}{I_0(y, z) - I_b(y, z)} \right], \tag{4.5.2}$$

where I(y, z) is the intensity related to the image with atoms, $I_0(y, z)$ is only related to the intensity of the laser beam on the image without atoms, and $I_b(y, z)$ is the intensity when there is not light on the camera, the background image. Finally, σ_0 is the scattering cross-section. The law physics below of this treatment is the Beer-Lambert law. In the next section, we going to discuss how we analyze the atomic cloud picture and obtain its parameters (i.e. number of atoms, temperature and sizes).

4.5.2 Thermal atomic cloud

The 2D profile density of a thermal cloud is a Gaussian distribution.(42) The equation of the 2D profile becomes

$$n_{2Dth}(y, z) = \frac{\eta_{th}}{\sigma_0} \exp\left[-\frac{(y-y_0)^2}{2\sigma_y^2} - \frac{(z-z_0)^2}{2\sigma_z^2}\right]$$
(4.5.3)

The size of the cloud can be defined using two widths σ_x and σ_y . y_0 and z_0 are the distribution centers in the image, and η_{th}/σ_0 is the peak value of the distribution. The atom number of the thermal cloud is obtained by the integral of the 2D density profile n_{2Dth} .

$$N_{th} = \int dy dz \, n_{2Dth}(y, z) = \frac{2\pi}{\sigma_0} \eta_{th} \sigma_y \sigma_z \tag{4.5.4}$$

This show that the atom number of the thermal cloud is proportional to the widths of the Gaussian distributions and the peak value of the density profile. Furthermore, the temperature of the cloud can be extracted using the energy conservation. The velocity distribution correspond to the expansion velocities in two directions at time $t_{exp} = TOF$. The kinetic energy associated to the velocity distributions is equal to the thermal energy of the system given by

$$k_B T = \frac{1}{2} m v^2 \to T = \frac{1}{2} \frac{m}{k_B} v^2,$$
 (4.5.5)

m is the mass of the atoms and $v = \frac{d\sigma(t_{exp})}{dt_{exp}}$ is the expansion velocity. The temperature of the thermal cloud after a certain expansion time is

$$T = \frac{1}{2} \frac{m}{k_B} \left[\frac{(\sigma_y - \sigma_{0y})^2 + (\sigma_z - \sigma_{0z})^2}{\Delta^2 t} \right],$$
(4.5.6)

where σ_{0i} is the initial width of the thermal cloud at a initial time t_0 . For long TOF we can consider that σ_{0i} is smaller than σ_i , so the temperature of the cloud at TOF is

$$T = \frac{m}{2k_B} \left[\frac{\sigma_y^2 + \sigma_z^2}{t_{TOF}^2} \right]. \tag{4.5.7}$$

One of the characteristics of the thermal cloud is the isotropic expansion during time of flight. The cloud expands with the same aspect ratio, which is ratio between the widths of the cloud. Its dynamic can be described classically. A expansion in TOF of the thermal cloud is showed in the fig. 4.5.2

Sequence of images during the TOF



Figure 4.5.2 – Expansion of the thermal cloud for different times of flight. On the figure we can observe that the aspect ratio is constant while the cloud is falling, explaining the isotropic expansion. Source: By the author.

4.5.3 Condensate atomic cloud

The profile of the condensate cloud density distribution is given by the Thomas-Fermi approximation, in which the shape of the atoms have the "potential's face", in our case an inverted parabola. So, the optical density density profile for the condensate cloud can be written as

$$n_{2DBEC}(y, z) = \frac{\eta_{TF}}{\sigma_0} \max\left[\left(1 - \frac{(y - y_0)^2}{R_y^2} - \frac{(z - z_0)^2}{R_z^2} \right)^{3/2}, 0 \right],$$
(4.5.8)

where η_{TF}/σ_0 is the peak value of the distribution and R_y and R_z are the Thomas-Fermi radius (BEC radius) in a y and z direction, respectively. To calculate the atom number we as the same way with the thermal cloud, integrate the optical density to obtain the atom number in the BEC cloud

$$N_{BEC} = \int dy dz \, n_{2DBEC}(y, \, z) = \frac{5\eta_{TF}}{4\sigma_0} R_y R_z.$$
(4.5.9)



Figure 4.5.3 – BEC expansion of the condensed cloud for different times of flights. In the graph we can see the aspect ratio inversion, which is a important characteristic that define a BEC. Source: By the author.

The atom number is proportional to the Thomas-Fermi radius of the condensed cloud and the peak value of the distribution. Contrary to the thermal cloud, the TOF expansion of the condensate cloud is much faster on the direction in which the confinement trap potential is strongest. The cloud in time of flight undergoes an aspect ratio inversion as show in fig. 4.5.3.

The Global Thermodynamic Variables

The global thermodynamics variables are appropriate variables to describe a thermodynamic system in which the state variables are not very well defined. In (9) Romero-Rochín and V. Bagnato defines the global variables comparing the results obtained for a Bose gas in a 3D harmonic potential with the results in a box potential, relating an extensive variable with the frequencies of the trap, because, they are not depend on the size of the system. The volume parameter \mathcal{V} is associated to the volume in the case of a harmonic potential. Consequently, the conjugated variable of the volume is the pressure, in the approach of the global variables, the pressure parameter Π is an intensive variable that depend on the number of particles, the density distributions, and the harmonic potential of the cloud. Together, the \mathcal{V} and Π describe macroscopically a quantum system as a BEC, because his product result in the total energy of the system. In this chapter we will define the global thermodynamics variables and also we will show the results obtained employing the formalism of these variables.

5.1 Volume and pressure parameter

we will introduce the variable \mathcal{V} , an extensive variable that depends on the potential frequencies, this variable was defined as

$$\mathcal{V} = \frac{1}{\bar{\omega}^3} = \frac{1}{\omega_x \omega_y \omega_z}.$$
(5.1.1)

The volume parameter \mathcal{V} , does not have volume units, but his product with another quantity, his conjugated variable, the *pressure parameter* Π give units of energy. Theses two variables are related through of the relation

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$$\Pi = -\left(\frac{\partial\Omega(\mu, T, \mathcal{V})}{\partial\mathcal{V}}\right)_{\mu, T}.$$
(5.1.2)

We use the macrocanonical partition function to obtain the pressure parameter, in the case that exist an interaction between the particles. The expression of the macrocanonical partition function in terms of the macrocanonical operator \hat{K} is

$$\Xi = \operatorname{Tr}\left[\exp(-\beta \hat{K})\right],\tag{5.1.3}$$

where $\hat{K} = \hat{H}_N - \mu \hat{N}$ is the macrocanonical operator . Using the Hamiltonian with the interaction between the particles, eq. 2.3.4 we have

$$\Xi = \text{Tr}\left[\exp\left[-\beta \sum_{i}^{N} \frac{\hat{P}_{i}}{2m} + \frac{1}{2} \sum_{i}^{N} m \mathcal{V}^{-2/3} \hat{r}_{i}^{2} + \sum_{i < j}^{N} \hat{V}(r_{ij}) - \mu \hat{N}\right]\right].$$
 (5.1.4)

In which the harmonic potential was rewritten in term of the volume parameter \mathcal{V} . Thus, we can obtain the pressure parameter directly of the eq. 5.1.2, given by

$$\Pi = \frac{2}{3\mathcal{V}} \frac{1}{\Xi} \operatorname{Tr} \left[\sum_{i}^{N} \frac{1}{2} m \mathcal{V}^{-2/3} \hat{r}_{i}^{2} \exp\left(-\beta \hat{K}\right) \right], \qquad (5.1.5)$$

using the identity

$$\sum_{i}^{N} \frac{1}{2} m \bar{\omega}^{2} \hat{r}_{i}^{2} = \int d^{3}r \frac{1}{2} m \bar{\omega}^{2} r^{2} \sum_{i}^{N} \delta(r - r_{i}), \qquad (5.1.6)$$

in this form

$$\Pi = \frac{2}{3\mathcal{V}} \int d^3r \frac{1}{2} m \bar{\omega}^2 r^2 \frac{1}{\Xi} \operatorname{Tr}\left[\sum_i^N \delta(r - r_i) \exp(-\beta \hat{K})\right], \qquad (5.1.7)$$

$$\Pi = \frac{m}{3\mathcal{V}} \int d^3r \, n(r) \left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right), \tag{5.1.8}$$

where the density $n(r) = \frac{1}{\Xi} \text{Tr} \left[\sum_{i}^{N} \delta(r - r_i) \exp(-\beta \hat{K}) \right]$. This shows that the pressure parameter can be expressed in term of the cloud density, the external potential of the trap and also inversely proportional to the *volume parameter* \mathcal{V} . If the system it is below of the critical temperature, the density will be n_0 which correspond to the density of the condensate, given by TFA. Otherwise the density follows a classical behavior. All those approach to reach the new variable Π and \mathcal{V} is called global variable approximation and it has been developed by Romero-Rochin and V. S Bagnato.(1, 9, 61)

5.2 Achieved measurements

In our group the global thermodynamic variables has been used to measure some thermodynamics susceptibilities as the heat capacity(10), isothermal compressibility(11), the thermal expansion coefficient(62) and also hydrodynamics properties as the sound velocity in a box gas.(63) In this section, we will see the measurements of this quantities and also how the global thermodynamic approach has been successes in explain the behavior of the phase transition of this system.

5.2.1 Isothermal compressibility

To obtain the frequencies of our 3D harmonic trap, we have to take in consideration the equation for the hybrid potential 4.4.4.

$$U_{HT} = \mu B'_x \sqrt{x^2 + \frac{y^2}{4} + \frac{z^2}{4}} - \frac{U_0}{(1 + y^2/y_R^2)} \exp\left[-\frac{2x^2 + 2(z - z_0)^2}{\omega_0^2(1 + y^2/y_R^2)}\right] + mg(z - z_0) + E_0.$$

If we expand this expression in the Taylor's series, we can approximate this potentials in terms of a polynomial equation as

$$U_{HT} = \sum_{n=0}^{\infty} \frac{U_{OH}^{(n)}(x, y, z)(x - x_0, y - y_0, z - z_0)^n}{n!},$$
(5.2.1)

$$U_{HT} \simeq \frac{1}{2}\mu B'_{x}z_{0} - U_{0} + E_{0} + \left(\frac{1}{2}\mu B'_{x} + mg\right)(z - z_{0}) + \frac{1}{2}\left(\frac{4U_{0}}{\omega_{0}^{2}} + \frac{2\mu B'_{x}}{|z_{0}|}\right)x^{2} + \frac{1}{2}\left(\frac{\mu B'_{x}}{2|z_{0}|} + \frac{2U_{0}}{y_{R}^{2}}\right)y^{2} + \frac{1}{2}\left(\frac{4U_{0}}{\omega_{0}^{2}}\right)(z - z_{0})^{2} + (5.2.2)$$
$$\mathcal{O}(x^{3}, y^{3}, z^{3}).$$

We consider that $y/y_R \ll 1$ and we can identify the frequencies as

$$\omega_x = \sqrt{\frac{4U_0}{m\omega_0^2} + \frac{2\mu B'_x}{m|z_0|}}, \quad \omega_y = \sqrt{\frac{\mu B'_x}{2m|z_0|}}, \quad \omega_z = \sqrt{\frac{4U_0}{m\omega_0^2}}, \quad (5.2.3)$$

where the radial frequencies ω_x and ω_z have a strong contribution of the optical trap depth. The axial frequency ω_y depend only of the magnetic field gradient, which remains constant in the final stage of the process to achieve the BEC. This means that the geometry of our trap only will be changed by the laser power of the ODT. As the magnetic field gradient B'_x is very smaller than the power of the dipole laser, we can approximate the radial frequencies as $\omega_x \simeq \omega_z = \omega_\rho$ which correspond and a cylindrical approximations. In this case, the frequency ω_ρ can be expressed as the mean value of the radial frequencies as

$$\omega_{\rho} = \frac{1}{2}(\omega_x + \omega_z). \tag{5.2.4}$$

As we saw in the chapter 3, second-order phase transitions (in the Ehrenfest classifications) or continuous phase transitions (in the modern classification), are characterized by the no presence of the latent heat when the system is at the critical point. Particularly, his susceptibilities are discontinuous at the critical point. In this chapter we going to show how the isothermal compressibility k_T was measured, and how we related it with a second-order phase transition. In eq. 3.2.4 was defined the isothermal compressibility k_T in terms of the thermodynamic variables volume V and pressure P. To define the the isothermal compressibility parameter κ_T in our system, its necessary to defined it in terms of the new thermodynamics variables, the volume parameter \mathcal{V} and the pressure parameter Π as follow

$$\kappa_T = -\frac{1}{\mathcal{V}} \left(\frac{\partial \mathcal{V}}{\partial \Pi} \right)_{T,N}.$$
(5.2.5)

The isothermal compressibility parameter κ_T is a quantity with the same properties of the standard compressibility k_T and indicates the thermodynamic stability defined by the second derivative of Gibbs free energy. The convexity property of the free energy is maintained with the condition, $0 \leq \kappa_T \leq \infty$. Our system its able to achieve a pure BEC of ~ 10⁵ atoms at typical temperatures 100 - 200 nK.

We characterize the atomic cloud using the imaging absorption system which was described in the section 4.5.1. For all images obtained, the free expansion time (TOF) is 30 ms. Varying the power laser of the ODT, the frequencies of the trap can be changed, and a set of different frequencies results in a different volume parameters. To measure the frequencies of the trap when the Bose-Einstein is achieved we give a "kick" on the cloud with a external magnetic field. After of the kick, the cloud remains a few mili-seconds into the hybrid trap, after that the cloud is released in TOF and the position into the trap will be change in function of the time after the kick. The behavior of the center of mass of the cloud will be a sinusoidal wave, characterized by a frequency $f_i = \omega_i/2\pi$; i = x, y, z for each axis in consideration. In the fig 5.2.1 we show the three frequencies f_x , f_y and f_z for two volume parameters \mathcal{V}_1 and \mathcal{V}_2 . In the references (40, 48) it can find all the total experimental description and measurements of the trap frequencies. We summarize in the table 5.1 all the volume parameters used to calculate the isothermal compressibility

parameter and also the thermal expansion coefficient was obtained later using the eq. 5.1.1.



Figure 5.2.1 – Measure of the trap frequencies for two volume parameter \mathcal{V}_1 (left) and \mathcal{V}_2 (right). The graphs shows the positions of the center of mass of the cloud in pixels (px). The solid lines represent the fitting for a sinusoidal curve which the frequency $f_i = \omega_i/2\pi$ was extracted. Also we can see the differences between the radial frequencies and the axial frequencies in which $\omega_x \simeq \omega_z$ and ω_y is different of them. In the frequency ω_z for \mathcal{V}_2 shows how to change the power laser of the ODT the volume parameter can be changed. Source: By the author.

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		2
	$\mathcal{V}\left(rad/s^{3} ight)$	$\Delta \mathcal{V}\left(rad/s^{3} ight)$
\mathcal{V}_1	1.9×10^{-7}	8.2×10^{-9}
\mathcal{V}_2	6.4×10^{-8}	2.02×10^{-9}
\mathcal{V}_3	3.2×10^{-8}	1.01×10^{-9}
\mathcal{V}_4	1.75×10^{-8}	5.5×10^{-10}
\mathcal{V}_5	1×10^{-8}	3.14×10^{-10}
Source: By the author.		

Table 5.1 - Volume parameters

Phase Diagrams



Figure 5.2.2 – Phase Diagram for Π vs T and Π vs N/\mathcal{V} curves from Romero-Rochín.(1) In both cases we can use the change in the behavior when occurs the transitions from thermal to condensate regime. Source: ROMERO-ROCHÍN et al.(1)

Equilibrium lines where two or more phases can coexist in thermodynamic equilibrium. When we mention phases in this thesis we refer to the property of the bosons to occupy the ground state and excited states, i.e. a quantum phase and classical phase, respectively. The equilibrium lines in this kind of system are typically represented by critical lines where quantum degeneresence begins to occur. A phase transition occurs when we go from one region to another through a critical line. In the reference (1) we can see how the phase diagram Π vs T and Π vs N/\mathcal{V} for a thermodynamic system in a harmonic trap fig.5.2.2. In order to calculate the pressure parameter Π by performing the integral in eq. 5.1.8, it is necessary to reconstruct the density profile of the atoms in the trap n(r), from the measured profiles in the time of flight, and the trap frequencies.(11) The density profile below of the critical temperature T_C will be the sum of the thermal and condensate contributions. In this way we can rewrite the equations for the pressure parameter 5.1.8 as follow

$$\Pi = \Pi_q + \Pi_{th} = \frac{2}{3\mathcal{V}} \left[\int d^3 r \, n_q(r) U(r) + \int d^3 r \, n_{th}(r) U(r) \right], \quad (5.2.6)$$

where $n_q(r)$ and $n_{th}(r)$ are the densities for the condensate and thermal part of the cloud respectively, which are given by

$$n_q = \frac{15N_0}{8\pi R_x^0 R_y^0 R_z^0} \max\left[1 - \left\{\left(\frac{x}{R_x^0}\right)^2 + \left(\frac{y}{R_y^0}\right)^2 + \left(\frac{z}{R_z^0}\right)^2\right\}, 0\right], \quad (5.2.7)$$

$$n_{th} = \frac{N_{th}}{(2\pi)^{3/2} \sigma_x^0 \sigma_y^0 \sigma_z^0} \exp\left[-\frac{1}{2} \left\{ \left(\frac{x}{\sigma_x^0}\right)^2 + \left(\frac{y}{\sigma_y^0}\right)^2 + \left(\frac{z}{\sigma_z^0}\right)^2 \right\} \right],$$
 (5.2.8)

where R_x^0 , R_y^0 and R_z^0 are the insitu Thomas-Fermi radius, N_0 is the condensate number of particles, σ_x^0 , σ_y^0 and σ_z^0 are the insitu width of the thermal cloud and, finally, N_{th} correspond to non-condensate atoms number of particles. Replacing the equations 5.2.7 and 5.2.8 into 5.2.6, the pressure parameter Π below the critical temperature is the sum of the two expression below

$$\Pi_q = \frac{mN_0}{21\mathcal{V}} \left(\omega_x^2 (R_x^0)^2 + \omega_y^2 (R_y^0)^2 + \omega_z^2 (R_z^0)^2 \right)$$
(5.2.9)

$$\Pi_{th} = \frac{mN_{th}}{3\mathcal{V}} \left(\omega_x^2 (\sigma_x^0)^2 + \omega_y^2 (\sigma_y^0)^2 + \omega_z^2 (\sigma_z^0)^2 \right).$$
(5.2.10)

The equation 5.2.10 is totally equivalent to the equation of state for an ideal gas. This fact can be verified using the equipartition theorem, where $\frac{1}{2}m\omega_i^2\sigma_i^2 = \frac{1}{2}k_BT$, them

$$\Pi_{th} \mathcal{V} = N_{th} k_B T \tag{5.2.11}$$

This equation, is the equation of state above the critical temperature T_C as is expected, because the thermal part follow the Maxwell-Boltzmann distribution. Now, the quantum pressure parameter Π_q can be rewritten with an analytical expression replacing the equations 2.2.22, 2.3.8 and 2.2.21 into 5.2.9, we obtain an analytical expression for the pressure parameter due to the condensed atoms, as follow(40)

$$\Pi_{q} = \frac{1}{7} \left[15a_{s}\hbar^{2}\sqrt{m} \left[\frac{N}{\mathcal{V}} - \left(\frac{k_{B}T}{0.94\hbar} \right)^{3} \right]^{7/2} \right].$$
(5.2.12)



Figure 5.2.3 – Phase diagram II vs T for a fixed atoms number $N = 1 \times 10^5$ atoms, the values of the volume parameter are showed in the table 5.1. Source: POVEDA-CUEVAS et al.(11)

For each volume parameter we have performed many experimental runs for temperature within the range 40 – 400 nK and post-selected atomic cloud containing $N = (1 \pm 0.1) \times 10^5$ atoms to be taken in consideration.(11) The result is presented in the fig 5.2.3 in which we are plotted the pressure parameter Π as a function of T, for different values of the volume parameter \mathcal{V} , remaining fixed the atoms number N. In the graph we can see clearly two regions: below the critical temperature T_C and above the T_C . The pressure parameter below the critical temperature is the result of the sum for the thermal and condensate contribution, follow the behavior of the equation $\Pi = \Pi_q + \Pi_{th}$, represented by the solid lines in the figure 5.2.3 below the T_C for each volume parameter. Above of the critical temperature, the behavior of the pressure parameter is the expected, the classical behavior of the state equation for an ideal gas (the straight lines in the fig. 5.2.3). Near of the BEC-thermal transition we can appreciate a abrupt change in in the behavior of the pressure parameter, revealing that at T_C is possible to find a continuous phase transitions. It is interesting to remark, when the temperature $T \rightarrow 0$ the pressure parameter in not zero.(12) The critical temperature curve can be expressed independent of the volume parameter \mathcal{V} and plotted in the middle of the transition in the fig. 5.2.3 which is given by

$$\Pi_C = (3.4284 \times 10^{10}) T_C^4 \to \Pi T^{-4} = const.$$
 (5.2.13)

The transition line from thermal state and condensate state in a $\Pi - \mathcal{V}$ diagram is plotted fig. 5.2.4. From the measurement in the fig. 5.2.3 we extract different isotherms and plotted in the fig. 5.2.4 relating the volume and pressure parameter $\mathcal{V} = \mathcal{V}_T(\Pi)$. From this graph, we can extract the isothermal compressibility parameter using the equation 5.2.5. Applying the derivative of the volume parameter respect to the pressure parameter and dividing by each volume parameter point by point, we obtain the isothermal compressibility parameter for a Bose gas in a harmonic trap. In the fig. 5.2.5 we plot these results, the isothermal compressibility parameter κ_T vs Π for different temperatures T.

In the fig 5.2.5(a) in clearly a thermal situation in which the temperature of the cloud is T = 150 nK. In this situation, κ_T follows the classical behavior $1/\Pi$, which correspond to the isothermal compressibility k_T for an ideal gas. When the temperature is slightly lower, T = 80 nK, which is approximately the critical temperature, the curve have an abrupt change for a certain pressure parameter fig. 5.2.5(b). The critical pressure parameter Π_C is between 20 and 30 (×10⁻¹⁹) J s⁻³, the sudden increase of κ_T indicates the transition. The compressibility reaches a maximum value before returning to the baseline after $40 \times 10^{-19} \,\mathrm{J \, s^{-3}}$ fig 5.2.5(b). In this pressure range the compressibility acquires values 4 to 8 times higher than the baseline. The behavior of the κ_T in fig. 5.2.5 is typical for a second-order phase transition (continuous transition).(11) In the last isotherm curve, T = 40 nK, the situation in which we have a pure BEC, the compressibility decrease with pressure parameter much faster than in the thermal regime. This can be explained saying that, in the thermal regime the expansion of the cloud have an anisotropic expansion, equal in all directions. But in the condensate regime, the interaction is more strongest in one direction produced by the harmonic potential, for this the expansion is much faster in one direction than another direction.



Figure 5.2.4 – Phase diagram \mathcal{V} vs Π for different isotherms $T = 175 \,\mathrm{nK}, T = 150 \,\mathrm{nK}, T = 175 \,\mathrm{nK}, T = 100 \,\mathrm{nK}, T = 75 \,\mathrm{nK}, T = 50 \,\mathrm{nK}, \text{ and } T = 40 \,\mathrm{nK}.$ For each isotherm we select a set of pressure and volume parameter points. They are separated by the critical pressure Π_C in a thermal and condensate region(gray region). The solid lines represent the best polynomial fitting and they are not a theoretical model. Source: POVEDA-CUEVAS et al.(11)



Figure 5.2.5 – Isothermal compressibility parameter κ_T in function of the pressure parameter II for three different isotherms, T = 150 nK, T = 80 nK and T = 40 nK, in which we can see the the behavior of κ_T in the thermal regime, near the transition and in the complete condensate regime. Source: POVEDA-CUEVAS et al.(11)

5.2.2 Heat capacity

The heat capacity using the global thermodynamic variables can be defined as

$$C_{\mathcal{V}} = \frac{3}{\bar{\omega}^3} \left(\frac{\partial \Pi}{\partial T} \right)_{N,\,\omega},\tag{5.2.14}$$

As a function of the volume parameter \mathcal{V} and its intensive conjugate variable Π , one can show that the internal energy of a harmonically trapped thermal cloud and pure BEC are $u_{th} = 3\Pi\mathcal{V}$ and $u_0 = 5\Pi\mathcal{V}/2$, respectively. These expressions can be found from the virial theorem. The first is the expected result for a noninteracting gas held in a three-dimensional (3D) harmonic oscillator potential. The second results from a contact interaction potential combined with the Thomas-Fermi approximation. Therefore it is valid to separate the thermal and the condensed fractions to determine the total internal energy(10)

$$u = 3\Pi_{th}\mathcal{V} + \frac{5}{2}\Pi_q\mathcal{V} \tag{5.2.15}$$



Figure 5.2.6 – a). Phase diagram IIvs T at constant volume parameter \mathcal{V} and three different number of particles N. b). Heat capacity $C_{\mathcal{V}}$ in a BEC system plotted around the condensation temperature T_C for two different atom numbers. Source: SHIOSAKI et al.(10)

where the total pressure parameter has been considered as the sum of the two components $\Pi = \Pi_{th} + \Pi_q$.(10) To obtain the pressure parameter, the density distribution is extracted

from the absorption image and, for a constant volume parameter, was obtained the phase diagram Π vs T at constant volume parameter, as shown in fig. 5.2.6(a). Using the equation 5.2.14 over each point in the fig. 5.2.6(a) the heat capacity is obtained and presented in the fig. 5.2.6(b) as a function of the temperature, where near the critical point is observed a spontaneous change in the heat capacity. The behavior of this result is accepted in the literature (64) as a property of a second-order phase transition. Thus, the investigation of the heat capacity steep change in a trapped gas, near Tc, is very significant to the overall understanding of the phase transition itself, especially for non-homogeneous density distributions.(10)

5.2.3 Pressure parameter at zero temperature

In the reference (12) was studied the behavior of the pressure parameter near of the absolute zero temperature. Again, we start from the phase diagram from Π vs T, fig. 5.2.7(a), in which we shows the behavior of the pressure parameter in function of the temperature, for a given atom number $N = 3 \times 10^5$ and the volume parameter $\mathcal{V} = 3 \times 10^8 \,\mathrm{s}^3$. The interpolation of the curve Π vs T below to $T < T_C$ allows to identify the pressure parameter when the temperature approximate to zero, reaching a finite value Π_0 . In the fig. 5.2.7(b) we can see the behavior of the pressure parameter at zero temperature, Π_0 , as function of the atoms number, showing that, as the atom number decrease, Π_0 also decreases. The theoretical curve is obtained using the eq. 5.2.12, in the limit of $T \to 0$, Π_0 depends only of the s-wave scattering lenght of the atomic cloud a_s and on its total atom number as follows the equation:

$$\Pi_0(T \to 0) = \frac{m}{21} \left(\frac{15\hbar^2 a_s}{m^2}\right)^{2/5} \left(\frac{N}{\mathcal{V}}\right)^{7/5}.$$
(5.2.16)

The pairs of conjugated variables $\Pi - \mathcal{V}$ in the quantum limit, obey an uncertainty relation that is able to describes the behavior of the quantum system when the temperature is near of the lowest possible value, T = 0. The preceding demonstration reveals ideas for the thermodynamic variables are sufficient to calculate some thermodynamic variables as we saw before. The fact that an equivalent compromise can exist between pressure and volume for a confined gas near absolute zero temperature is totally different from what is expected in traditional classical thermodynamics.(12) Therefore, we can say that the global thermodynamic variables are a powerful tool to explore the state of the thermodynamic quantum system and his behavior around the critical points, even near the absolute zero.



Figure 5.2.7 – (a). Pressure parameter Π as a function of the temperature T, for a fixed atom number and volume parameter. (b) Behavior of the pressure parameter at zero temperature function of the atom number. Source: CASTILHO et al.(12)

Chapter 6

Results and Discussion

In this chapter, the result of measuring the coefficient of thermal expansion of a BEC is displayed, showing how the transition from the thermal regime to condensate regime can be a continuous phase transition, and also how can be express the thermal expansion coefficient as critical phenomena in terms of the critical exponents and its scale law. So, the isobaric thermal expansion coefficient β_T can be defined as

$$\beta_{\Pi} = \frac{1}{\mathcal{V}} \left(\frac{\partial \mathcal{V}}{\partial T} \right)_{\Pi, N}, \tag{6.0.1}$$



Figure 6.0.1 – Phase diagram II vs T for a fixed atoms number $N = 1 \times 10^5$ atoms. Source: POVEDA-CUEVAS et al.(11)



Figure 6.0.2 – Phase Diagram \mathcal{V} vs T for different isobaric curves. In the graph we can see the the critical temperature showing the separation between the thermal and condensate regime. Source: By the author.

its means that, the capacity of the system of change its volume when we apply energy or temperature, normalized by the volume at constant pressure. As we know, the volume in our system is not the physical volume. In this case, the volume was changed by the frequencies of the confinement potential, like an effective volume of dilute gases in vacuum. To measure the isobaric thermal expansion coefficient it is necessary, as in the isothermal compressibility, a phase diagram, but in this case, a \mathcal{V} vs T diagram. Taking the phase diagram Π vs T in the fig. 6.0.1, it is possible to select a few isobaric (horizontal lines) and take the points that cross the volume parameters. Each point its plotted as a function of temperature for each isobaric curve with the same number of atom N. The corresponding phase diagram \mathcal{V} vs T is plotted in a log-log scale in fig. 6.0.2, in which each set of point correspond to an isobaric curve (constant pressure parameter). Many different isobaric curves are plotted, as well. Is clearly to see the behavior of the volume parameter as a function of temperature in two regions: the gray zone and the white zone, representing the condensate and thermal regime respectively. The solid lines above the critical temperature follows the behavior of the ideal gas law $\Pi \mathcal{V} = Nk_B T$ as expected for thermal clouds. The curves below the critical temperature are not theoretical models, they are the best curve fit over those points, following a similar behavior that the isothermal compressibility parameter κ_T , because is not possible to predict in fig. 6.0.2 what is the behavior of the volume parameter at T = 0.

In order to obtain the isobaric thermal expansion coefficient of a Bose gas, using the fig. 6.0.2 and evaluating the derivative in eq. 6.0.1, we obtain β_{Π} at constant pressure parameter $\Pi_{20} = 20 \times 10^{-19} \,\mathrm{J\,s^{-3}}$ which is plotted in the fig 6.0.3. Below to the critical temperature, the thermal expansion coefficient grow up faster than above the critical temperature. Near of this point, we can see a high peak very close of the transition point, revealing a continuous phase transition for the isobaric thermal expansion coefficient. The same was done for three different pressure parameters $\Pi_3 = 3 \times 10^{-19} \,\mathrm{J\,s^{-3}}$, $\Pi_{20} = 20 \times 10^{-19} \,\mathrm{J\,s^{-3}}$ and $\Pi_{80} = 80 \times 10^{-19} \,\mathrm{J\,s^{-3}}$ showing in fig 6.0.4 a similar behavior, each one near of the critical temperature. It is important to note that the collection of the thermal coefficient plots in fig. 6.0.4 indicate that high pressure parameters promotes condensation at high temperature as expected. For all pressure, the typical shape β_{Π} vs T is present.



Figure 6.0.3 – Isobaric thermal expansion coefficient for a Bose gas with a constant pressure parameter $\Pi_{20} = 20 \times 10^{-19} \, \mathrm{J \, s^{-3}}$ as a function of the temperature. Source: By the author.



Figure 6.0.4 – Thermal expansion coefficient for three different isobaric $\Pi_3 = 3 \times 10^{-19} \,\mathrm{J \, s^{-3}}$, $\Pi_{20} = 20 \times 10^{-19} \,\mathrm{J \, s^{-3}}$ and $\Pi_{80} = 80 \times 10^{-19} \,\mathrm{J \, s^{-3}}$. Source: By the author.

To analyses the behavior of β around T_C , we consider the case in fig. 6.0.3 in which we consider the reduced temperature $t_r = |T - T_C|/T_C$ and the thermal expansion coefficient as a function of a critical exponent α given by

$$\beta_{\Pi} \sim t_r^{-\alpha},\tag{6.0.2}$$

which is valid for $T < T_C$. Taking the limit when $T = T_C$ or $t_r \to 0$ we can find the value of α , thus

$$\alpha = -\lim_{t_r \to 0} \frac{d\ln\beta}{d\ln t_r}.$$
(6.0.3)

In fig. 6.0.5 we illustrate the behavior of β vs t_r , showing that the limit of the eq. 6.0.3 is finite as t_r approximates to 0. The dashed line represent the curve which slope is $\alpha = 0.15$. Equivalents values for alpha are obtained for other pressure parameters and the combined values results in
In 2007 Donner et. al. (65) investigate the correlation length as a critical phenomena as $\xi \propto t_r^{-\nu}$. The observation enable then to obtain a critical exponent through the correlation length, revealing a critical exponent $\nu = 0.67 \pm 0.13$. Considering this value of ν and our value for α and applying the scaling law $d\nu = 2 - \alpha$ it is possible to obtain the value for the dimension for the system

$$d = 2.76 \pm 0.16, \tag{6.0.5}$$

which is slightly smaller than 3, the expected value for our geometry. This deviation can come from the finite size of the system or effects no yet considered. Since the global variable is fully related to the thermodynamics in a formal sense, it should not introduce variations on d. In doing that another limitation arises from technical difficulties to obtain data for t_r very close to zero. The capability to measure for smaller t_r could improve the value of α . A deep theoretical evaluation on the critical exponent using global variables could also elucidate differences that are however out of the scope of this work. Besides the technical limitation, it seems clear that the use of global thermodynamics variables may open up a whole new window of opportunities to investigate universality and scaling laws for those non-homogeneous systems. In special, interactions play an important role in this field. While it is practically impossible to vary the interaction in 4He λ -transition, it is possible for trapped atoms. The new possibilities for universality in strong correlated systems may be quite exciting since it is very unknown. In all new possible exciting situations, the global variable concept may well be a nice tool of great relevance as demonstrated with this present walk.

Our experiment procedure, allow to investigate the system across the critical temperature T_C and the extraction of the susceptibilities which its divergences provide us information about the critical exponent. In this sense, we are near the critical point. It would be very nice if we could explore a whole collection of point around T_C , this is however technically very hard and the best that we can do is observe around and extrapolate the best behavior near the critical point.



Figure 6.0.5 – Critical exponent α for the thermal expansion coefficient β_{Π} . Source: By the author.

Chapter 7

Conclusion

We can conclude that formalism of global thermodynamics variables has successfully describes the system by mean the volume and pressure parameter. The volume parameter is defined as $\mathcal{V} = 1/\bar{\omega}^3$, where $\bar{\omega}$ is the product trapping frequencies. The pressure parameter Π , was defined as product of density distributions and harmonic potential. Eq. 5.1.8 shows that Π and \mathcal{V} are conjugated variables. In experiment we reached a BEC of $^{87}\mathrm{Rb}$ atoms with an average number of atoms approximately \sim 10^5 in a range of temperature of 40 - 300 nK. Using dipolar oscillations of the BEC it was possible to measure the frequencies of the hybrid trap composed by a magnetic trap and optical dipole trap. The volume parameter could be modified by variation of laser power of the ODT. It allows us to construct a phase diagram Π vs T, where each curve assume the constant number of atoms and volume parameter. By means the constructed phase diagram, we can build another phase diagram Π vs \mathcal{V} to then extract the derivatives of volume parameter respect to pressure parameter and thus obtain the isothermal compressibility κ_T . Around critical temperature, the isothermal compressibility shows a discontinuity that indicates the existence of the second-order phase transition. The thermal expansion coefficient β_{Π} has been obtained in the same way. Applying the thermodynamic definition of the thermal expansion coefficient, we obtained its dependence on temperature. The results shows that also near the critical temperature T_C , β_{Π} demonstrates an abrupt change in the thermal expansion coefficient, growing up 10 times more than the baseline. The calculations of the thermal expansion coefficient has been made for three different pressure parameters; We found out, for each pressure parameter the critical temperature has a different value, higher pressure parameter corresponds to a higher critical temperature. The behavior of β_{Π} near the critical temperature could be explained by using the critical exponent of Landau's theory, where $\beta \sim t_r^{-\alpha}$ (t_r is reduced temperature $t_r = |T - T_C/T_C|$, α is the critical exponent then). The critical exponent was calculated taking the derivative of β_{Π} respect to T and evaluating this value at the limit $T \to 0$. As result, the value for the critical exponent, $\alpha = 0.15 \pm 0.09$, has been found and then checked within scaling theory. One relates the dimensionality d and another critical exponent ν .(65). With obtained our values of α and ν we get that dimensionality of the system is $d = 2.76 \pm 0.16 \sim 3$, which correspond to real one. Due to behavior of the thermal expansion coefficient near the critical temperature, we can conclude that this quantity also demonstrates the second-order phase transitions, like the isothermal compressibility.

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