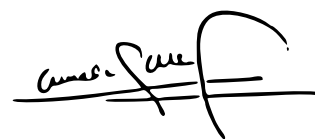Universidade de São Paulo
Instituto de Física

Propriedades termodinâmicas de condensados de Bose-Einstein confinados utilizando a abordagem canônica recursiva

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Dissertação de mestrado apresentada ao Instituto de Física da Universidade de São Paulo, como requisito parcial para a obtenção do título de Mestre(a) em Ciências.

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São Paulo
2024

University of São Paulo
Physics Institute

Thermodynamic properties of confined Bose-Einstein condensates using the recursive canonical approach

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Dissertation submitted to the Physics Institute of the University of São Paulo in partial fulfillment of the requirements for the degree of Master of Science.

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São Paulo
2024

Eu dedico esta dissertação aos meus pais e a
todos que me ajudaram até aqui

Agradecimentos

Primeiro de tudo, quero agradecer a Deus por ter conseguido realizar este trabalho. Meus primeiros agradecimentos vão aos meus pais, que são as pessoas que mais amo na vida e são os meus maiores ídolos, que me ensinaram a ser o que sou, e me deram todo o apoio emocional, intelectual e financeiro, novamente, o meu muito obrigado, tenho muito orgulho e honra de ser filho de vocês, que nunca mediram esforços para que eu estudasse e fizeram a pessoa que sou hoje. Segundo, à minha família, que sempre acreditou em mim e me apoiaram nessa jornada, especialmente minhas tias e meus primos.

Ao meu orientador, Prof. Dr. Arnaldo Gammal pela paciência, pelas inúmeras discussões, por ter me ensinado a falar inglês, pela disposição em me ajudar, pelos conselhos e me mostrar de fato a área de pesquisa na qual me apaixonei. Quero agradeçer ao Dr. Axel Pelster pelas inúmeras discussões a respeito de teoria quântica de campos aplicada a mecânica estatística, pelos conselhos, e pela oportunidade de ir para a Alemanha como visitante por um mês, que foi certamente, uma das grandes experiências da minha vida. Também quero agradeçer aos professores Dr. Antonio Piza e Dr. Emerson Passos pelas discussões nos semanais JC.

Aos meus amigos, Pedro, David, Will, Gabriel, Bruno, Quinsan e Lucas por serem os melhores amigos que conheci na USP, e por todas as discussões, cafés, conselhos e risadas. Vocês são incríveis e moldaram parte do que sou hoje. Também quero agradeçer aos meus amigos desde o colégio há mais de 10 anos, Marcelo, Alessandro, Jonas, Guilherme por todas as risadas, conselhos e histórias. Também queria agradeçer aos meus colegas de grupo, ao Gustavo, Rafael, Leonardo e Alex pelas inúmeras discussões na nossa sala e no JC.

Resumo

Estudamos a termodinâmica de condensados de Bose-Einstein confinados usando dois ensembles estatísticos: grande-canônico e canônico. Quando nós temos um sistema armadilhado, o conceito de limite termodinâmico é diferente em relação ao caso homogêneo, assim nós temos que uma melhor desrição física do sistema com poucas partículas é feita pelo ensemble canônico. Primeiro, nós reproduzimos a teoria grande canônica não interagente, mas agora incluindo as correções de tamanho finito e, seguindo a mesma ideia, em outras situações, com o gás de Bose fracamente interagente. Segundo, nós fazemos a mesma ideia só que agora no ensemble canônico, inicialmente reproduzindo os cálculos padrões não interagentes, depois, nós apresentamos uma teoria canônica fracamente interagente usando o tratamento perturbativo. Como uma aplicação, nós estudamos os gases diluídos confinados em diferentes potenciais externos.

Palavras-chave: Mecânica estatística, condensados de Bose-Einstein, tepria quântica de campos, mecânica quântica.

Abstract

We study the thermodynamics of confined Bose-Einstein condensates using two statistical ensembles: grand canonical and canonical. When we have a trapped system, the concept of the thermodynamic limit is different in relation to the homogeneous case - and for this, for a better physical description of a system with a small number of particles, we use the canonical ensemble. First, we reproduced the non-interacting grand canonical theory but now include the finite-size corrections and follow the same procedure, in other situations, with a weakly interacting Bose gas. Second, we do the same idea but now in the canonical ensemble, initially reproducing the standard non-interacting calculations, and after, we present a weakly interacting canonical theory using the perturbative treatment.

Key words: Statistical mechanics, Bose-Einstein condensates, quantum field theory, quantum mechanics.

List of Figures

List of Tables

Contents

Chapter 1

Introduction

In this chapter we will recover the history of Bose-Einstein condensation (BEC) starting of Bose paper published in 1924 in which have a derivation of Planck's law from photon statistics, after by Einstein's works based in Bose article, and finally experimental techniques and their relations with finite-size systems which changes the theoretical results. Also we will outline dissertation sections.

1.1 A brief history about Bose-Einstein condensate

In 1924 by Satyendra Nath Bose presented a new derivation of Planck's formula using a the concept of indistinguishability in the photons statistics. First, this work was rejected in the Philosophical Magazine of London. Bose then asked Einstein to use his influence to publish the paper. Einstein decided to translate the paper by himself to German and submitted it to the journal Zeitschrift für Physik [5]. At the end of the article, he included: "Translator's Note. Bose's derivation of Planck's formula represents, in my understanding, an important progress. The method used here applies also to the theory of quantum theory of ideal gases that I will carry out in another place."[1]

So in 1924-1925, Einstein explored the Bose statistics in three articles for quantum statistics of ideal quantum gases [6–8], and then, the same idea of Bose statistics (called Bose gas). He used the matter wave idea developed by Louis de Broglie [9] to describe the particle's behavior and hence, it is applied to the Bose statistics. In your second paper [7], Einstein showed that for a homogeneous gas described by Bose statistics with constant temperature, a gas fraction occupies the lowest energy level (ground-state) - called the Bose-Einstein condensate.

One illustrative description of Bose gases is given in Fig. 1.1, where for high temperatures, we have the "billiard balls" situation, and then when we decrease the temperature, the "wave packets" appear going to "giant matter wave" in zero temperature. The result showed by Einstein about heat capacity discontinuity was contested by George E. Uhlenbeck for finite systems [10]. The discussion about the thermodynamics of Bose gas for homogeneous and finite systems during that time was

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[1]In German: *Anmerkung des Übersetzers. Boses Ableitung der Planckschen Formel bedeutet nach meiner Meinung einen wichtigen Fortschritt. Die hier benutzte Methode liefert auch die Quantentheorie des idealen Gases, wie ich an anderer Stelle ausführen will.*
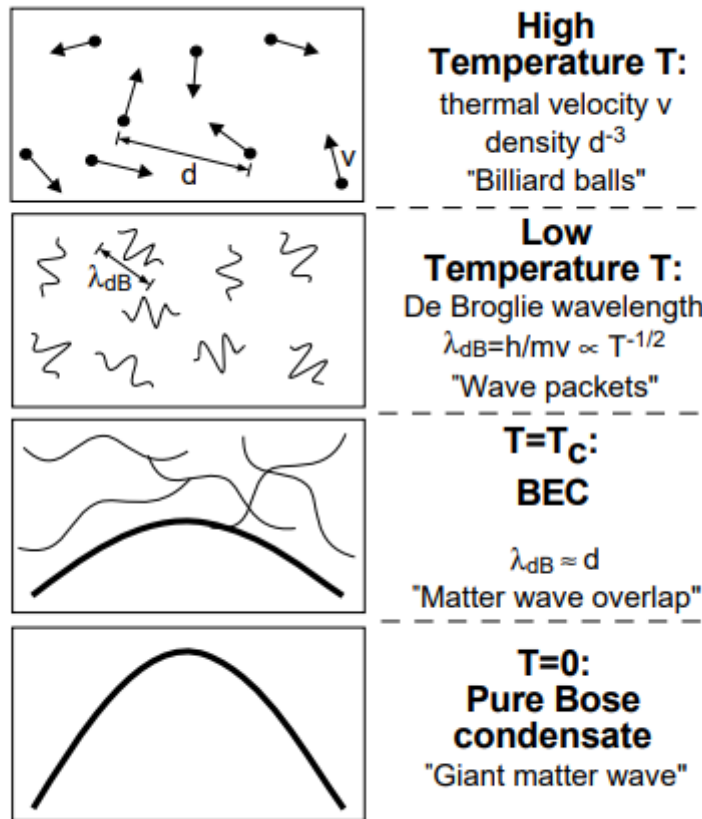
Figure 1.1: This figure shows the scheme of the thermal Bose gas given in [1] - first, for high temperatures, we have the classical billard balls representation for particles, and with the decreases of temperature, the wave packets appear; but for a certain temperature T_c, we have the BEC phase, here with the matter wave overlap and this situation extend at zero temperature, when we have the pure BEC.

increasing due to the experimental realizations with a fixed number of particles [11, 12]. But the first theoretical discussion about the thermodynamic limit is in [13] for the ideal Bose gas revisited, where we have the suggestion of canonical ensemble to calculate the confined Bose gas properties. After, the canonical description of ideal Bose gas was studied in [14, 15], but with inclusion of the interactions, the problem is open in its general case, some cases were studied as the dilute gas in a finite box [16].

On the other hand, the theoretical studies about the Bose-Einstein condensates motivated their experimental realizations. Laser cooling [17–21] were the starting point to do the BEC experiment in gases. The additional problem is to obtain the BEC temperature that is less than the usual ultracold experiment temperature. To solve this, magnetic traps were included to confine the bosons inside of the chamber, characterizing the magneto-optical trap (MOT), and with radio frequency evaporation, in 1995 were realized the first Bose-Einstein condensates in gases [2, 22], and the first images produced of this new state of matter were given by the BEC velocity distribution picture
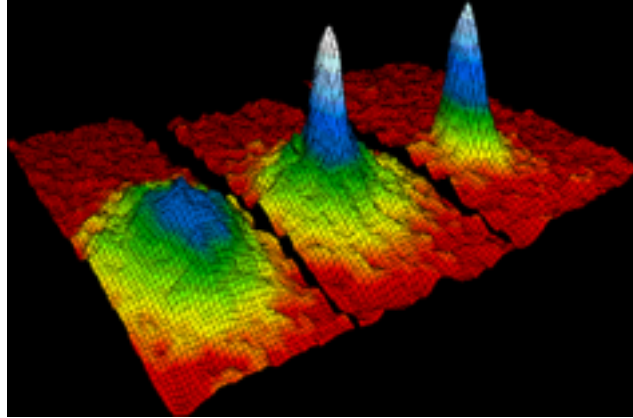
Figure 1.2: Velocity distribution of the BEC produced in [2], here the first image, on left, we have the case for high temperatures $T > T_c$, in the middle figure, characterizing the condensed state $T < T_c$, and the right plot for very low temperatures $T << T_c$.

in Fig. 1.2.

One of the most interesting of ultracold physics is its thermodynamic study which is a big challenge in this research area. The inclusion of interactions, i.e., the more realistic model, requires the solution of a many-body problem. The addition of interactions implies a change in critical temperature [23, 24], condensed fraction, heat capacity, and ground-state fluctuations with respect to ideal results [25, 26]. To solve these questions in this dissertation we use the perturbation theory which treats the interaction as a perturbation of a non-interacting system. But here the focus is in the weakly interactions, and so, the use of perturbation theory is consistent [27] - the systems with finite number of particles was discussed in [13] about the ideal Bose gas considering trapped systems, and it was suggested the use of canonical ensemble because in these situations, the number of particles is fixed, having one better description of thermodynamic properties. Besides, given the recent experiments with few number of particles [11, 12], the use of canonical ensemble at this time is even more important in our theoretical models.

The connection between the statistical ensembles is a good point to check the validity of the quantities in the thermodynamic limit. When we have a homogeneous gas, the thermodynamic quantities converge in all ensembles. But there is one that do not converge, that is the ground-state fluctuation, and this situation opens a great theoretical discussion about the certain statstical distribution to describe specific experimental situations. We have many papers about this [28, 29] for ideal case, but with the inclusion of interactions, the problem is more complicated, however in 2022, one good discussion was done in [26]. In this dissertation, we discussed this fluctuations in the both cases, but by perturbation overview, and after, comparing these results with the previous discussion.

1.2   About this dissertation

The main purpose of this dissertation is to study the thermodynamics of trapped Bose gases by two different ensembles: canonical and grand canonical. With recent papers

about Bose-Einstein condensates for a few particles, the canonical ensemble is a great approach to calculate the thermodynamic properties of these systems because is precisely in the description of few particles and it is physically similar to experimental realizations. In contrast, the grand canonical systems have a fixed density and due to it is a precise method to determine the critical temperature of a Bose gas, but the other thermodynamic properties as the condensed fraction, heat capacity, and principally the ground-state fluctuations diverge for high temperatures, are not adequate for finite systems. An additional motivation was to obtain, in the interacting canonical ensemble, that the heat capacity goes to zero as temperature goes to zero. Previous calculations by ref. [30] omit these results or get inconsistency [31]. As we show, renormalization of the self energy solves this long standing problem and finally gives consistent results.

In this dissertation, we have six chapters divided into two principal schemes: for non-interacting case and the interacting case for two statistical ensembles: grand canonical and canonical. For the grand canonical ensemble, we have in Chapter 2, the semiclassical theory for the ideal Bose gas trapped in an external power-law potential but we put the finite-size corrections expanding the idea done in [32]. Here, we calculate the thermodynamic properties as the heat capacity, condensed fraction, ground-state fluctuation and the critical temperature. However, for the case when the spectrum is quantized as in the finite-box trap, we have other semiclassical overview, similar to the presented in [15] and here we reproduce this calculation, including the condensed fraction for this system. Finally, we finish our study doing the exact calculation solving the summations of the quantum numbers by numerical methods and later, we calculate the thermodynamic properties in the same form of the semiclassical approach.

Following the developments of Chapter 2, we expanded these ideas for the weakly interacting systems in Chapter 3. First, we show the grand canonical theory for weakly interacting systems using the perturbation theory [3,33] for a semiclassical system - for the same potential applied in Chapter 2 and calculating the same thermodynamic properties, and finally comparing the results with the standard limits, for example in the harmonic trap [34–36]. The exact approach for this situation was not studied here because when we shall build the interacting spectrum, we have to solve the Schrödinger equation including the interacting potential or to include the quantum depletions via Bogoliubov-Popov spectrum [27]. Therefore, in Chapters 2 and 3 we have the grand canonical overview of ultracold trapped Bose gases.

On chapters 4 and 5, we have the main calculation of this thesis, a complete canonical theory for Bose gases in which we study the non-interacting Bose gases on Chapter 4 and the weakly interacting Bose gas on Chapter 5. The starting point is the grand canonical theory and to find the canonical quantity we used the connection between these ensembles [37–39] and we obtain the same formulas obtained of different approaches [14,15], the first reference by path-integral decomposition and the second, by counting statistics. For each canonical theory, we calculate the thermodynamic properties using the classical statistical mechanics and the ground-state properties decomposing the partition function in two contributions, building the canonical probability to find particles in the ground-state, after using the classical probability formulas, to calculate the moments of our condensed canonical distribution. These calculations are valid for any recursive systems and are in Chapter 4 joined with the

non-interacting results - the homogeneous gas, trapped in the finite box and in harmonic trap and its comparison with the grand canonical results.

In Chapter 5, we expand the canonical idea for the weakly interacting Bose gases, doing a perturbative canonical representation, using the calculations done in Chapter 3 as a guide. We realize that the canonical quantities have the same Feynman representation but with different mathematical representation. The idea was presented in [31], but here we complete the theory solving the problem in the low temperatures, building a correct recursive formula renormalizing the energy spectrum for an interacting quantum particles using the interpretation of divergence of the Green's function done in [4, 40]. After the detailed presentation of this theory, we apply for the same systems studied in Chapter 4 to compare the influence of the interactions in the thermodynamics previously done in Chapter 3. Further, we present a discussion about energies in the canonical representation.

In Chapter 6 we present our conclusions and future perspectives.

Chapter 2

Grand canonical trapped Bose gas

In an initial study about quantum gases, in textbooks [4,37,40], the calculations are done in the grand canonical, so as in this ensemble there is the exchange of heat and particles. Remembering the initial ideas of this ensemble, we have that the chemical potential μ is fixed besides particle density N/V in the thermodynamic limit. First, let us show the functional approach of grand canonical distribution starting with grand canonical partition function $\Xi(\beta, z)$ for non-interacting systems.

With $\Xi(\beta, z)$, we can calculate the main thermodynamic properties of the system: the critical temperature, the heat capacity, and the condensate fraction. As we want to study the trapped Bose gases, we must include the finite-size corrections which depend on the number of particles because the thermodynamic limit is modified as seen in [13]. The motivation is to extend the study about the non-interacting power-law trap done in [32] including now the finite-size corrections that are inserted in the chemical potential excluding the ground-state energy. With this correction, we have a more precise grand partition function $\Xi^{(0)}$, and using the standard statistical mechanics procedure, we calculate the thermodynamic properties cited in the second line of this paragraph.

2.1 Non-interacting functional theory

Consider a grand canonical D dimensional ideal Bose gas. By the concept of the partition function, we shall sum over all states and so in a path integral representation corresponds to the integral of all possible paths for a particle of Boltzmann exponential action [39]

$$\Xi^{(0)} = \oint D\psi^* \, D\psi \, e^{-A^{(0)}[\psi^*,\psi]/\hbar} \,, \tag{2.1}$$

where the Bose fields $\psi(\mathbf{x}, \tau)$ are periodic in Euclidean time $\psi(\mathbf{x}, 0) = \psi(\mathbf{x}, \hbar\beta)$, $D\psi^* D\psi$ is the measure over these fields, and

$$A^{(0)}[\psi^*, \psi] = \int_0^{\hbar\beta} d\tau \int d^D x \, \psi^*(\mathbf{x}, \tau) \left(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2M} \nabla^2 + V^{(\text{ext})}(\mathbf{x}) - \mu \right) \psi(\mathbf{x}, \tau) \tag{2.2}$$

is the non-interacting action in Euclidean time. Here, we will use the Euclidean time τ to include the temperature in our calculations. The technique to calculate Eq. (2.2) is to

decompose the Bose field in a function that depends on Euclidean time term and position contribution (eigenfunctions of time-independent Schrödinger equation) of form

$$\psi(\mathbf{x}, \tau) = \sum_{\mathbf{k},m} c_{\mathbf{k},m} \psi_{\mathbf{k}}(\mathbf{x}) \, e^{-i\omega_m \tau} \tag{2.3}$$

where $c_{\mathbf{k},m}$ are complex numbers, $\omega_m = 2\pi m/\hbar\beta$ is the bosonic Matsubara frequency and $\psi_{\mathbf{k}}(\mathbf{x})$ are the eigenfunctions such that

$$\hat{H} \, \psi_{\mathbf{k}}(\mathbf{x}) = E_{\mathbf{k}} \, \psi_{\mathbf{k}}(\mathbf{x}) \tag{2.4}$$

with

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla^2 + V^{(\text{ext})}(\mathbf{x}). \tag{2.5}$$

Inserting Eqs. (2.4), (2.3) in Eq. (2.2),

$$A^{(0)}[\psi^*, \psi] = \hbar\beta \sum_{\mathbf{k}} \sum_{m=-\infty}^{\infty} [-i\hbar\omega_m + E_{\mathbf{k}} - \mu] \, c_{\mathbf{k},m}^* c_{\mathbf{k},m}. \tag{2.6}$$

The measure depends on complex numbers because now our action is given by Eq. (2.6). All paths are represented by differential over $c_{\mathbf{k},m}$ of form [33]

$$\oint D\psi^* D\psi = \prod_{\mathbf{k}} \prod_{m=-\infty}^{\infty} \frac{1}{2\pi} \int dc_{\mathbf{k},m}^* dc_{\mathbf{k},m} \tag{2.7}$$

With Eqs. (2.7), (2.6), we can calculate our formula for $\Xi^{(0)}$,

$$\Xi^{(0)} = \prod_{\mathbf{k}} \prod_{m=-\infty}^{\infty} \frac{1}{2\pi} \int dc_{\mathbf{k},m}^* dc_{\mathbf{k},m} \, e^{-\beta \sum_{\mathbf{k}} \sum_{m=-\infty}^{\infty} [-i\hbar\omega_m + E_{\mathbf{k}} - \mu] c_{\mathbf{k},m}^* c_{\mathbf{k},m}} \tag{2.8}$$

$$\Xi^{(0)} = \prod_{\mathbf{k}} \prod_{m=-\infty}^{\infty} \frac{1}{2\pi} \int dc_{\mathbf{k},m}^* dc_{\mathbf{k},m} \, e^{-\beta[-i\hbar\omega_m + E_{\mathbf{k}} - \mu] c_{\mathbf{k},m}^* c_{\mathbf{k},m}} \tag{2.9}$$

As $c_{\mathbf{k},m}$ are complex, we may represent its in a general decomposition:

$$c_{\mathbf{k},m} = x_{\mathbf{k},m} + i \, y_{\mathbf{k},m} \tag{2.10}$$

and therefore,

$$c_{\mathbf{k},m}^* c_{\mathbf{k},m} = x_{\mathbf{k},m}^2 + y_{\mathbf{k},m}^2 \tag{2.11}$$

$$dc_{\mathbf{k},m}^* dc_{\mathbf{k},m} = 2 \, dx_{\mathbf{k},m} \, dy_{\mathbf{k},m} \tag{2.12}$$

Then including these formulas in Eq. (2.9) we will obtain two Gaussian integrals for each number,

$$\Xi^{(0)} = \prod_{\mathbf{k}} \prod_{m=-\infty}^{\infty} \frac{1}{\pi} \int dx_{\mathbf{k},m} e^{-\beta[-i\hbar\omega_m + E_{\mathbf{k}} - \mu] x_{\mathbf{k},m}^2} \int dy_{\mathbf{k},m} e^{-\beta[-i\hbar\omega_m + E_{\mathbf{k}} - \mu] y_{\mathbf{k},m}^2}, \tag{2.13}$$

therefore,

$$\Xi^{(0)} = \prod_{\mathbf{k}} \prod_{m=-\infty}^{\infty} \frac{\beta}{-i\hbar\omega_m + E_{\mathbf{k}} - \mu}. \tag{2.14}$$

But to continue the thermodynamic calculations, we shall connect the partition function with thermodynamics calculating the grand canonical free energy

$$\mathcal{F}^{(0)} = -\frac{1}{\beta} \ln \Xi^{(0)} \tag{2.15}$$

$$\mathcal{F}^{(0)} = -\frac{1}{\beta} \left[\sum_{\mathbf{k}} \sum_{m=-\infty}^{\infty} \ln \beta \left(-i\hbar\omega_m + E_{\mathbf{k}} - \mu \right) \right] \tag{2.16}$$

and this sum is an example of Matsubara sum calculated using the residue theorem detailed in Appendix A. Then, for a Matsubara function
$f(\omega_m) = \ln \beta \left(-i\hbar\omega_m + E_{\mathbf{k}} - \mu \right) / \beta$ in Eq. (2.16), the final non-interacting GC free energy given by Eq. (2.16) is

$$\mathcal{F}^{(0)} = -\frac{1}{\beta} \ln \Xi^{(0)} = \frac{1}{\beta} \sum_{\mathbf{k}} \ln \left(1 - e^{-\beta(E_{\mathbf{k}} - \mu)} \right) . \tag{2.17}$$

Here, let's discuss the possible calculations of $\mathcal{F}^{(0)}$ because we have an interesting discussion.

2.2 Semiclassical approximation

As said previously, we have many possibilities to calculate the grand canonical free energy by Eq. (2.17). The most intuitive possibility is to write the summation over the quantum numbers as an integral that is equivalent to representing the energy eigenvalues as a continuum spectrum similar to classical energy representation which is the Hamiltonian. This situation can be viewed in the case of many particles due to the total energy forming a band energy structure as seen in Fig. 2.1 in the case of the quantum harmonic oscillator. Then, as the ground state is not zero, we divide the free energy into two parts: first refers to the condensed state (in ground-state - $\mathbf{k} = 0$) which is unique, and second refers to excited states ($\mathbf{k} \neq 0$) that in this approximation will be given by integral

$$\mathcal{F}^{(0)} = \frac{1}{\beta} \ln \left(1 - e^{-\beta(E_G - \mu)} \right) + \frac{1}{\beta} \sum_{\mathbf{k} \neq 0} \ln \left(1 - e^{-\beta(E_{\mathbf{k}} - \mu)} \right) . \tag{2.18}$$

As the excited states are given by summation excluding the ground-state, then the semiclassical approximation is based on two considerations: first, the chemical potential is shifted by ground-state energy denoted now by $\hat{\mu}$ called reduced chemical potential, and as the energies will be represented in phase-space by Hamiltonian H. In summary,

$$\mu \rightarrow \hat{\mu} \equiv \mu - E_G \tag{2.19}$$

$$E_{\mathbf{k}} \rightarrow H(\mathbf{p}, \mathbf{x}) \tag{2.20}$$
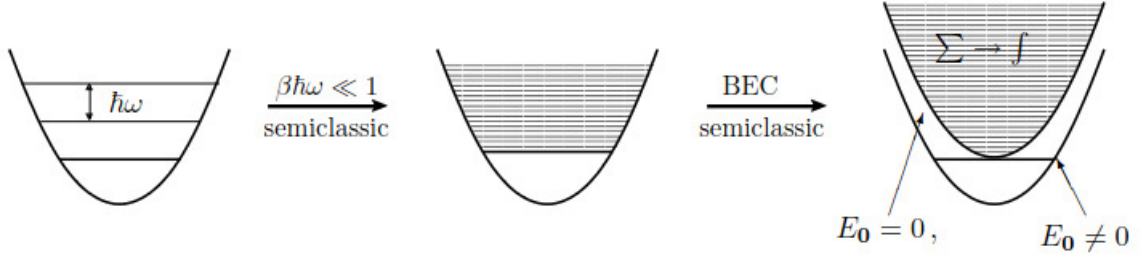
Figure 2.1: Explanation about semiclassical approximation using as an example, the energy levels of the quantum harmonic oscillator. Here, we have that the level shift given by $\hbar\omega$ - when this shift is small, these discrete levels become a band, then this small division can be treated using integration as the equivalence of the summation over the quantum numbers, but for the BEC semiclassical approximation, we must exclude the ground-state because that in this energy level, we have the condensate phase.

therefore,

$$\mathcal{F}^{(0)} = \frac{1}{\beta} \ln \left(1 - e^{-\beta(E_G - \mu)}\right) + \frac{1}{\beta} \int \frac{d^D p \, d^D x}{(2\pi\hbar)^D} \ln \left(1 - e^{-\beta(H(\mathbf{p},\mathbf{x}) - \mu)}\right) \tag{2.21}$$

where

$$H(\mathbf{p}, \mathbf{x}) = \frac{\mathbf{p}^2}{2M} + V^{(\text{ext})}(\mathbf{x}) \tag{2.22}$$

is the classical Hamiltonian. The inclusion of reduced chemical potential will be discussed now because our purpose is to study the trapped Bose gas. When we have finite systems the finite-size corrections must be included in $\mathcal{F}^{(0)}$ and its effects modify the chemical potential μ (the quantity which is fixed in grand canonical distribution). From Eq. (2.21), the logarithm function can be expanded in a series,

$$\ln(1 - x) = -\sum_{n=1}^{\infty} \frac{x^n}{n} \tag{2.23}$$

and then

$$\mathcal{F}^{(0)} = \frac{1}{\beta} \ln \left(1 - e^{-\beta(E_G - \mu)}\right) - \frac{1}{\beta} \int \frac{d^D p \, d^D x}{(2\pi\hbar)^D} \sum_{n=1}^{\infty} e^{-n\beta(H(\mathbf{p},\mathbf{x}) - \mu)} \tag{2.24}$$

By Eq. (2.22), we can divide our free energy into two parts: one for momentum p and the other for coordinate x, then Eq. (2.24) becomes

$$\mathcal{F}^{(0)} = \frac{1}{\beta} \ln \left(1 - e^{-\beta(E_G - \mu)}\right) - \frac{1}{\beta \lambda_T^D} \sum_{n=1}^{\infty} \frac{z^n}{n^{D/2+1}} \int d^D x \, e^{-n\beta V^{(ext)}(\mathbf{x})} \tag{2.25}$$

where

$$\lambda_T \equiv \sqrt{\frac{2\pi\hbar^2\beta}{M}} \tag{2.26}$$

is the thermal wavelength, by simplicity, we defined the ground-state contribution by $\mathcal{F}_0^{(0)}$. Therefore,

$$\mathcal{F}^{(0)} = \mathcal{F}_0^{(0)} - \frac{1}{\beta \lambda_T^D} \sum_{n=1}^{\infty} \frac{z^n}{n^{D/2+1}} \int d^D x \, e^{-n\beta V^{(ext)}(\mathbf{x})}, \qquad (2.27)$$

where $z \equiv e^{\beta\mu}$ is the fugacity and now we will insert the reduced chemical potential to include the finite-size effects in grand canonical results. For this, we shall expand the fugacity z in terms of $\hat{\mu}$. By Eq. (2.20), the fugacity power is now written as

$$z^n = e^{n\beta\mu} = e^{n\beta(\hat{\mu}+E_G)} = \hat{z}\,(1 + n\beta E_G) \qquad (2.28)$$

where $\hat{z}$ is the reduced fugacity defined as $e^{n\beta\hat{\mu}}$. Finally, inserting this formula in Eq. (2.27), we have that

$$\mathcal{F}^{(0)} = \mathcal{F}_0^{(0)} - \frac{1}{\beta \lambda_T^D} \sum_{n=1}^{\infty} \frac{\hat{z}^n}{n^{D/2+1}} \, (1 + n\beta E_G) \int d^D x \, e^{-n\beta V^{(ext)}(\mathbf{x})}. \qquad (2.29)$$

The grand canonical free energy is the starting point of our thermodynamic analysis because using the classical relations of thermodynamics, we may calculate the average number of particles N, entropy S, critical temperature $T_c^{(0)}$ and heat capacity C. One observation is that the ground-state fluctuations will be calculated in section about exact calculations. The number of particles N is

$$N = -\left(\frac{\partial \mathcal{F}}{\partial \mu}\right)_T \qquad (2.30)$$

the entropy S,

$$S = -\left(\frac{\partial \mathcal{F}}{\partial T}\right)_\mu \qquad (2.31)$$

and the heat capacity C,

$$C = \left(\frac{\partial U}{\partial T}\right)_N \qquad (2.32)$$

The critical temperature in the non-interacting system T_c is obtained by formula Eq. (2.30) when the condensed N is zero, the critical chemical potential is zero (because $\mu_c = E_G$ - all particles are in ground-state) and it occurs when $\beta = \beta_c$. As seen in Eq. (2.29), the equation depends on the external potential, then the details of the calculation of critical temperature $T_c^{(0)}$ will be made for each system. To find the other thermodynamic quantities is need to calculate this temperature due to the bosons have two phases: the condensed phase (when $T \leq T_c$) and the normal phase (when $T \geq T_c$) and the difference between these states are that inside a condensate $\hat{\mu}$ is zero while in thermal gas $\hat{\mu} \neq 0$. As an example, let's study the ideal Bose gas confined in a general power law external potential $V(x) \, (x/l)^a$ in D dimensions, and when $a = 2$ we have a harmonic trap and $a \to \infty$ is the finite box. The calculations for ideal systems in a thermodynamic limit were calculated in Ref. [32]. Here, let's expand this idea including the finite-size corrections following the previous discussion in semiclassical approximation.

Ideal Power law trap

Consider a general power law external potential in D dimensions [32],

$$V(\mathbf{x}) = \sum_{i=1}^{D} \left(\frac{x_i}{l_i} \right)^{a_i} \tag{2.33}$$

where l_i corresponds at a term with a dimension of length over energy in $\hbar\omega$ units. The generalization of the power law trap is an interesting idea to represent the two most common traps: the finite box, when l_i tends to infinity, and the harmonic trap when $a_i = 2$. For a power law trap, the total Hamiltonian given by Eq. (2.22) now is

$$H(\mathbf{p}, \mathbf{x}) = \frac{p^2}{2M} + \sum_{i=1}^{D} \left(\frac{x_i}{l_i} \right)^{a_i} \tag{2.34}$$

with

$$p^2 = \sum_{i=1}^{D} p_i^2. \tag{2.35}$$

By Eq. (2.29) for this Hamiltonian, our work will make the coordinate integral for potential Eq. (2.33) which here is denoted by B below

$$\int d^D x e^{-n\beta V(\mathbf{x})} \equiv B \tag{2.36}$$

Using Eq. (2.33) in Eq. (2.36) will have an integral of type,

$$\int e^{-b(x/l)^a} dx \tag{2.37}$$

B is written as

$$B = \prod_{i=1}^{D} \int e^{-n\beta(x_i/l_i)^{a_i}} dx_i \tag{2.38}$$

and it can be solved using the gamma function $\Gamma(z)$,

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt \tag{2.39}$$

Looking the integral of Eq. (2.38), we have that

$$\int e^{-n\beta(x_i/l_i)^{a_i}} dx_i = 2^i l_i \int_0^\infty e^{-n\beta u^{a_i}} du \tag{2.40}$$

where $u \equiv x_i/l_i$. Putting the gamma function in this integral, we have

$$\int e^{-n\beta(x_i/l_i)^{a_i}} dx_i = 2^i l_i \int_0^\infty e^{-n\beta u^{a_i}} du = 2^i l_i \frac{1}{n^{a_i} \beta^{a_i} a_i} \Gamma\left(\frac{1}{a_i} \right) \tag{2.41}$$

and so, inserting Eq. (2.41) in Eq. (2.38),

$$B = \prod_{i=1}^{D} \int e^{-n\beta(x_i/l_i)^{a_i}} dx_i = \frac{1}{n^{\sum_i 1/a_i} \beta^{\sum_i 1/a_i}} \prod_{i=1}^{D} 2^i l_i \frac{1}{a_i} \Gamma\left(\frac{1}{a_i} \right). \tag{2.42}$$

Putting this integral in Eq. (2.29), we have that

$$\mathcal{F}^{(0)} = \mathcal{F}_0^{(0)} - \frac{1}{\beta \lambda_T^D} \sum_{n=1}^{\infty} \frac{\hat{z}^n}{n^{D/2+1}} \left(1 + n\beta E_G\right) \frac{1}{n^{\sum_i 1/a_i} \beta^{\sum_i 1/a_i}} \prod_{i=1}^{D} 2^i l_i \frac{1}{a_i} \Gamma \left(\frac{1}{a_i}\right). \quad (2.43)$$

We can simplify this equation with definition of polylogarithm function $\zeta_a(x)$ whose definition is

$$\zeta_a(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^a}. \quad (2.44)$$

But before following our calculations we use a simplification about the power of the trap. By Eq. (2.33) the principal power is given by a_i parameter, however, we can use a new general parameter α defined as

$$\alpha \equiv \frac{D}{2} + \sum_{i=1}^{D} \frac{1}{a_i} \quad (2.45)$$

and in terms of it, for example, when have a three-dimensional harmonic trap, $D = 3$ and $a_i = 2$ for all i giving $\alpha = 3$ and for $3 - D$ finite box, $a_i \to \infty \Rightarrow \alpha = 3/2$. Thus, Eq. (2.43) can be written as

$$\mathcal{F}^{(0)} = \mathcal{F}_0^{(0)} - \frac{1}{\beta^{\alpha+1}} \eta \left(\zeta_{\alpha+1}(\hat{z}) + \beta E_G \zeta_\alpha(\hat{z})\right) \quad (2.46)$$

where

$$\eta \equiv \left(\frac{M}{2\pi\hbar^2}\right)^{D/2} \prod_{i=1}^{D} \frac{2^i l_i}{a_i} \Gamma \left(\frac{1}{a_i}\right). \quad (2.47)$$

Now, using Eq. (2.46), we can calculate N by Eq. (2.30) and with it, have a critical temperature. Then,

$$N^{(0)} = N_0^{(0)} + \frac{1}{\beta^\alpha} \eta \left(\zeta_\alpha(\hat{z}) + \beta E_G \zeta_{\alpha-1}(\hat{z})\right). \quad (2.48)$$

In critical point, $N_0^{(0)} = 0$, $\beta = \beta_c$ and $\hat{\mu} = 0$, then,

$$N^{(0)} = N = \frac{1}{\beta_c^\alpha} \eta \left(\zeta_\alpha(1) + \beta E_G \zeta_{\alpha-1}(1)\right). \quad (2.49)$$

but $\zeta_a(1) = \zeta(a)$, then

$$N^{(0)} = N = \frac{1}{\beta_c^\alpha} \eta \left(\zeta(\alpha) + \beta E_G \zeta(\alpha - 1)\right). \quad (2.50)$$

In ref. [32], it was made the case of homogeneous power law Bose gas when the finite-size effect is not considered. Here in the first step, we inserted these effects. The non-interacting critical temperature in thermodynamic limit is denoted by $T_c^{(0)}$ and it occurs when E_G-term do not contribute in Eq. (2.50), then Eq. (2.50) becomes

$$N = \frac{\eta \zeta(\alpha)}{\beta_c^{(0)\alpha}}; \quad (2.51)$$

therefore,

$$T_c^{(0)} = \frac{1}{k_B} \left(\frac{N}{\eta\, \zeta(\alpha)} \right)^{1/\alpha}. \tag{2.52}$$

The equation (2.52) is our starting point because the inclusion of the finite-size effect will shift this homogeneous temperature and this same idea will be applied to interacting systems. So,

$$T_c = T_c^{(0)} + \Delta T_c \Rightarrow \frac{T_c}{T_c^{(0)}} \equiv t_c = 1 + \frac{\Delta T_c}{T_c^{(0)}} \tag{2.53}$$

Now, we can write T_c. By Eq. (2.50)

$$1 = \frac{1}{\beta_c^\alpha N} \eta \left(\zeta(\alpha) + \beta E_G \zeta(\alpha - 1) \right). \tag{2.54}$$

and inserting here in Eq. (2.52), we have

$$1 = \left(\frac{T_c}{T_c^{(0)}} \right)^\alpha + E_G\, \beta_c^{(0)} \frac{\zeta(\alpha - 1)}{\zeta(\alpha)} \left(\frac{T_c}{T_c^{(0)}} \right)^{\alpha - 1} \tag{2.55}$$

$$t_c = 1 - \frac{E_G}{\alpha}\, \beta_c^{(0)} \frac{\zeta(\alpha - 1)}{\zeta(\alpha)} t_c^{\alpha - 1} \tag{2.56}$$

But the ratio $T_c/T_c^{(0)}$ is given by Eq. (2.53) then we have that

$$\frac{\Delta T_c}{T_c^{(0)}} = -\frac{E_G}{\alpha}\, \beta_c^{(0)} \frac{\zeta(\alpha - 1)}{\zeta(\alpha)} \;. \tag{2.57}$$

This formula generalizes the critical temperature shift for a power-law trap. The most common power-law trap is the three-dimensional harmonic trap and this system has a potential given by

$$V(\mathbf{x}) = \frac{M}{2} \sum_{j=1}^{3} \omega_j^2\, x_j^2, \tag{2.58}$$

and comparing it with Eq. (2.33), we have that

$$l_j = \left(\frac{2}{M} \right)^{1/2} \frac{1}{\omega_j}, \tag{2.59}$$

$D = 3$ and $a_j = 2, \forall j$. So by definition of α (2.45), we have that $\alpha = 3$. From Eq. (2.47) for these values of D, α, we obtain that

$$\eta = \frac{1}{(\hbar\, \tilde{\omega})^3}, \tag{2.60}$$

where

$$\tilde{\omega} \equiv (\omega_1\, \omega_2\, \omega_3)^{1/3} \tag{2.61}$$

is the geometric mean value of the frequencies. On the other hand, η relates with the critical temperature $T_c^{(0)}$ by Eq. (2.52),

$$T_c^{(0)} = \frac{\hbar\, \tilde{\omega}}{k_B} \left(\frac{N}{\zeta(3)} \right)^{1/3} \tag{2.62}$$

that is the same obtained in [41]. The finite-size correction of this system can be calculated from Eq. (2.57) and we need the ground-state energy E_G, then starting with the Hamiltonian,

$$H = \frac{-\hbar^2}{2M}\nabla^2 + \frac{M}{2}\sum_{j=1}^{3}\omega_j^2\, x_j^2 \tag{2.63}$$

however, to solve the Schrödinger equation of this Hamiltonian it is convenient to write Eq. (2.63) in terms of $a, a^\dagger$ operators [10]

$$H = \hbar\omega_1\left(a_1^\dagger a_1 + \frac{1}{2}\right) + \hbar\omega_2\left(a_2^\dagger a_2 + \frac{1}{2}\right) + \hbar\omega_3\left(a_3^\dagger a_3 + \frac{1}{2}\right) \tag{2.64}$$

whose eigenstates are given by a tensor product

$$|n_1, n_2, n_3\rangle = |n_1\rangle|n_2\rangle|n_3\rangle \tag{2.65}$$

and the eigenvalues are

$$E_{k_1,k_2,k_3} = \hbar\omega_1\left(k_1 + \frac{1}{2}\right) + \hbar\omega_2\left(k_2 + \frac{1}{2}\right) + \hbar\omega_3\left(k_3 + \frac{1}{2}\right) \tag{2.66}$$

The equation (2.66) admits a ground-state energy, that is when $k_1 = k_2 = k_3 = 0$,

$$E_G = \frac{3\hbar\overline{\omega}}{2} \quad and \quad \overline{\omega} \equiv \frac{\omega_1 + \omega_2 + \omega_3}{3} \tag{2.67}$$

and then Eq. (2.66) becomes

$$E_{k_1,k_2,k_3} = E_G + \hbar(k_1\,\omega_1 + k_2\,\omega_2 + k_3\,\omega_3). \tag{2.68}$$

Therefore, using Eqs. (2.67), (2.61), (2.59) in Eq. (2.57), we have that the shift of the critical temperature for this system is given by

$$\frac{\Delta T_c}{T_c^{(0)}} = -\frac{\overline{\omega}\,\zeta(2)}{2\,\tilde{\omega}\,N^{1/3}\,\zeta^{2/3}(3)}. \tag{2.69}$$

which is the same result obtained from [42].

Now, we can calculate the other thermodynamic properties because now we have the measure of the critical point and may separate the two phases of the system. The first quantity calculated is the condensed fraction $N_0^{(0)}/N$ which occurs when we have in condensed state $\hat{\mu} = 0$. By Eq. (2.48), we can divide it by N in both sides,

$$1 = \frac{N_0^{(0)}}{N} + \frac{1}{\beta^\alpha N}\eta\left(\zeta(\alpha) + \beta E_G\zeta(\alpha - 1)\right). \tag{2.70}$$

writing this result in terms of $T_c^{(0)}$, we have the formula of condensed fraction,

$$\frac{N_0^{(0)}}{N} = 1 - \left(\frac{T}{T_c^{(0)}}\right)^\alpha - E_G\,\beta_c^{(0)}\frac{\zeta(\alpha - 1)}{\zeta(\alpha)}\left(\frac{T}{T_c^{(0)}}\right)^{\alpha - 1}. \tag{2.71}$$

Its formula is a function of the non-interacting critical temperature in the thermodynamic limit $T_c^{(0)}$, but when we have a trapped gas, then is more convenient to represent Eq. (2.71) on T/T_c-dependence. We see that

$$\frac{T}{T_c^{(0)}} = \frac{T}{T_c} \frac{T_c}{T_c^{(0)}} \tag{2.72}$$

with $T_c/T_c^{(0)}$ given by Eq. (2.53). As made in the calculation of $\Delta T_c/T_c^{(0)}$, we will use the binomial theorem, and the terms with order above 1 with respect to the ground-state energy will be neglected. Then,

$$\frac{N_0^{(0)}}{N} = 1 - \left(\frac{T}{T_c}\right)^\alpha \left(1 + \alpha \frac{\Delta T_c}{T_c^{(0)}}\right) - E_G \, \beta_c^{(0)} \frac{\zeta(\alpha-1)}{\zeta(\alpha)} \left(\frac{T}{T_c}\right)^{\alpha-1}, \tag{2.73}$$

therefore,

$$\frac{N_0^{(0)}}{N} = 1 - \left(\frac{T}{T_c}\right)^\alpha - E_G \, \beta_c^{(0)} \frac{\zeta(\alpha-1)}{\zeta(\alpha)} \left[\left(\frac{T}{T_c}\right)^{\alpha-1} - \left(\frac{T}{T_c}\right)^\alpha\right]. \tag{2.74}$$

We can check this formula for the same system studied in the case of T_c which is the three-dimensional harmonic trap. Substituting Eqs. (2.67), (2.61), (2.59) in Eq. (2.74), we obtain that

$$\frac{N_0^{(0)}}{N} = 1 - \left(\frac{T}{T_c}\right)^3 - \frac{3\,\overline{\omega}\,\zeta(2)}{2\,\tilde{\omega}\,N^{1/3}\,\zeta^{2/3}(3)} \left[\left(\frac{T}{T_c}\right)^2 - \left(\frac{T}{T_c}\right)^3\right]. \tag{2.75}$$

This result is the same obtained by [39,42]. To see the difference between this quantity with and without finite-size corrections in the harmonic trap, first, let us do the plot of the condensed fraction for isotropic case $\overline{\omega} = \tilde{\omega}$ for $10, 100, 1000$ particles and comparing these with the plot for the thermodynamic limit as seen in Fig. 2.2. With this plot is clear that for a few number of particles, this semiclassical result is not good for analysing the finite-size correction in a box. Then, due to this, we need another semiclassical treatment of the finite box, and this calculation is calculated in our final section. When we don't count the finite-size corrections, the result is the standard calculations given in [7,37,38,40]. However, for finite systems, we need to include the corrections due to the ground-state E_G and in the case of a finite box, its homogeneous ground-state is zero in a semiclassical overview - thus, by [10], we have that the correct box ground-state is not zero and when this result is included, our condensed fraction has a strange behavior. Of fact, using the ground-state of finite box given by [10] in Eq. (2.75), we have that

$$\frac{N_0^{(0)}}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2} - \frac{3\,\pi\,\zeta(1/2)}{4\,N^{2/3}\,\zeta^{1/3}(3/2)} \left[\left(\frac{T}{T_c}\right)^{1/2} - \left(\frac{T}{T_c}\right)^{3/2}\right]. \tag{2.76}$$

This situation is discussed in the section about non-interacting finite box. As $\zeta(1/2)$ is a negative number, we see that for low values of T/T_c, the condensed fraction is greater than 1 and this behavior can be viewed in Fig. 2.3. With this plot is clear that for a few number of particles, this semiclassical result is not good. Then, due to it, we need another semiclassical treatment of the finite box, and this calculation is performed in our final section.
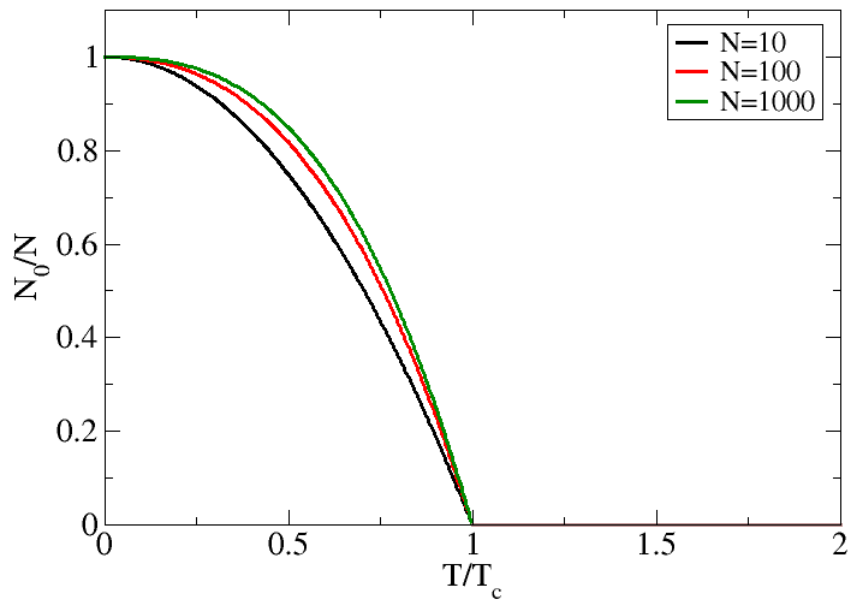
Figure 2.2: Condensate fraction for an isotropic three-dimensional harmonic trap in the semiclassical approximation as a function of reduced temperature given by Eq. (2.75) for a different number of particles N. The brown line in zero corresponds to all plots after the critical point due to, independently of N, the condensate fraction being zero for high temperatures in the grand canonical ensemble.
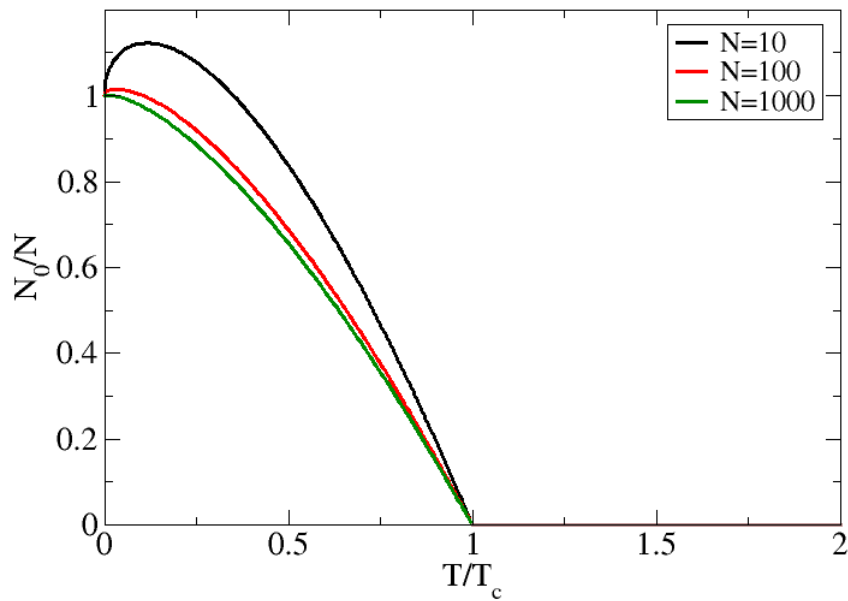
Figure 2.3: Condensate fraction for a three-dimensional finite box using the homogeneous semiclassical approximation as a function of reduced temperature given by Eq. (2.76) for different numbers of particles N. The brown line in zero corresponds to all plots after the critical point due to, independently of N, the condensate fraction being zero for high temperatures in the grand canonical ensemble. Here is clear that this semiclassical approximation for a box trap is not good enough to describe the finite-size correction, so we need to do a semiclassical treatment using the discrete energy representation.

Internal energy and heat capacity

We will calculate the internal energy and heat capacity to finalize our calculations for a non-interacting power-law trap. These quantities have different mathematical formulas for $T < T_c$ and $T > T_c$ because for the Boson gases, below the critical temperature, the fugacity is fixed by critical chemical potential and so, in this case, the polylogarithms converge to the Riemann zeta function; and when under the critical temperature, the fugacity depends of the temperature, then we must operate with these functions. In both cases, the condensed contribution of the grand canonical free energy $\mathcal{F}_0^{(0)}$ and $N_0^{(0)}$ is zero.

The internal energy is calculated through the grand canonical probability P_j for a state j given by

$$P_j(\beta, \hat{\mu}) = \frac{1}{\Xi^{(0)}} \, e^{-\beta(E_j - \hat{\mu} N_j)} \tag{2.77}$$

and this formula can be written in terms of the fugacity,

$$P_j(\beta, \hat{z}) = \frac{1}{\Xi^{(0)}} \, \hat{z}^{N_j} \, e^{-\beta E_j}. \tag{2.78}$$

So, we know that we can calculate the mean value of the energy using the classical equation for an average value of a given probability distribution,

$$U(\beta, \hat{z}) = \langle E_j \rangle = \sum_j E_j \, P_j(\beta, \hat{z}), \tag{2.79}$$

and here inserting Eq. (2.78) in Eq. (2.79), we have that

$$U = -\frac{\partial}{\partial \beta} \ln(\beta, \hat{z}) \,, \tag{2.80}$$

where to obtain this formula, we used a common procedure of statistical mechanics, writing

$$E_j \, e^{-\beta E_j} = -\frac{\partial}{\partial \beta} e^{-\beta E_j}. \tag{2.81}$$

But the natural logarithm of $\Xi^{(0)}$ have connection with the thermodynamics given by $-\beta \mathcal{F}^{(0)}$. Then, Eq. (2.80) becomes

$$U = \frac{\partial}{\partial \beta} (\beta \, \mathcal{F}^{(0)}). \tag{2.82}$$

To obtain the heat capacity C_N, let's derivate the internal energy U with respect to the temperature T for fixed N,

$$c_N = \frac{1}{N} \left(\frac{\partial U}{\partial T} \right)_N = -\frac{k_B \beta^2}{N} \left(\frac{\partial U}{\partial \beta} \right)_N, \tag{2.83}$$

where $c_N \equiv C_N / N$. But as we see here, the derivative is fixed in N but N also depends on T, then is necessary to use the Jacobian technique as made in [38]

$$\left(\frac{\partial U}{\partial \beta} \right)_N = \left(\frac{\partial U}{\partial \beta} \right)_{\hat{z}} - \left(\frac{\partial U}{\partial \hat{z}} \right)_\beta \frac{\left(\frac{\partial N}{\partial \beta} \right)_{\hat{z}}}{\left(\frac{\partial N}{\partial \hat{z}} \right)_\beta}. \tag{2.84}$$

Remembering that the grand canonical free energy and the average number of particles are given by Eqs. (2.46) and (2.48), and now together with Eqs. (2.82) and (2.84), is possible to calculate the internal energy in condensed and normal phases. By simplicity, let us start with the condensed measures (when $T < T_c$).

Condensed phase - $T < T_c$

In the condensed phase as discussed previously, the reduced fugacity is fixed in critical reduced chemical potential. Then, $\hat{z}_c = 1 \Rightarrow \zeta_a(\hat{z}_c) = \zeta(a)$. So, Eq. (2.46) becomes

$$\mathcal{F}_0(T < T_c) = -\frac{\eta}{\beta^{\alpha+1}} \left[\zeta(\alpha + 1) + \beta\, E_G\, \zeta(\alpha) \right] \tag{2.85}$$

and putting Eq. (2.85) in Eq. (2.82),

$$U(T < T_c) = \alpha\, \eta\, \zeta(\alpha + 1)\, \beta^{-\alpha-1} - \eta\, E_G\, (1 - \alpha)\, \zeta(\alpha)\, \beta^{-\alpha}. \tag{2.86}$$

To find the heat capacity, we need Eq. (2.48) for condensed state, and then

$$N = \frac{\eta}{\beta^{\alpha}} \left(\zeta(\alpha) + \beta\, E_G\, \zeta(\alpha - 1) \right) \tag{2.87}$$

and as Eqs. (2.87), (2.86) not depend of $\hat{z}$, then Eq. (2.83) becomes

$$c_N(T < T_c) = -\frac{k_B \beta^2}{N} \left(\frac{\partial U(T < T_c)}{\partial \beta} \right)_{\hat{z}}, \tag{2.88}$$

therefore,

$$c_N(T < T_c) = \frac{\alpha(\alpha + 1)k_B\, \eta\, \zeta(\alpha + 1)}{N \beta^{\alpha}} - \frac{k_B E_G\, \alpha(1 - \alpha)\, \eta\, \zeta(\alpha)}{N \beta^{\alpha-1}}. \tag{2.89}$$

Normal phase - $T > T_c$

In the normal phase, the fugacity is not fixed, thus the heat capacity calculations are more complicated. From Eqs. (2.46) and (2.48),

$$\mathcal{F}_0 = -\frac{\eta}{\beta^{\alpha+1}} \left[\zeta_{\alpha+1}(\hat{z}) + \beta\, E_G\, \zeta_{\alpha}(\hat{z}) \right], \tag{2.90}$$

$$N_0 = \frac{\eta}{\beta^{\alpha}} \left[\zeta_{\alpha}(\hat{z}) + \beta\, E_G\, \zeta_{\alpha-1}(\hat{z}) \right]. \tag{2.91}$$

By Eq. (2.82), we have that

$$U(T > T_c) = \alpha\, \eta\, \zeta_{\alpha+1}(\hat{z})\, \beta^{-\alpha-1} - \eta\, E_G\, (1 - \alpha)\, \zeta_{\alpha}(\hat{z})\, \beta^{-\alpha}. \tag{2.92}$$

As all formulas depend on the $\hat{z}$, then to calculate the heat capacity, we need to solve the Jacobian Eq. (2.85). So,

$$\left(\frac{\partial U}{\partial \beta} \right)_{\hat{z}} = -\alpha\, (\alpha + 1)\, \eta\, \beta^{-\alpha-2}\, \zeta_{\alpha+1}(\hat{z}) + \alpha\, (1 - \alpha)\, \eta\, E_G\, \beta^{-\alpha-1}\, \zeta_{\alpha}(\hat{z}) \tag{2.93}$$

$$\left(\frac{\partial U}{\partial \hat{z}} \right)_{\beta} = \frac{1}{\hat{z}} \left(\alpha\, \eta\, \beta^{-\alpha-1}\, \zeta_{\alpha}(\hat{z}) - (1 - \alpha)\, \eta\, E_G\, \beta^{-\alpha}\, \zeta_{\alpha-1}(\hat{z}) \right) \tag{2.94}$$

$$\left(\frac{\partial N}{\partial \beta}\right)_{\hat{z}} = -\alpha\,\eta\,\beta^{-\alpha-1}\,\zeta_\alpha(\hat{z}) + (1-\alpha)\,\eta\,E_G\,\beta^{-\alpha}\,\zeta_{\alpha-1}(\hat{z}) \tag{2.95}$$

$$\left(\frac{\partial N}{\partial \hat{z}}\right)_{\beta} = \frac{1}{\hat{z}}\left(\eta\,\beta^{-\alpha}\,\zeta_{\alpha-1}(\hat{z}) + \eta\,E_G\,\beta^{1-\alpha}\,\zeta_{\alpha-2}(\hat{z})\right) \tag{2.96}$$

By Eqs. (2.96) and (2.95) in Eq. (2.84), the denominator can be calculated using the binomial theorem $(1+x)^{-1} \approx 1-x$, besides we multiply Eq. (2.94) and finally, we do not consider the terms which depend of E_G^n with $n > 1$ because it corresponds to the higher orders. Therefore, denoting

$$A \equiv \left(\frac{\partial U}{\partial \hat{z}}\right)_{\beta} \frac{\left(\frac{\partial N}{\partial \beta}\right)_{\hat{z}}}{\left(\frac{\partial N}{\partial \hat{z}}\right)_{\beta}}, \tag{2.97}$$

we have that

$$A \approx -\alpha^2\,\eta\,\beta^{-\alpha-2}\,\frac{\zeta_\alpha^2(\hat{z})}{\zeta_{\alpha-1}(\hat{z})} + \alpha^2\,E_G\,\eta\,\beta^{-\alpha-1}\,\frac{\zeta_\alpha^2(\hat{z})\,\zeta_{\alpha-2}(\hat{z})}{\zeta_{\alpha-1}^2(\hat{z})}$$
$$+ \alpha\,\eta\,\beta^{-\alpha-1}\,E_G\,(1-\alpha)\,\zeta_\alpha(\hat{z}) + \alpha\,(1-\alpha)\,E_G\,\eta\,\beta^{-\alpha-1}\,\zeta_\alpha(\hat{z}). \tag{2.98}$$

With this result, we can calculate the heat capacity $c_N(T > T_c)$ using Eqs. (2.98), (2.93) in Eqs. (2.83) and (2.84), obtaining

$$c_N(T > T_c) = \frac{k_B\,\beta^{-\alpha}\,\alpha\,(\alpha+1)\,\eta}{N}\,\zeta_{\alpha+1}(\hat{z}) - \frac{k_B\,\beta^{-\alpha}\,\alpha^2\,\eta}{N}\,\frac{\zeta_{\alpha1}^2(\hat{z})}{\zeta_{\alpha-1}(\hat{z})}$$
$$+ \frac{k_B\,\beta^{-\alpha+1}\,\alpha^2\,\eta\,E_G}{N}\,\frac{\zeta_{\alpha-2}(\hat{z})\,\zeta_\alpha^2(\hat{z})}{\zeta_{\alpha-1}^2(\hat{z})} + \frac{k_B\,\beta^{-\alpha+1}\,\alpha\,(1-\alpha)\,\eta\,E_G}{N}\,\zeta_\alpha(\hat{z}) \tag{2.99}$$

The equations Eqs. (2.89) and (2.99) can be written as a function of the critical temperature in the thermodynamic limit $T_c^{(0)}$ given by Eq. (2.52) and hence, the value of the Boltzmann factor $\beta_c^{(0)}$ from Eq. (2.51). So, Eq. (2.89) is now

$$C_N(T < T_c) = N\,k_B\left[\alpha\,(\alpha+1)\,\frac{\zeta(\alpha+1)}{\zeta(\alpha)}\left(\frac{T}{T_c^{(0)}}\right)^\alpha + \alpha\,(\alpha-1)\,E_G\,\beta_c^{(0)}\left(\frac{T}{T_c^{(0)}}\right)^{\alpha-1}\right] \tag{2.100}$$

$$C_N(T > T_c) = N\,k_B\left[\alpha\,(\alpha+1)\,\frac{\zeta_{\alpha+1}(\hat{z})}{\zeta(\alpha)} - \alpha^2\,\frac{\zeta_\alpha^2(\hat{z})}{\zeta(\alpha)\,\zeta_{\alpha-1}(\hat{z})}\right]\left(\frac{T}{T_c^{(0)}}\right)^\alpha$$
$$+ N\,k_B\left[\alpha^2\,E_G\,\beta_c^{(0)\alpha}\,\frac{\zeta_\alpha^2(\hat{z})\,\zeta_{\alpha-2}(\hat{z})}{\zeta(\alpha)\,\zeta_{\alpha-1}^2(\hat{z})} - \alpha\,(\alpha-1)\,\beta_c^{(0)}\,E_G\,\frac{\zeta_\alpha(\hat{z})}{\zeta(\alpha)}\right]\left(\frac{T}{T_c^{(0)}}\right)^{\alpha-1}. \tag{2.101}$$

In the limit of the three-dimensional harmonic trap, we have that this result is similar to that obtained in [39]. Before continuing the calculations, let us check the limit of high temperatures. We know that when $T \to \infty$, C_N is given by the Dulong-Petit law, in fact, this limit is satisfied on Eq. (2.101),

$$C_N(T \to \infty) = \lim_{T \to \infty} C_N(T > T_c) = N\,k_B\,\alpha\,, \tag{2.102}$$

and again, this result agrees with [32] for a general Dulong-Petit law.

2.2.1   Non-interacting finite box

The power law trap is a good method to generalize the traps in which the spectrum can be approximated by continuous form. But when we concentrate on studying trapped systems with boundary conditions, we will have that the energies are quantized by quantum mechanics, so a semiclassical treatment is different. Here, we studied the three-dimensional Bose gas in a finite box with length L using an integral approach with Robinson's formula and Jacobi elliptic theta function. Consider N bosons in a cubic box with length L. The potential for its system is given by

$$
V(\mathbf{x}) = \begin{cases} 0 & |x_j| \leq L \\ \infty & |x_j| \geq L \end{cases}
$$

First, we will calculate the wave function $\psi_{\mathbf{k}}(\mathbf{x})$ using the Schrödinger equation,

$$
\hat{H}\psi_{\mathbf{k}}(\mathbf{x}) = E_{\mathbf{k}}\psi_{\mathbf{x}}(\mathbf{x}), \tag{2.103}
$$

where E_k are the energy eigenvalues and $\hat{H}$ is the Hamiltonian, whose expression is

$$
\hat{H} = -\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{x}). \tag{2.104}
$$

This problem in three dimensions can be written as a tensor product

$$
\psi_k(\mathbf{x}) = \prod_{j=1}^{3} \psi_{k_j}(x_j) \tag{2.105}
$$

and

$$
E_k = \sum_{j=1}^{3} E_{k_j} \tag{2.106}
$$

with each $\psi_{k_j}(x_j)$ and E_{k_j} functions in one dimension. In form, we'll make the details for a one-dimension system, and then, Eq. (2.104) can be written as

$$
\frac{d^2}{dx^2}\psi(x) + k^2\psi(x) = 0 \tag{2.107}
$$

where

$$
k^2 \equiv \frac{2ME_k}{\hbar^2}. \tag{2.108}
$$

The boundary conditions for each component are equal because is a cubic trap, so $\psi(0) = \psi(L) = 0$. Solving Eq. (2.107) with its conditions, we have that

$$
\psi_{n_j}(x_j) = \frac{1}{(2L)^{1/2}} \left[e^{in_j\pi x_j/L} - (-1)^{n_j}e^{-in_j\pi x_j/L} \right], \tag{2.109}
$$

where k_j is equal to

$$
k_j = \frac{\pi n_j}{L}, \tag{2.110}
$$

with n_j an integer number, and

$$E_{n_j} = \frac{\hbar^2 \pi^2 n_j^2}{2ML^2}. \tag{2.111}$$

With (2.111), we can generalize the energy for three dimensions using Eq. (2.106). Expanding the logarithm by Eq. (2.23), we have that

$$\mathcal{F} = \mathcal{F}_0^{(0)} - \frac{1}{\beta} \sum_{n=1}^{\infty} \frac{\hat{z}^n}{n} \left[\hat{Z}_1(n\beta) - 1 \right] , \tag{2.112}$$

where

$$\hat{Z}_1(n\beta) \equiv \left[\sum_{m=1}^{\infty} e^{-n\beta \hbar^2 \pi^2 (m^2-1)/2ML^2} \right]^3 . \tag{2.113}$$

For simplicity, we can write Eq. (2.113) in terms of dimensionless parameter τ here defined as

$$\tau \equiv V^{2/3} \frac{M}{2\pi \hbar^2 \beta} \tag{2.114}$$

then Eq. (2.113) becomes

$$\hat{Z}_1(n\beta) = \left[\sum_{m=1}^{\infty} e^{-n\pi(m^2-1)/4\tau} \right]^3 \equiv [X_1(n\tau)]^3 \tag{2.115}$$

with

$$X_1(n\tau) = \sum_{m=1}^{\infty} e^{-n\pi(m^2-1)/4\tau} = 1 + \sum_{m=2}^{\infty} e^{-n\pi(m^2-1)/4\tau} \tag{2.116}$$

but (2.116) can be written as

$$X_1(n\tau) = 1 + e^{-3n\pi/4\tau} \sigma(\tau/n) \tag{2.117}$$

where

$$\sigma(\tau/n) \equiv \sum_{m=2}^{\infty} e^{-n\pi(m^2-4)/4\tau} \tag{2.118}$$

For $\sigma(\tau/n)$ in a semiclassical treatment, we can expand it in a polynomial formula using Poisson's summation formula,

$$\sum_{m=-\infty}^{\infty} f(m) = \sum_{q=-\infty}^{\infty} \int_{-\infty}^{\infty} dx \, f(x) \, e^{2\pi i q x} \tag{2.119}$$

By Eq. (2.116),

$$\sigma(\tau/n) = \sum_{m=1}^{\infty} e^{-n\pi(m^2-4)/4\tau} - e^{3\pi n/4\tau} \tag{2.120}$$

and the summation over m from 1 to ∞ is equal to

$$\sum_{m=1}^{\infty} e^{-n\pi(m^2-4)/4\tau} = \frac{e^{n\pi/\tau}}{2} \left[\sum_{m=-\infty}^{\infty} e^{-n\pi(m^2-4)/4\tau} - 1 \right] \tag{2.121}$$

now we can use Eq. (2.119) here, then Eq. (2.121) becomes

$$\sum_{m=1}^{\infty} e^{-n\pi(m^2-4)/4\tau} = e^{n\pi/\tau}\left[\sqrt{\frac{\tau}{n}} - \frac{1}{2} + 2\sqrt{\frac{\tau}{n}}\sum_{q=1}^{\infty} e^{-4\pi q^2\tau/n}\right] \tag{2.122}$$

Therefore, the polynomial formula of $\sigma(\tau/n)$ by Eq. (2.120) using Eq. (2.122) is

$$\sigma(\tau/n) = \sqrt{\frac{\tau}{n}}\left(1 - \frac{3}{2}\sqrt{\frac{n}{\tau}} + \frac{\pi n}{\tau}\right). \tag{2.123}$$

So, by Eq. (2.111), and remembering that the number of particles given by Eq. (2.30), we have that

$$N^{(0)} = N_0^{(0)} + \sum_{n=1}^{\infty} \hat{z}^n\left(X_1(n\tau)^3 - 1\right) \tag{2.124}$$

but

$$(1+x)^3 = 1 + 3x^2 + 3x + 1 \tag{2.125}$$

then, we obtain that

$$N^{(0)} = N_0^{(0)} + \sum_{n=1}^{\infty} \hat{z}^n\left(3\,e^{-3n\pi/4\tau}\,\sigma(\tau/n) + 3\,e^{-6n\pi/4\tau}\,\sigma^2(\tau/n) + e^{-9n\pi/4\tau}\,\sigma^3(\tau/n)\right). \tag{2.126}$$

The first calculation is to find the critical temperature. Therefore, for a non-interacting case, $\hat{\mu}_c = 0$ with $\tau = \tau_c^{(0)}$ and $N_0^{(0)} = 0$, so

$$N^{(0)} = N = \sum_{n=1}^{\infty}\left(3\,e^{-3n\pi/4\tau_c^{(0)}}\,\sigma(\tau_c^{(0)}/n) + 3\,e^{-6n\pi/4\tau_c^{(0)}}\,\sigma^2(\tau_c^{(0)}/n) + e^{-9n\pi/4\tau_c^{(0)}}\,\sigma^3(\tau_c^{(0)}/n)\right). \tag{2.127}$$

and using Eq. (2.123) in Eq. (2.127), we shall see the each $\tau_c^{(0)}$-contribution,

$$\sigma(\tau_c^{(0)}/n) = \sqrt{\frac{\tau_c^{(0)}}{n}}\left[1 - \frac{3}{2}\sqrt{\frac{n}{\tau_c^{(0)}}} + \frac{n\pi}{\tau_c^{(0)}}\right], \tag{2.128}$$

$$\sigma^2(\tau_c^{(0)}/n) = \frac{\tau_c^{(0)}}{n}\left[1 - \frac{3}{2}\sqrt{\frac{n}{\tau_c^{(0)}}} + \frac{n\pi}{\tau_c^{(0)}}\right]^2, \tag{2.129}$$

$$\sigma^3(\tau_c^{(0)}/n) = \left(\frac{\tau_c^{(0)}}{n}\right)^{3/2}\left[1 - \frac{3}{2}\sqrt{\frac{n}{\tau_c^{(0)}}} + \frac{n\pi}{\tau_c^{(0)}}\right]^3. \tag{2.130}$$

Therefore,

$$N = 3\sum_{n=1}^{\infty} e^{-3n\pi/4\tau_c^{(0)}}\sqrt{\frac{\tau_c^{(0)}}{n}}\left[1 - \frac{3}{2}\sqrt{\frac{n}{\tau_c^{(0)}}} + \frac{n\pi}{\tau_c^{(0)}}\right] + 3\sum_{n=1}^{\infty} e^{-6n\pi/4\tau_c^{(0)}}\frac{\tau_c^{(0)}}{n}\left[1 - \frac{3}{2}\sqrt{\frac{n}{\tau_c^{(0)}}} + \frac{n\pi}{\tau_c^{(0)}}\right]^2$$
$$+ \sum_{n=1}^{\infty} e^{-9n\pi/4\tau_c^{(0)}}\left(\frac{\tau_c^{(0)}}{n}\right)^{3/2}\left[1 - \frac{3}{2}\sqrt{\frac{n}{\tau_c^{(0)}}} + \frac{n\pi}{\tau_c^{(0)}}\right]^3, \tag{2.131}$$

and separating Eq. (2.131) in polylogarithm contributions,

$$N = \tau_c^{(0)3/2}\, \zeta_{3/2}\left(e^{-9n\pi/4\tau_c^{(0)}}\right) + \frac{3}{2}\,\tau_c^{(0)}\left[2\,\zeta_1\left(e^{-6n\pi/4\tau_c^{(0)}}\right) - 3\,\zeta_1\left(e^{-9n\pi/4\tau_c^{(0)}}\right)\right]$$
$$+ \frac{3\tau_c^{(0)1/2}}{4}\left[4\,\zeta_{1/2}\left(e^{-3n\pi/4\tau_c^{(0)}}\right) - 12\,\zeta_1\left(e^{-6n\pi/4\tau_c^{(0)}}\right) + (4\pi+9)\zeta_{1/2}\left(e^{-9n\pi/4\tau_c^{(0)}}\right)\right] \tag{2.132}$$

In Eq. (2.132), we have some polylogarithms in the critical points, and it can be calculated by Robinson's formula (Appendix B),

$$\zeta_{3/2}\left(e^{-9n\pi/4\tau_c^{(0)}}\right) \cong \zeta(3/2) \tag{2.133}$$

$$\zeta_{1/2}\left(e^{-3n\pi/4\tau_c^{(0)}}\right) = \zeta_{1/2}\left(e^{-6n\pi/4\tau_c^{(0)}}\right) = \zeta_{1/2}\left(e^{-9n\pi/4\tau_c^{(0)}}\right) \cong \zeta(1/2) \tag{2.134}$$

$$\zeta_1\left(e^{-6n\pi/4\tau_c^{(0)}}\right) = -\ln\left(\frac{6n\pi}{4\tau_c^{(0)}}\right) + \sum_{k=1}^{\infty}\frac{\zeta(1-k)}{k!}\left(\frac{-6n\pi}{4\tau_c^{(0)}}\right)^k \tag{2.135}$$

$$\zeta_1\left(e^{-9n\pi/4\tau_c^{(0)}}\right) = -\ln\left(\frac{9n\pi}{4\tau_c^{(0)}}\right) + \sum_{k=1}^{\infty}\frac{\zeta(1-k)}{k!}\left(\frac{-9n\pi}{4\tau_c^{(0)}}\right)^k \tag{2.136}$$

Then, putting Eqs. (2.136), (2.135), (2.134), (2.133) in Eq. (2.132), we have that

$$N = \tau_c^{(0)3/2}\,\zeta(3/2) + \frac{3}{4}\,(\pi+1)\,\zeta(1/2)\,\tau_c^{(0)1/2} + \frac{3}{2}\,\tau_c^{(0)}\ln\left(0.9574\,\frac{\pi}{2\,\tau_c^{(0)}}\right). \tag{2.137}$$

The thermodynamic limit of the finite box system is the homogeneous case, then from Eq. (2.114) for $V = L^3$, we can write the dimensionless temperature $\tau_c^{(0)}$ in the function of $t_c^{(0)}$ defined as

$$t_c^{(0)} \equiv \frac{T_c}{T_c^{(0)}}, \tag{2.138}$$

where T_c is the exact critical temperature and $T_c^{(0)}$ is the critical temperature in the thermodynamic limit. So,

$$\tau_c^{(0)} = \left(\frac{N}{\zeta(3/2)}\right)^{2/3} t_c^{(0)}. \tag{2.139}$$

From Eq. (2.139), Eq. (2.137) becomes

$$1 = t_c^{(0)3/2} + \frac{3}{2}\,t_c^{(0)}\,\frac{1}{N^{1/3}\,\zeta^{2/3}(3/2)}\ln\left(\frac{0.9574\,\pi\,\zeta^{2/3}(3/2)}{2\,N^{2/3}\,t_c^{(0)}}\right) \tag{2.140}$$

and therefore,

$$t_c^{(0)} = 1 - \frac{1}{N^{1/3}\,\zeta^{2/3}(3/2)}\ln\left(\frac{0.9574\,\pi\,\zeta^{2/3}(3/2)}{2\,N^{2/3}}\right). \tag{2.141}$$

This result is the same obtained in [15, 36] at the first order. To find the high-order contributions is only to expand the logarithm function in many terms of its power series representation. Following the same method that was employed in the previous section

about semiclassical representation, let's calculate the condensed fraction N_0/N starting by Eq. (2.126) with $\sigma(\tau/n)$ given by Eqs. (2.128), (2.129) and (2.130). When we have the condensed state, the fugacity is equal to 1 and the polylogarithms function reduces according to Robinson's formula (Appendix B), then doing the similar method that was employed in $t_c^{(0)}$ calculation, we have that

$$
N = N_0^{(0)} + \tau^{3/2}\,\zeta_{3/2}\left(e^{-9\pi/4\tau}\right) + \frac{3}{2}\,\tau\left[2\,\zeta_1\left(e^{-6\pi/4\tau}\right) - 3\,\zeta_1\left(e^{-9\pi/4\tau}\right)\right]
$$
$$
+ \frac{3\tau^{1/2}}{4}\left[4\,\zeta_{1/2}\left(e^{-3\pi/4\tau}\right) - 12\,\zeta_1\left(e^{-6\pi/4\tau}\right) + (4\pi+9)\zeta_{1/2}\left(e^{-9\pi/4\tau}\right)\right] \quad (2.142)
$$

The parameter τ is given by Eq. (2.133) but now the temperature in numerator is not critical. As the temperature is shifted by finite-size corrections and τ is a function of $T_c^{(0)}$, we shall include the new critical temperature dependence T_c, for this,

$$
\frac{T}{T_c^{(0)}} = \frac{T}{T_c}\frac{T_c}{T_c^{(0)}}, \quad (2.143)
$$

where $T_c/T_c^{(0)}$ given by Eq. (2.141). As the finite-size correction is small, then we can use the binomial approximation to calculate the powers of Eq. (2.143). As

$$
1 = \frac{N_0^{(0)}}{N} + \frac{\tau^{3/2}}{N}\,\zeta(3/2) + \frac{3}{4}\,(\pi+1)\,\zeta(1/2)\,\frac{\tau^{1/2}}{N} + \frac{3}{2}\,\frac{\tau}{N}\,\ln\left(0.9574\,\frac{\pi}{2\,\tau_0}\right). \quad (2.144)
$$

and therefore,

$$
\tau = \left(\frac{N}{\zeta(3/2)}\right)^{2/3}\frac{T}{T_c}\left(1 + \frac{\Delta T_c}{T_c^{(0)}}\right) \quad (2.145)
$$

and hence,

$$
1 = \frac{N_0^{(0)}}{N} + \left(\frac{T}{T_c}\right)^{3/2}\left[1 - \frac{3}{2}\frac{1}{N^{1/3}\,\zeta^{2/3}(3/2)}\,\ln\left(0.9574\,\frac{\pi}{2\,\tau_0}\right)\right], \quad (2.146)
$$

where $\tau_0 = N^{2/3}/\zeta^{2/3}(3/2)$. Therefore, not considering the second-order finite-size corrections, we obtain that the condensed fraction is

$$
\frac{N_0^{(0)}}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2} + \frac{3}{2}\frac{1}{N^{1/3}\,\zeta^{2/3}(3/2)}\,\ln\left(0.9574\,\frac{\pi\,\zeta^{2/3}(3/2)}{2\,N^{2/3}}\right)\left[\left(\frac{T}{T_c}\right)^{3/2} - \left(\frac{T}{T_c}\right)\right]
$$
$$
(2.147)
$$

and this formula agrees with that obtained by [36]. As an illustrative result, we have a plot with the condensed fraction for many values of N. Here, we see that this semi-classical approximation gives us the correct plots seen in Fig. 2.4. In this figure, when we do this approximation, we eliminate the problem of low temperatures which appears for Eq. (2.76) specially for a few particles - but when the LDA approximation is done according to the integral representation of the summation over the quantum numbers excluding correctly the ground-state contribution given by Eq. (2.147); and now, this divergence is eliminated.
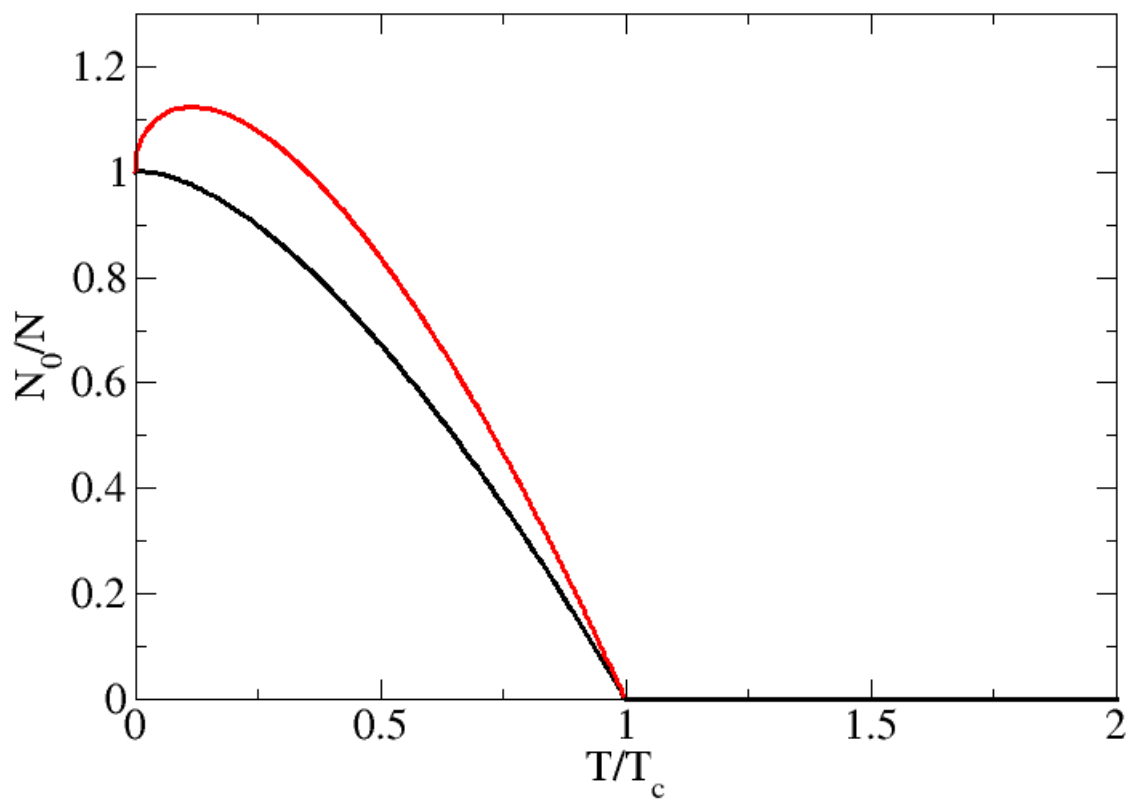
Figure 2.4: The comparision of the condensate fraction for 10 particles calculated by two formulas: the red line with Eq. (2.76) and the black line with Eq. (2.147). Is quite clear that this last formula corresponds to the correct formulation of our primary semi-classical approximation.
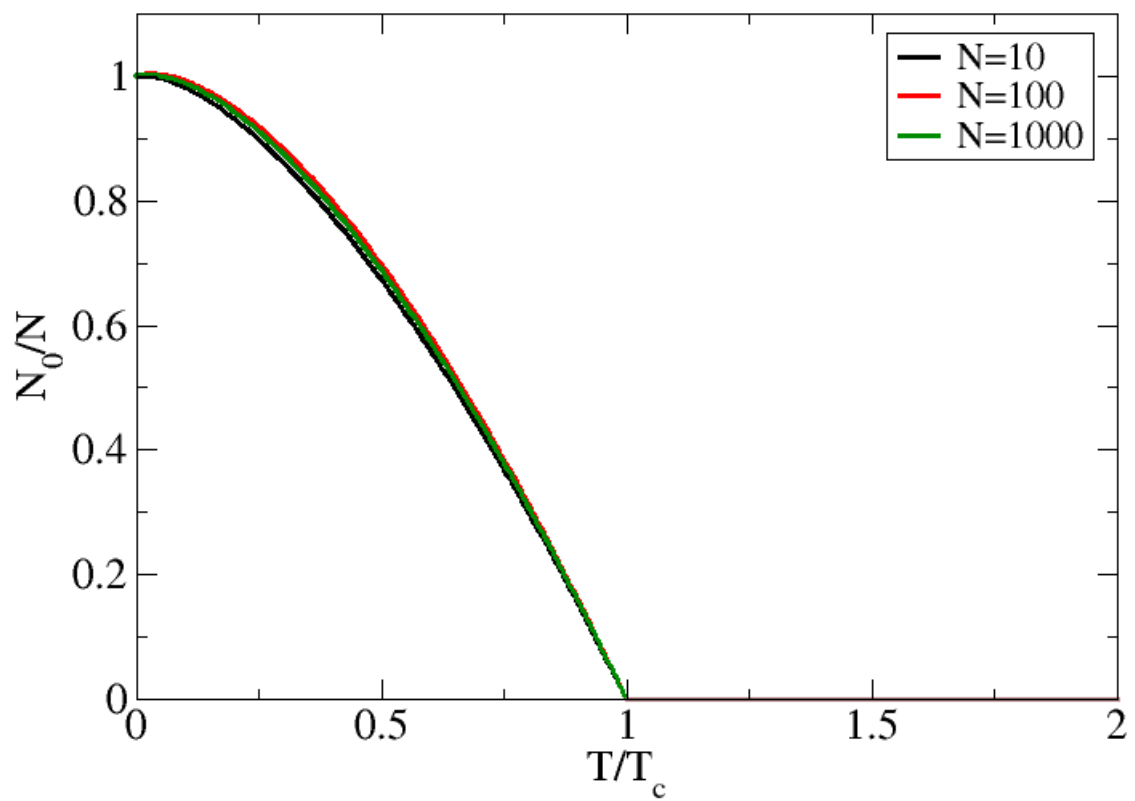
Figure 2.5: The condensate fraction of the three-dimensional finite box for $10, 100$ and 1000 particles calculated by Eq. (2.147). The behavior is similar as seen in Fig. 2.3 but now the problem for a few particles in low temperatures was solved, therefore, we have the correct semi-classical approximation for the box trap.

Chapter 3

Weakly interacting Bose gas

In real situations, the atoms have interactions between them. However, the inclusion of the interactions creates a difficulty in our calculations, and the form to study this influence can be seen by different approaches [4,33,40]. In general, the most common is the perturbation theory treating the interaction as a perturbation under the non-interacting situation using, as done in this text, with a path integral representation, considering until the first-order contribution that is known as the Hartree-Fock approximation. Different from Chapter 2 when we did the study for an ideal D-dimensional power-law trap, here we will do the calculations for a three-dimensional case because of the problems of the dimensional crossover as discussed in [43]. So, in this Chapter, we extend the calculations done in Chapter 2 for three-dimensional dilute gases whose interaction is described by the delta potential using the perturbative treatment, calculating the critical temperature shift, the condensed fraction, and the heat capacity for the power-law traps. As the fully interacting contribution is independent of the finite-size corrections, we can apply this formalism to see the behavior for the harmonic trap and the homogeneous box that are derivations of the power-law external potential.

3.1 Semiclassical approach of an interacting Bose gas

The procedure here is the same as done in the non-interacting case. The semiclassical treatment of the weakly interacting Bose gas is given by the integral of the ideal Green's function used in the perturbative formulas of the Hartree and Fock terms as will be viewed in the next subsection. Following the rules for the standard local density approximation, the chemical potential μ is shifted by its reduced quantity $\hat{\mu}$ and the respective fugacity $\hat{z}$, and the energy eigenvalues are written as the Hamiltonian. Another difference concerning the non-interacting system is that the chemical potential in the critical point will be modified due to interactions. All these points will be shown in this Chapter.

3.1.1 First-order perturbation theory in a power law trap

When we include the interactions in the system, the total action is modified by interacting action so, let's resort to statistical field theory and first, write the grand

canonical partition function Ξ in a functional form,

$$\Xi = \int D\psi^* \, D\psi \; e^{-\left(A^{(0)}[\psi^*,\psi] + A^{(\text{int})}[\psi^*,\psi]\right)/\hbar} \tag{3.1}$$

where

$$A^{(0)}[\psi^*,\psi] = \int_0^{\hbar\beta} d\tau \int d^3x \; \psi^*(\mathbf{x},\tau)\left[\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\Delta}{2M} + V(x) - \mu\right]\psi(\mathbf{x},\tau) \tag{3.2}$$

and

$$A^{(\text{int})}[\psi^*,\psi] = \frac{1}{2}\int_0^{\hbar\beta} d\tau \int d^3x \int d^3x' V^{(\text{int})}(\mathbf{x}-\mathbf{x}')\psi^*(\mathbf{x},\tau)\psi(\mathbf{x},\tau)\,\psi^*(\mathbf{x}',\tau)\psi(\mathbf{x}',\tau). \tag{3.3}$$

is the interacting action for a two-body interaction. As said in the second paragraph, for a weak interaction we can calculate Ξ expanding the interacting term in Eq. (3.1) in a Taylor series over $V^{(\text{int})}(\mathbf{x})$. So, using Eq. (3.3), we have

$$e^{-A^{(\text{int})}[\psi^*,\psi]/\hbar} \cong 1 - \frac{1}{2\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, d^3x' V^{(\text{int})}(\mathbf{x}-\mathbf{x}')\psi^*(\mathbf{x},\tau)\psi(\mathbf{x},\tau)\,\psi^*(\mathbf{x}',\tau)\psi(\mathbf{x}',\tau) + \dots, \tag{3.4}$$

and inserting Eq. (3.4) in Eq. (3.1),

$$\Xi = \oint D\psi^* \, D\psi \, e^{-A^{(0)}[\psi^*,\psi]/\hbar}$$
$$-\frac{1}{2\hbar}\oint D\psi^* \, D\psi \, e^{-A^{(0)}[\psi^*,\psi]/\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, d^3x' V^{(\text{int})}(\mathbf{x}-\mathbf{x}')\psi^*(\mathbf{x},\tau)\psi(\mathbf{x},\tau)\,\psi^*(\mathbf{x}',\tau)\psi(\mathbf{x}',\tau) + \dots. \tag{3.5}$$

The first term in Eq. (3.5) is the non-interacting grand canonical partition function $\Xi^{(0)}$ while the second term can be written using the average functional value given by the general formula,

$$\langle F[\psi*,\psi]\rangle^{(0)} \equiv \frac{1}{\Xi^{(0)}}\oint D\psi^* \, D\psi \, F[\psi^*,\psi]\, e^{-A^{(0)}[\psi^*,\psi]/\hbar}, \tag{3.6}$$

and now we may write Ξ in terms of non-interacting partition function $\Xi^{(0)}$ using Eq. (3.6), then Eq. (3.5) becomes

$$\Xi = \Xi^{(0)}\left(1 - \frac{1}{2\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, d^3x'\, V^{(\text{int})}(\mathbf{x}-\mathbf{x}')\langle\psi^*(\mathbf{x},\tau)\,\psi(\mathbf{x},\tau)\,\psi^*(\mathbf{x}',\tau)\psi(\mathbf{x}',\tau)\rangle^{(0)} + \dots\right). \tag{3.7}$$

The connection between grand canonical ensemble and thermodynamics is given by the formula

$$\mathcal{F} = -\frac{1}{\beta}\ln\Xi\,, \tag{3.8}$$

then inserting Eq. (3.7) in Eq. (3.8), we obtain that

$$\mathcal{F} = -\frac{1}{\beta}\ln\Xi^{(0)} - \frac{1}{\beta}\ln\left(1 - \frac{1}{2\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, d^3x'\, V^{(\text{int})}(\mathbf{x}-\mathbf{x}')\langle\psi^*(\mathbf{x},\tau)\,\psi(\mathbf{x},\tau)\,\psi^*(\mathbf{x}',\tau)\psi(\mathbf{x}',\tau)\rangle^{(0)} + \dots\right). \tag{3.9}$$

$$\mathcal{F} = \mathcal{F}^{(0)} - \frac{1}{2\beta} \, \text{⬭⬭} - \frac{1}{2\beta} \, \text{⬭} + \dots$$

Figure 3.1: Diagrammatic expansion of the grand canonical free energy up to first order perturbation theory, where the two diagrams correspond to the Hartree contribution (H) and Fock contribution (F) respectively. The Feynman rules are in Fig. 3.2 and their respective mathematical formulas are given by Eqs. (3.12) and (3.13).

$$\mathbf{x}, \tau \longleftarrow \mathbf{x}', \tau' \equiv G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau')$$

$$\mathbf{x} \text{≻•⌇⌇•≺} \mathbf{x}' \equiv -\frac{1}{\hbar} \int_0^{\hbar\beta} \mathrm{d}\tau \int \mathrm{d}^3x \int \mathrm{d}^3x' \, V^{(\text{int})}(\mathbf{x} - \mathbf{x}')$$

Figure 3.2: The grand canonical Feynman rules, the line corresponds to Green's function, and the vertex with a wiggly line is the interacting integral. With these rules, we have a scheme to determine the perturbative contribution of free energy for any order.

The term $\langle \psi^*(\mathbf{x}, \tau) \, \psi(\mathbf{x}, \tau) \, \psi^*(\mathbf{x}', \tau) \psi(\mathbf{x}', \tau) \rangle^{(0)}$ is known as the four-point correlation function, to calculate this term we shall consider the all possible combinations and it is solved using the Wick's theorem which will decompose this function in clusters of two-body correlations. These functions have a very important in our discussions because it is equal to Green's function in a grand canonical system, and the first term is the non-interacting free energy given by Eq.(2.25). The logarithm term can be expanded in a series, and therefore, we have that

$$\mathcal{F} = \mathcal{F}^{(0)} + \mathcal{F}^{(1)} + \dots , \tag{3.10}$$

where $\mathcal{F}^{(1)}$ is the first-order term whose equation is

$$\mathcal{F}^{(1)} = \mathcal{F}^{(H)} + \mathcal{F}^{(F)} , \tag{3.11}$$

with (H) referring to Hartree channel and (F) to Fock channel and their mathematical formulas are

$$\mathcal{F}^{(H)} = \frac{1}{2\hbar\beta} \int_0^{\hbar\beta} d\tau \int d^D x \, d^D x' \, G^{(0)}(\mathbf{x}, \tau; \mathbf{x}, \tau) \, V^{(\text{int})}(\mathbf{x} - \mathbf{x}') \, G^{(0)}(\mathbf{x}', \tau; \mathbf{x}', \tau) \,, \quad (3.12)$$

$$\mathcal{F}^{(F)} = \frac{1}{2\hbar\beta} \int_0^{\hbar\beta} d\tau \int d^D x \, d^D x' \, G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau) \, V^{(\text{int})}(\mathbf{x} - \mathbf{x}') \, G^{(0)}(\mathbf{x}', \tau; \mathbf{x}, \tau) \,, \quad (3.13)$$

where $G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau)$ is the non-interacting Green's function. This expansion can be represented in a diagrammatic form by the Feynman diagrams given by Fig. 3.1, where the equations (3.12) and (3.13) are the mathematical representation of the first-order diagrams following the Feynman rules [3].

As we are using the contact interaction [27] given by

$$V^{(\text{int})}(\mathbf{x} - \mathbf{x}') = g \, \delta(\mathbf{x} - \mathbf{x}') \,, \quad (3.14)$$

where g is the coupling constant

$$g = \frac{4\pi\hbar^2 a_s}{M} \,, \quad (3.15)$$

with scattering length a_s and the mass M. Inserting this interaction potential in Eq. (3.11), we have that the Hartree and Fock terms are equal, thus Eq. (3.11) becomes

$$\mathcal{F}^{(1)} = g \int d^D x \, G^{(0)}(\mathbf{x}, \tau; \mathbf{x}, \tau) \, G^{(0)}(\mathbf{x}, \tau; \mathbf{x}, \tau) \quad (3.16)$$

and now our next step is to calculate Green's function for a three-dimensional system. We know that the two-body correlation function $\langle \psi(\mathbf{x}, \tau) \, \psi^*(\mathbf{x}', \tau') \rangle^{(0)}$ is the Green's function. In general, $G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau')$ is given by [39]

$$\langle \psi(\mathbf{x}, \tau) \, \psi^*(\mathbf{x}', \tau') \rangle^{(0)} = G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau')$$
$$= \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{x}) \psi_{\mathbf{k}}^*(\mathbf{x}') \frac{\theta(\tau - \tau') e^{-(E_{\mathbf{k}} - \hat{\mu})(\tau - \tau' - \hbar\beta/2)/\hbar} + \theta(\tau' - \tau) e^{-(E_{\mathbf{k}} - \hat{\mu})(\tau' - \tau + \hbar\beta/2)/\hbar}}{2 \sinh(\beta(E_{\mathbf{k}} - \hat{\mu})/2)} \,.$$
$$(3.17)$$

As we have that $\tau - \tau' > 0$, then we shall consider the first term of the previous equation,

$$G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{x}) \psi_{\mathbf{k}}^*(\mathbf{x}') \frac{e^{-(E_{\mathbf{k}} - \mu)(\tau - \tau')/\hbar}}{1 - e^{-\beta(E_{\mathbf{k}} - \mu)}} \,. \quad (3.18)$$

As we have a power-law trap, we can use the semi-classical representation of Eq. (3.18), where now following the same rules written in Chapter 2, but now for the Green's function, the integral is over the relative coordinate $\delta x \equiv \mathbf{x} - \mathbf{x}'$, and the wave function is represented as a plane wave in momentum space; therefore Eq. (3.18) becomes

$$G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \int \frac{d^3 p \, d^3 \Delta x}{(2\pi\hbar)^3} \, e^{-i\mathbf{p} \cdot \Delta\mathbf{x}} \frac{e^{-(H[\mathbf{p}, \mathbf{X} - \hat{\mu}](\tau - \tau')/\hbar}}{1 - e^{-\beta(H[\mathbf{p}, \mathbf{X} - \hat{\mu})}} \,, \quad (3.19)$$

where $\mathbf{X}$ is the center of mass coordinate given by

$$\mathbf{X} \equiv \frac{\mathbf{x} + \mathbf{x}'}{2} . \tag{3.20}$$

Writing Eq. (3.19) for a diagonal term and writing the denominator using the geometric series, we have that

$$G^{(0)}(\mathbf{x}, \tau; \mathbf{x}, \tau) = \lim_{\tau' \downarrow \tau} G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \sum_{n=1}^{\infty} \int \frac{d^3 p}{(2\pi\hbar)^3} \exp\left(-n\beta\left(\frac{\mathbf{p}^2}{2M} + V(\mathbf{x}) - \hat{\mu}\right)\right) \tag{3.21}$$

$$G^{(0)}(\mathbf{x}, \tau; \mathbf{x}, \tau) = \frac{1}{\lambda_T^3} \sum_{n=1}^{\infty} \frac{\hat{z}^n}{n^{3/2}} e^{-n\beta V(\mathbf{x})} \tag{3.22}$$

where λ_T is the thermal wavelength,

$$\lambda_T = \sqrt{\frac{2\pi\hbar^2\beta}{M}}. \tag{3.23}$$

Inserting Eq. (3.23) in Eq. (3.16),

$$\mathcal{F}^{(1)} = \frac{g}{\lambda_T^6} \sum_{n,m=1}^{\infty} \frac{\hat{z}^{n+m}}{n^{3/2}m^{3/2}} \int e^{-(n+m)\beta V(\mathbf{x})} \, d^3 x \tag{3.24}$$

again, using Eq. (2.33) in Eq. (3.24) will have an integral of the same type of Eq. (2.38) with the difference is that now

$$\int e^{-(n+m)\beta V(\mathbf{x})} \, d^3 x = \frac{1}{\beta^{\sum 1/a_i} (n+m)^{\sum 1/a_i}} \prod_{i=1}^{3} \frac{l_i}{a_i} \Gamma\left(\frac{1}{a_i}\right) \tag{3.25}$$

$$\mathcal{F}^{(1)} = \frac{g}{\lambda_T^6} \sum_{n,m=1}^{\infty} \frac{z^{n+m}}{n^{3/2}m^{3/2}} \frac{1}{\beta^{\sum 1/a_i} (n+m)^{\sum 1/a_i}} \prod_{i=1}^{3} \frac{l_i}{a_i} \Gamma\left(\frac{1}{a_i}\right) \tag{3.26}$$

and writing it in terms of α and multiple polylogarithm function $\zeta_{a,b,c}(z)$:

$$\zeta_{a,b,c}(z) = \sum_{n,m=1}^{\infty} \frac{z^{n+m}}{n^a m^b (n+m)^c} \tag{3.27}$$

besides the thermal wavelength and therefore, we have that the first-order formula for grand canonical free energy $\mathcal{F}^{(1)}$

$$\mathcal{F}^{(1)} = \frac{g}{\lambda_T^6 \beta^{\alpha-3/2}} \prod_{i=1}^{3} 2^i \frac{l_i}{a_i} \Gamma\left(\frac{1}{a_i}\right) \zeta_{3/2,3/2,\alpha-3/2}(\hat{z}) \tag{3.28}$$

Writing Eq. (3.28) in terms of β and denoting

$$g \left(\frac{M}{2\pi\hbar^2}\right)^3 \prod_{i=1}^{3} 2^i \frac{l_i}{a_i} \Gamma\left(\frac{1}{a_i}\right) \equiv \xi \tag{3.29}$$

we have

$$\mathcal{F}^{(1)} = \frac{\xi}{\beta^{\alpha+3/2}} \zeta_{3/2,3/2,\alpha-3/2}(\hat{z}) \tag{3.30}$$

and hence,

$$N^{(1)} = -\frac{\xi}{\beta^{\alpha+1/2}} \zeta_{3/2,3/2,\alpha-5/2}(\hat{z}) \tag{3.31}$$

This form, the total free energy $\mathcal{F}$ and number of particles N are equal to

$$\mathcal{F} = \mathcal{F}_0^{(0)} - \frac{1}{\beta^{\alpha+1}} \eta \left(\zeta_{\alpha+1}(\hat{z}) + \beta E_G \zeta_\alpha(\hat{z}) \right) + \frac{\xi}{\beta^{\alpha+3/2}} \zeta_{3/2,3/2,\alpha-3/2}(\hat{z}) \tag{3.32}$$

where $\mathcal{F}_0^{(0)}$ is the condensed free energy

$$N = N_0^{(0)} + \frac{1}{\beta^{\alpha}} \eta \left(\zeta_\alpha(\hat{z}) + \beta E_G \zeta_{\alpha-1}(\hat{z}) \right) - \frac{\xi}{\beta^{\alpha+1/2}} \zeta_{3/2,3/2,\alpha-5/2}(\hat{z}). \tag{3.33}$$

With Eqs. (3.32) and (3.33) we have complete quantities to study the thermodynamic properties of the system. As done in Chapter 2, we must calculate the critical point between the two phases: the BEC and the thermal gas. In the case of non-interacting gas, the critical point occurs when $\hat{\mu} = 0$, however, the inclusion of the interactions changes the critical point through a chemical potential shift, and this situation is studied by calculating the poles of Green's function as we show in next subsection.

3.1.2 Green's function for an interacting system

Let's start with the two-body correlation function:

$$\langle \psi(\mathbf{x}, \tau) \psi^*(\mathbf{x}', \tau') \rangle \equiv G(\mathbf{x}, \tau; \mathbf{x}', \tau'). \tag{3.34}$$

By quantum field theory, for any functional $F[\psi^*, \psi]$, we have a path integral representation. So, we can write the Green's function as

$$G(\mathbf{x}, \tau; \mathbf{x}', \tau') = \frac{1}{\Xi} \oint D\psi^* \, D\psi \; \psi(\mathbf{x}, \tau) \psi^*(\mathbf{x}', \tau') \, e^{-A[\psi^*, \psi]/\hbar} \tag{3.35}$$

where $A[\psi^*, \psi]$ is the total action given by $A^{(0)}[\psi^*, \psi] + A^{(int)}[\psi^*, \psi]$. The denominator was expanded in the previous subsection about grand canonical free energy. But now we shall expand the numerator following the same idea of the Ξ expansion, doing a perturbation theory in the interacting action given by Eq. (3.3) with respect to the interacting potential. So,

$$G(\mathbf{x}, \tau; \mathbf{x}', \tau') = \frac{1}{\Xi} \oint D\psi^* \, D\psi \; \psi(\mathbf{x}, \tau) \psi^*(\mathbf{x}', \tau') \, e^{-A^{(0)}[\psi^*, \psi]/\hbar} \left(1 - \frac{A^{(int)}[\psi^*, \psi]}{\hbar} \right), \tag{3.36}$$

where Ξ is given by Eq. (3.1). The numerator can be written using Wick's theorem [4,39], in terms of correlation function $\langle F[\psi^*, \psi] \rangle$ for any functional $F[\psi^*, \psi]$ following

$$\langle F[\psi^*, \psi] \rangle^{(0)} \equiv \frac{1}{\Xi^{(0)}} \oint D\psi^* \, D\psi \, F[\psi^*, \psi] \, e^{-A^{(0)}[\psi^*, \psi]/\hbar}, \tag{3.37}$$

then the numerator in Eq. (3.36) becomes

$$\Xi^{(0)} \left(\langle \psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau') \rangle^{(0)} - \frac{1}{\hbar} \langle \psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau') A^{(\text{int})}[\psi^*,\psi] \rangle^{(0)} \right) , \quad (3.38)$$

and therefore

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{\langle \psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau') \rangle^{(0)} - \frac{1}{\hbar} \langle \psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau') A^{(\text{int})}[\psi^*,\psi] \rangle^{(0)}}{1 - \frac{1}{\hbar} \langle A^{(\text{int})}[\psi^*,\psi] \rangle^{(0)}}. \quad (3.39)$$

However, now the denominator can be approximated using the binomial theorem $(1-x)^n \cong 1 - nx$, then $G(\mathbf{x},\tau;\mathbf{x}',\tau')$ is

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = \langle \psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau') \rangle^{(0)} - \frac{1}{\hbar} \langle \psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau') A^{(\text{int})}[\psi^*,\psi] \rangle^{(0)}$$

$$+ \frac{1}{\hbar} \langle A^{(\text{int})}[\psi^*,\psi] \rangle^{(0)} \langle \psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau') \rangle^{(0)} + ... , \quad (3.40)$$

where we neglected the second-order term with respect to the interacting action. Here, this approximation can be used because we have weak interactions. Again, we must apply Wick's theorem for the last two correlations in Eq. (3.40), remembering that the two-body correlation function is, by definition, the grand canonical Green's function [4,39,40]. When we do this expansion, the interacting Green's function is written as

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = G^{(0)}(\mathbf{x},\tau;\mathbf{x}',\tau') - \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau'' \int d^3x'' d^3x''' V^{(int)}(\mathbf{x}'' - \mathbf{x}''') \quad (3.41)$$

$$[G^{(0)}(\mathbf{x},\tau;\mathbf{x}'',\tau'') G^{(0)}(\mathbf{x}'',\tau'';\mathbf{x}',\tau') G^{(0)}(\mathbf{x}''',\tau'';\mathbf{x}''',\tau'') \quad (3.42)$$

$$+ G^{(0)}(\mathbf{x},\tau;\mathbf{x}'',\tau'') G^{(0)}(\mathbf{x}''',\tau'';\mathbf{x}',\tau') G^{(0)}(\mathbf{x}'',\tau'';\mathbf{x}''',\tau'')] , \quad (3.43)$$

where the second line corresponds to the Hartree channel and the last line is the Fock channel. This equation can be written in a compact form as

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = G^{(0)}(\mathbf{x},\tau;\mathbf{x}',\tau')$$

$$+ \int_0^{\hbar\beta} d\tau'' d\tau''' \int d^3x'' d^3x''' G^{(0)}(\mathbf{x},\tau;\mathbf{x}'',\tau'') \Sigma(\mathbf{x}'',\tau'';\mathbf{x}''',\tau''') G(\mathbf{x}''',\tau''';\mathbf{x}',\tau'),$$

$$(3.44)$$

where $\Sigma(\mathbf{x},\tau;\mathbf{x}',\tau')$ is self-energy operator. This is known as Dyson's equation, and as done in the case of the grand canonical free energy, this equation can be represented in a diagrammatic form given by Fig. 3.3. Doing the comparison between Eqs. (3.43) and (3.44), the first order contributions of $\Sigma(\mathbf{x},\tau;\mathbf{x}',\tau')$ are given by

$$\Sigma^{(D)}(\mathbf{x},\tau;\mathbf{x}',\tau') = -\frac{1}{\hbar} \delta(\mathbf{x}-\mathbf{x}') \delta(\tau-\tau') \int d^3x'' V^{(\text{int})}(\mathbf{x}-\mathbf{x}'') G^{(0)}(\mathbf{x}'',\tau;\mathbf{x}'',\tau), \quad (3.45)$$

$$\Sigma^{(E)}(\mathbf{x},\tau;\mathbf{x}',\tau') = -\frac{1}{\hbar} \delta(\tau-\tau') V^{(\text{int})}(\mathbf{x}-\mathbf{x}') G^{(0)}(\mathbf{x}',\tau;\mathbf{x}',\tau) , \quad (3.46)$$

where these formulas also are obtained following the Feynman rules developed in the previous subsection. The correspondent Hartree and Fock self-energies diagrams are in

Figure 3.3: Diagrammatic expansion of Dyson's equation Eq. (3.44) up to first order perturbation theory, where $1 \equiv (\mathbf{x}, \tau)$ and $2 \equiv (\mathbf{x}', \tau')$, the two lines correspond to the interacting G, the one line is non-interacting $G^{(0)}$, the first diagram corresponds to the Hartree term and the second, the Fock term. The difference between the self-energy diagrams and the free energy is that in the self-energy, we cut one line following [3].

$$\Sigma^{(D)}(\boldsymbol{x}, \tau; \boldsymbol{x}', \tau') = \underset{\boldsymbol{x}\,\tau\ \ \boldsymbol{x}'\tau'}{\vcenter{\hbox{}}} \quad , \quad \Sigma^{(E)}(\boldsymbol{x}, \tau; \boldsymbol{x}', \tau') = \underset{\boldsymbol{x}\,\tau \qquad \boldsymbol{x}'\tau'}{\vcenter{\hbox{}}}$$

Figure 3.4: Diagrammatic representation of the Hartree and Fock self-energy given by Eqs. (3.45) and (3.46).

Fig. 3.4. These self-energies depend on grand canonical non-interacting Green's function $G^{(0)}$ and this result is a function of the chemical potential μ. From Euclidean time-position representation, the divergent points are not clear, then we need to go to the Fourier-Matsubara space. Given our representation of the Green's function by Eq. (3.18), we can extend that the general transformation is

$$G(\mathbf{k}; i\omega_m) \equiv \int_0^{\hbar\beta} d(\tau - \tau') \int d^3x\, d^3x'\, G(\mathbf{x}, \tau; \mathbf{x}', \tau')\, \psi_{\mathbf{k}}(\mathbf{x}) \psi_{\mathbf{k}}^*(\mathbf{x}')\, \frac{e^{-i\omega_m(\tau - \tau')}}{\hbar\beta} \quad (3.47)$$

for the fully G and for $G^{(0)}$. As we are interested in the power-law trap, is convenient to treat the problem in a semi-classical overview. So we will make this transformation which, in general, is made in three steps: First, let us introduce the center of mass coordinate $\mathbf{X}$ and the relative coordinate $\Delta\mathbf{x}$ as

$$\Delta\mathbf{x} \equiv \mathbf{x} - \mathbf{x}' \quad (3.48)$$

so, using Eqs. (3.20) and (3.48), we may represent the coordinates $\mathbf{x}$ and $\mathbf{x}'$ as

$$\mathbf{x} = \mathbf{X} + \frac{\Delta\mathbf{x}}{2} \quad (3.49)$$

$$\mathbf{x}' = \mathbf{X} - \frac{\Delta\mathbf{x}}{2} \quad (3.50)$$

then the dependence of $G(\mathbf{x}, \tau; \mathbf{x}', \tau')$ is

$$G(\mathbf{x}, \tau; \mathbf{x}', \tau') = G\left(\mathbf{X} + \frac{\Delta\mathbf{x}}{2}, \tau; \mathbf{X} - \frac{\Delta\mathbf{x}}{2}, \tau'\right). \quad (3.51)$$

Second, we shall make a Fourier transform with respect to the relative coordinates where will go to the momentum space,

$$G(\mathbf{p}; \mathbf{X}, \Delta\tau) \equiv \int d^3\Delta x \, e^{-i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar} \, G\left(\mathbf{X} + \frac{\Delta\mathbf{x}}{2}, \tau; \mathbf{X} - \frac{\Delta\mathbf{x}}{2}, \tau'\right) . \tag{3.52}$$

Third, to do a transformation with respect to the Euclidean time, we have the Mastubara representation given in function of its Matsubara frequencies ω_m

$$G(\mathbf{p}, i\omega_m; \mathbf{X}) \equiv \int_0^{\hbar\beta} d\Delta\tau \, e^{i\omega_m\Delta\tau} \, G(\mathbf{p}; \mathbf{X}, \Delta\tau) , \tag{3.53}$$

where

$$\omega_m \equiv \frac{2\pi m}{\hbar\beta} \tag{3.54}$$

is the bosonic Matsubara frequencies. In Appendix A, we have the details of the formula for $G^{(0)}$ in Fourier-Matsubara space using the previous transformations. So, we have that

$$G^{(0)}(\mathbf{p}, i\omega_m; \mathbf{X}) = \frac{\hbar}{-i\hbar\omega_m + \frac{\mathbf{p}^2}{2M} + V(\mathbf{X}) - \hat{\mu}}. \tag{3.55}$$

But when we include the interactions in our calculations, this interacting Green's function is shifted by self-energies following [4]

$$G^{-1}(\mathbf{p}, i\omega_m; \mathbf{X}) = G^{(0)^{-1}}(\mathbf{p}, i\omega_m; \mathbf{X}) - \Sigma(\mathbf{p}, i\omega_m; \mathbf{X}) \tag{3.56}$$

then

$$G(\mathbf{p}, i\omega_m; \mathbf{X}) = \frac{\hbar}{-i\hbar\omega_m + \frac{\mathbf{p}^2}{2M} + V(\mathbf{X}) - \hat{\mu} - \hbar\Sigma(\mathbf{p}, i\omega_m; \mathbf{X})}. \tag{3.57}$$

Now we have that Green's function is written in a complex form and so we see that there are poles and these points are equivalent to the critical point, but this point has a physical meaning which is the situation where occurs the phase transition, then it cannot be complex, then we shall consider the Matsubara frequency equal to zero. Using this condition in Eq. (3.57),

$$G(\mathbf{p}, 0; \mathbf{X}) = \frac{\hbar}{\frac{\mathbf{p}^2}{2M} + V(\mathbf{X}) - \hat{\mu} - \hbar\Sigma(\mathbf{p}, 0; \mathbf{X})}. \tag{3.58}$$

The critical point occurs when $\mathbf{p} = \mathbf{0}$ and the reduced chemical potential $\hat{\mu}$ is calculated in the minimum with respect to the center of mass coordinate $\mathbf{X}$,

$$\hat{\mu}_c \equiv \min_{\mathbf{X}} \left(V(\mathbf{X}) - \hbar\Sigma(\mathbf{0}, 0; \mathbf{X})\right) \tag{3.59}$$

and clearly, when we have without interactions, the self-energy contribution is zero and we recover that $\hat{\mu}_c = \min_{\mathbf{X}} V(\mathbf{X})$. We can calculate the self-energies contributions joined to Eqs. (3.45) and (3.46) remembering that the Fourier transform of Σ follows Eq.(3.52) and (3.53)

$$\Sigma(\mathbf{p}, i\omega_m; \mathbf{X}) = \int_0^{\hbar\beta} d\Delta\tau \, e^{i\omega_m\Delta\tau} \int d^3\Delta\mathbf{x} \, e^{-i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar} \, \Sigma\left(\mathbf{X} + \frac{\Delta\mathbf{x}}{2}, \tau; \mathbf{X} - \frac{\Delta\mathbf{x}}{2}, \tau'\right) . \tag{3.60}$$

Solving these formulas for $\mathbf{p} = \mathbf{0}, \omega_m = 0$, using that the total self-energy contribution is equal to the sum of the Hartree and the Fock contribution, we obtain that

$$\Sigma(\mathbf{0}, 0; \mathbf{X}) = -\frac{2g}{\hbar} G^{(0)}(\mathbf{X}, \tau; \mathbf{X}, \tau). \tag{3.61}$$

By Eqs. (3.22), (2.33) in Eq. (3.61) and after, in Eq. (3.59), we will have that

$$\hat{\mu}_c = \hat{\mu}_c^{(0)} + \frac{2g}{\lambda_T^3} \zeta_{3/2}(\hat{z}) \tag{3.62}$$

and now, we have the critical point of an interacting Bose system. In the next subsection, we calculate the critical temperature and the condensed fraction.

There is another physical discussion from Eq. (3.58). First, let us remember its non-interacting version given by Eq. (3.56) which occurs when $\omega_m = 0$ has a term dependent on the single particle Hamiltonian $H^{(0)}[\mathbf{p}, \mathbf{X}]$. When we include the interaction, this Hamiltonian is shifted by one self-energy contribution

$$H[\mathbf{p}, \mathbf{X}] \equiv \frac{\mathbf{p}^2}{2M} + V(\mathbf{X}) - \hbar\Sigma(\mathbf{p}, 0; \mathbf{X}) \tag{3.63}$$

and therefore, their eigenvalues can be interpreted as interacting single-particle energies. This topic will discussed in Chapter 5 with details.

3.1.3 Critical temperature and condensed fraction

From Eq. (3.33), we can calculate the critical temperature, it occurs when $N_0^{(0)} = 0$, N is fixed, and $\hat{\mu} = \hat{\mu}_c$ given by Eq. (3.62). First, we shall compute the critical fugacity $\hat{z}$ and after, the expansion of this polylogarithm $\zeta_a(\hat{z})$,

$$\zeta_a(\hat{z}_c) = \sum_{n=1}^{\infty} \frac{1}{n^a} \exp\left[n\beta\left(\hat{\mu}_c^{(0)} + \frac{2g}{\lambda_0^3}\zeta(3/2)\right)\right], \tag{3.64}$$

where λ_0 is the thermal wavelength Eq. (3.23) calculated in the non-interacting critical temperature $T_c^{(0)}$

$$\zeta_a(\hat{z}_c) = \zeta(a) + \frac{2g\beta_c^{(0)}}{\lambda_0^3} \zeta(a-1)\,\zeta(3/2). \tag{3.65}$$

Now, inserting Eq. (3.65) in Eq. (3.33) with the conditions discussed previously such that the finite-size term and the fully perturbative contribution do not depend on the interacting contribution of the fugacity. So, with $T_c^{(0)}$, we can write the critical temperature for interacting systems in terms of non-interacting results. Dividing Eq. (3.33) by N with $N_0^{(0)} = 0$ inserting Eq. (3.65) with definitions given by Eqs. (2.51), (3.29), we have

$$1 = \left(\frac{T_c}{T_c^{(0)}}\right)^{\alpha} + \frac{2g\beta_c^{(0)}}{\lambda_{(0)}^3} \frac{\zeta(\alpha-1)\zeta(3/2)}{\zeta(\alpha)} \left(\frac{T_c}{T_c^{(0)}}\right)^{\alpha} \tag{3.66}$$

$$+ E_G\, \beta_c^{(0)} \frac{\zeta(\alpha-1)}{\zeta(\alpha)} \left(\frac{T_c}{T_c^{(0)}}\right)^{\alpha-1} \tag{3.67}$$

$$- \frac{g}{\beta_c^{(0)1/2}} \left(\frac{M}{2\pi\hbar^2}\right)^{3/2} \frac{\zeta(3/2, 3/2, \alpha-5/2)}{\zeta(\alpha)} \left(\frac{T_c}{T_c^{(0)}}\right)^{\alpha}. \tag{3.68}$$

The ratio $T_c/T_c^{(0)}$ is denoted by t_c, $g\beta_c^{(0)}$ is equal to $2a_s\lambda_{(0)}^2$ and last term of Eq. (3.68) can be written as $2a_s/\lambda_{(0)}^3$ (to see the definition of thermal wavelength). So,

$$1 = \left(1 + \frac{4a_s}{\zeta(\alpha)\lambda_{(0)}}\left[\zeta\left(\frac{3}{2}\right)\zeta(\alpha-1) - \zeta\left(\alpha - \frac{5}{2}, \frac{3}{2}, \frac{3}{2}\right)\right]\right)t_c^\alpha \tag{3.69}$$

$$+ E_G\,\beta_c^{(0)}\frac{\zeta(\alpha-1)}{\zeta(\alpha)}t_c^{\alpha-1} \tag{3.70}$$

$$t_c = 1 - \frac{E_G}{\alpha}\,\beta_c^{(0)}\frac{\zeta(\alpha-1)}{\zeta(\alpha)}t_c^{\alpha-1} + c\frac{a_s}{\lambda_0}\ , \tag{3.71}$$

where c is a numeric constant defined as

$$c \equiv \frac{4}{\alpha\zeta(\alpha)}\left[\zeta\left(\alpha - \frac{5}{2}, \frac{3}{2}, \frac{3}{2}\right) - \zeta\left(\frac{3}{2}\right)\zeta(\alpha-1)\right]. \tag{3.72}$$

The critical reduced temperature t_c is

$$t_c = \frac{T_c}{T_c^{(0)}} = 1 + \frac{\Delta T_c}{T_c^{(0)}}. \tag{3.73}$$

writing Eqs.(3.65) and (3.70) in finite-size term and Eq. (3.65) in Eq. (3.71), we have the shift of critical temperature caused by the interaction

$$\frac{\Delta T_c}{T_c^{(0)}} = -\frac{E_G}{\alpha}\,\beta_c^{(0)}\frac{\zeta(\alpha-1)}{\zeta(\alpha)} + c\frac{a_s}{\lambda_0}. \tag{3.74}$$

To verify this formula, let's consider the three-dimensional harmonic trap, the same one studied in Chapter 2. Remembering Eq. (2.62) in Eq. (3.74), with $\alpha = D = 3$,

$$\frac{\Delta T_c}{T_c^{(0)}} = -\frac{\zeta(2)\,\overline{\omega}}{2\,\tilde{\omega}\,N^{1/3}\,\zeta^{2/3}(3)} + c\frac{a_s}{\lambda_0}. \tag{3.75}$$

where

$$c = \frac{4}{3\,\zeta(3)}\left[\zeta\left(\frac{1}{2}, \frac{3}{2}, \frac{3}{2}\right) - \zeta(2)\,\zeta(3/2)\right] \approx -3.427 \tag{3.76}$$

and therefore, we have the same result obtained in [35,42]. For a weakly homogeneous trap, $\alpha = 3/2$ and therefore, the constant c is equal to $8\zeta(1/2)/3$ and our temperature shift will be positive and given by

$$\frac{\Delta T_c}{T_c^{(0)}} = -\frac{8\zeta(1/2)}{3}\frac{a_s}{\lambda_0}\ , \tag{3.77}$$

that is the same obtained in [44].

Now we discuss the influence of the trap geometry in the critical temperature value due to interactions. The interacting correction is the last term of Eq. (3.74) denoted here by $\left(\Delta T_c/T_c^{(0)}\right)_{\text{int}}$,

$$\left(\frac{\Delta T_c}{T_c^{(0)}}\right)_{\text{int}} = \frac{4}{\alpha\zeta(\alpha)}\left[\zeta\left(\alpha - \frac{5}{2}, \frac{3}{2}, \frac{3}{2}\right) - \zeta\left(\frac{3}{2}\right)\zeta(\alpha-1)\right]\frac{a_s}{\lambda_0}\ . \tag{3.78}$$

As seen in this previous equation, its contribution depends on the parameter α which is given by Eq. (2.45) with $D = 3$. The result is a function of the Riemann zeta function, we shall see the points where this function diverges and when it occurs, we do not consider its contribution in Eq. (3.78).

The divergence is when we have $\zeta(1)$ and the multiple zeta functions have a negative argument, that is, these conditions may occur for two Riemann functions in our constant c: $\zeta(\alpha - 1)$ and $\zeta(\alpha - 5/2, 3/2, 3/2)$. The first quantity has two conditions: when $3/2 \leq \alpha < 2$, $\zeta(\alpha - 1) < 0$ and for $\alpha > 2$, $\zeta(\alpha - 1) > 0$ - for $\alpha = 2$, $\zeta(\alpha - 1) = \zeta(1)$ and it contribution is zero. On the other hand, for $\alpha < 5/2$, $\zeta(\alpha - 5/2, 3/2, 3/2)$ diverges and it does not contribute in Eq.(3.78), but for $\alpha \geq 5/2$, $\zeta(\alpha - 5/2, 3/2, 3/2) > 0$ such that it value is less than $\zeta(3/2)\zeta(\alpha - 1)$.

Therefore, we have two behaviors: when $3/2 \leq \alpha \leq 2$, the critical temperature increases, and for $\alpha > 2$, the critical temperature decreases. Then remembering that α depends on $1/a_i$ power of our external potential Eq. (2.24), we see that the harmonic confinement $\alpha = 3$ will have a negative shift but when the power increases, α decreases and the homogeneous trap $\alpha = 3/2$ has a positive shift.

Usually, the finite-size correction of critical temperature is represented in terms of N because its effects are important for low values of N but this contribution is in $\beta_c^{(0)}$. The calculation of condensed fraction $N_0^{(0)}/N$ is similar to the one done in the critical temperature case. When we compute the condensed properties, $T < T_c$, the fugacity is fixed by its polylogarithm expansion Eq. (3.65). To simplify our calculations, we know that the process of calculating the critical temperature and condensed fraction is similar, so let's use some previous results to obtain $N_0^{(0)}/N$. Then,

$$1 = \frac{N_0^{(0)}}{N} + \frac{\eta}{\beta^\alpha N}\zeta_\alpha(\hat{z}_c) + \frac{\eta E_G}{\beta^{\alpha-1}N}\zeta_{\alpha-1}(\hat{z}_c) - \frac{\xi}{N\beta^{\alpha+1/2}}\zeta_{3/2,3/2,\alpha-5/2}(\hat{z}_c)\,. \qquad (3.79)$$

As discussed in the previous section, the critical temperature T_c is shifted by perturbation contribution and finite-size corrections for finite traps, and usually, the condensed fraction is written in terms of T/T_c ratio because in function this is easier to find the discontinuity of heat capacity and of other thermodynamic quantities. Here, for simplicity, let us write it equation with $T/T_c^{(0)}$ besides this consideration implies in our plots. Using Eq. (3.65) in Eq. (3.74), we have

$$1 = \frac{N_0^{(0)}}{N} + \frac{\eta}{\beta^\alpha N}\left(\zeta(\alpha) + \frac{2g\beta_0}{\lambda_{T_0}^3}\zeta(3/2)\zeta(\alpha-1)\right) + \frac{\eta E_G}{\beta^{\alpha-1}N}\zeta(\alpha-1) \qquad (3.80)$$

$$- \frac{\xi}{N\beta^{\alpha+1/2}}\zeta(3/2, 3/2, \alpha - 5/2) \qquad (3.81)$$

and inserting Eq. (3.61) in Eq. (3.81),

$$1 = \frac{N_0^{(0)}}{N} + t^\alpha\left(1 + \frac{4a_s}{\lambda_{T_0}}\frac{\zeta(3/2)\zeta(\alpha-1)}{\zeta(\alpha)}\right)t^\alpha + \frac{\eta E_G}{\beta^{\alpha-1}N}\zeta(\alpha-1) \qquad (3.82)$$

$$- \frac{\xi}{N\beta^{\alpha+1/2}}\zeta(3/2, 3/2, \alpha - 5/2) \qquad (3.83)$$

for ξ expression we can write it in function of η and so, is possible to simplify our formula for $N_0^{(0)}/N$. By Eqs. (3.29) and (2.51), we have

$$\xi = g \left(\frac{M}{2\pi\hbar^2} \right)^{3/2} \eta \tag{3.84}$$

and therefore,

$$1 = \frac{N_0^{(0)}}{N} + \left(1 + \frac{4a_s}{\lambda_{T_0}} \frac{\zeta(3/2)\zeta(\alpha-1)}{\zeta(\alpha)} \right) t^\alpha + E_G \beta_c^{(0)} \frac{\zeta(\alpha-1)}{\zeta(\alpha)} t^{\alpha-1} \tag{3.85}$$

$$- \frac{1}{\beta^{\alpha+3/2}} g \left(\frac{M}{2\pi\hbar^2} \right)^{3/2} \frac{\zeta(3/2, 3/2, \alpha-5/2)}{\zeta(\alpha)} \tag{3.86}$$

$$1 = \frac{N_0^{(0)}}{N} + \left(1 + \frac{4a_s}{\lambda_{T_0}} \frac{\zeta(3/2)\zeta(\alpha-1)}{\zeta(\alpha)} \right) t^\alpha + E_G \beta_c^{(0)} \frac{\zeta(\alpha-1)}{\zeta(\alpha)} t^{\alpha-1} \tag{3.87}$$

$$- \frac{1}{\beta_{(0)}^{\alpha+3/2}} g \left(\frac{M}{2\pi\hbar^2} \right)^{3/2} \frac{\zeta(3/2, 3/2, \alpha-5/2)}{\zeta(\alpha)} t^\alpha, \tag{3.88}$$

and looking that

$$\frac{1}{\beta_{(0)}^{\alpha+1/2}} g \left(\frac{M}{2\pi\hbar^2} \right)^{3/2} = \frac{4a_s}{\lambda_0 \, \beta_0^\alpha}, \tag{3.89}$$

we have the condensed fraction of a weakly interacting power-law trap

$$\frac{N_0^{(0)}}{N} = 1 - \left(1 + \frac{4a_s}{\lambda_{T_0}} \frac{\zeta(3/2)\zeta(\alpha-1)}{\zeta(\alpha)} \right) t^\alpha - E_G \beta_c^{(0)} \frac{\zeta(\alpha-1)}{\zeta(\alpha)} t^{\alpha-1} \tag{3.90}$$

$$+ \frac{4\,a_s}{\lambda_0 \, \beta_0^\alpha} \frac{\zeta(3/2, 3/2, \alpha-5/2)}{\zeta(\alpha)} t^\alpha. \tag{3.91}$$

Doing the same representation made in a non-interacting case, let us put Eq. (3.91) as a function of T/T_c. So,

$$\frac{N_0^{(0)}}{N} = 1 - \left(1 + \frac{4a_s}{\lambda_{T_0}} \frac{\zeta(3/2)\zeta(\alpha-1)}{\zeta(\alpha)} \right) \left(\frac{T}{T_c} \right)^\alpha \left(1 + \alpha \frac{\Delta T_c}{T_c^{(0)}} \right)$$

$$- \beta_c^{(0)} E_G \frac{\zeta(\alpha-1)}{\zeta(\alpha)} \left(\frac{T}{T_c} \right)^{\alpha-1} \left(1 + (\alpha-1) \frac{\Delta T_c}{T_c^{(0)}} \right)$$

$$+ \frac{4\,a_s}{\lambda_0 \, \beta_c^{(0)\alpha}} \frac{\zeta(3/2, 3/2, \alpha-5/2)}{\zeta(\alpha)} \left(\frac{T}{T_c} \right)^\alpha \left(1 + \left(\alpha + \frac{1}{2} \right) \frac{\Delta T_c}{T_c^{(0)}} \right). \tag{3.92}$$

Finally, inserting Eq. (3.74) in Eq. (3.92) with the condition that the terms with $a_s E_G$, E_G^2 and a_s^2 are not considered , we have that

$$\frac{N_0^{(0)}}{N} = 1 - \left(\frac{T}{T_c} \right)^\alpha \left[1 - \beta_c^{(0)} E_G \frac{\zeta(\alpha-1)}{\zeta(\alpha)} - \frac{\alpha \, c \, a_s}{\lambda_0} \right] - \beta_c^{(0)} E_G \frac{\zeta(\alpha-1)}{\zeta(\alpha)} \left(\frac{T}{T_c} \right)^{\alpha-1}, \tag{3.93}$$

where c is given by Eq. (3.72). This result is for a general power-law trap. To check this result, let us see the limit for the three-dimensional harmonic trap that occurs when $\alpha = 3$. Then substituting Eq. (2.62) for the non-interacting critical temperature and Eq. (2.67) for the ground-state energy, we have that

$$\frac{N_0^{(0)}}{N} = 1 - \left(\frac{T}{T_c}\right)^3 \left[1 - \frac{3\zeta(2)\,\overline{\omega}}{2\,\tilde{\omega}\,N^{1/3}\,\zeta^{2/3}(3)} - \frac{3\,c\,a_s}{\lambda_0}\right] - \frac{3\zeta(2)\,\overline{\omega}}{2\,\tilde{\omega}\,N^{1/3}\,\zeta^{2/3}(3)}\left(\frac{T}{T_c}\right)^2 ,$$

(3.94)

and this result is the same as obtained in [34,41] and when $a_s = 0$, we recover our non-interacting result given by Eq. (2.75). In fact, the inclusion of the interactions decreases the condensed fraction plot with respect to the non-interacting formula, and we recover this idea. To see better the behavior of the condensed fraction, we have a plot for the three-dimensional isotropic harmonic trap given by Fig. 3.5. The constant c is negative in this case and therefore, the interacting contribution is greater than 1, so, this plot is less than the non-interacting plot. Following this same study, we can see the interaction influence in the box trap. For this, we consider the thermodynamic limit of this confinement which is the Eq. (3.93) without ground-state contributions. For the box, we have that $\alpha = 3/2$, therefore, inserting this condition in Eq. (3.93), we obtain

$$\frac{N_0^{(0)}}{N} = 1 - \left[1 - \frac{3\,c\,a_s}{2\,\lambda_0}\right]\left(\frac{T}{T_c}\right)^{3/2} ,$$

(3.95)

whose plot is in Fig. 3.6. Here, the interaction increases the critical temperature, while in the harmonic trap, it decreases with respect to the thermodynamic limit result. In both cases, we did the plots for Rubidium 87 as an example to see the behavior of the condensate fraction which is the most important of condensate properties. Another interesting point is that the perturbative contribution does not depend on the number of particles, that is, the finite-size term is independent of the interaction. The behavior of the plots is different for the traps: while the harmonic trap the plot is less than the non-interacting curve following the critical temperature value, the homogenous box is the inverse.

3.1.4   Internal energy and heat capacity

The most important quantities in the statistical mechanics of the Bose gas are the critical temperature and the condensed fraction. But there are other important quantities in the thermodynamic characterization which are the internal energy and the heat capacity. We know that in high temperatures, the heat capacity converges to the Dulong-Petit law. The calculations for the non-interacting case were performed in Chapter 2 with a general dimension D; for our interacting case we have the same idea but now the critical fugacity is shifted by interacting contributions, for the general terms, we have the fully perturbative contribution. Here, we calculated the heat capacity specially for the condensed state because in this state we have the maximum point, and consequently, we can compare this behavior with the canonical plots done in Chapter 5.

Then, let us start with the calculation of the internal energy U following the same formulas developed in Chapter 2. Starting with Eq. (2.82) but now we have that $\mathcal{F}^{(0)}$ is
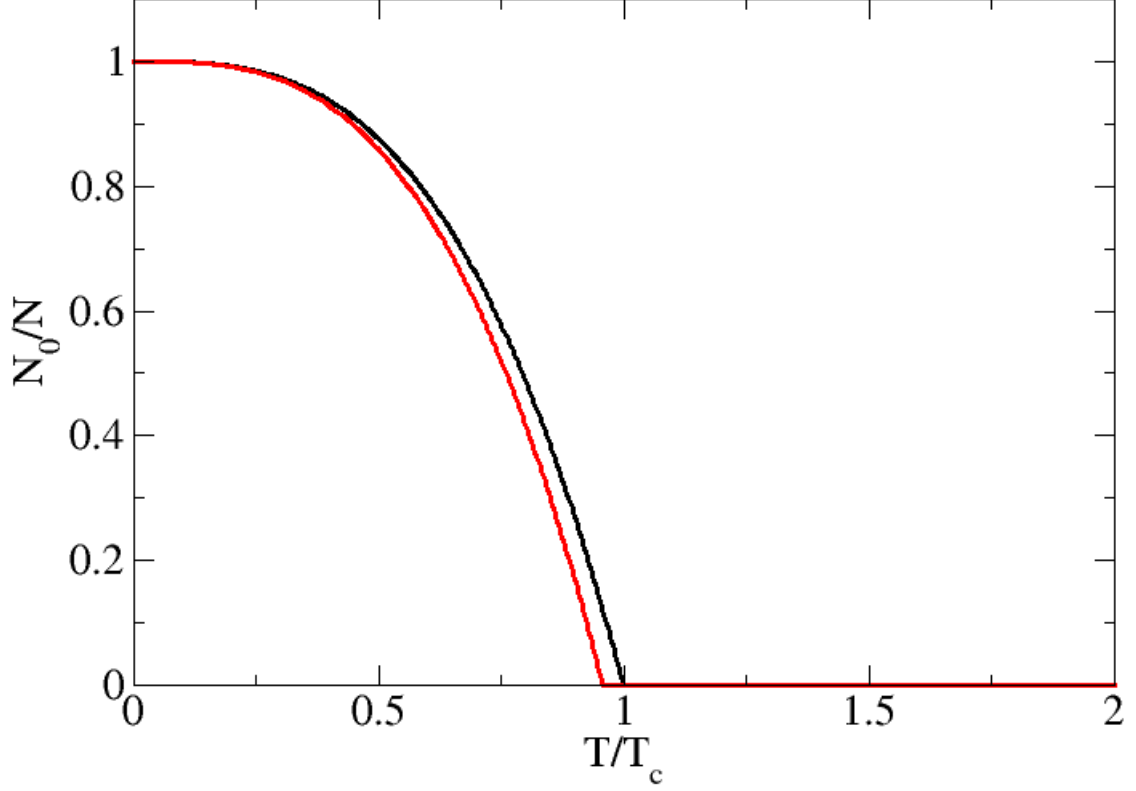
Figure 3.5: Condensate fraction of the isotropic three-dimensional harmonic trap in the thermodynamic limit. The black line corresponds to the non-interacting curve while the red line is the interacting plot - here we have that the interaction decreases the curve behavior, following the prevision given by the critical temperature calculation.

now $\mathcal{F}$ given by Eq. (3.32). We are interested in the calculations of the condensed state $(T \leq T_c)$ - then in this case, by Eq. (3.33), the number of particles is fixed by this equation in the critical temperature point. Besides, the fugacity is equal to the critical fugacity polylnarithm expansion Eq. (3.65) and $N_0^{(0)} = \mathcal{F}_0^{(0)} = 0$. Then, first doing the derivative of Eq. (3.32) in Eq. (2.82), we have that

$$
U(T < T_c) = -\eta \zeta_{\alpha+1}(\hat{z}_c)\beta^{-\alpha-1} - \eta E_G \zeta_\alpha(\hat{z}_c)\beta^{-\alpha} + g \left(\frac{M}{2\pi\hbar^2} \right)^{3/2} \eta \, \zeta \left(\frac{3}{2}, \frac{3}{2}, \alpha - \frac{3}{2} \right) \beta^{-\alpha-3/2} ,
$$
$$(3.96)$$

where ξ was substituted by $g(M/2\pi\hbar^2)^{3/2}\eta$. However, the second step, that is the calculation of the heat capacity, we have that the derivative must be done with N constant. Then, this situation is solved by substituting η from Eq. (3.33) with $\beta = \beta_c$.
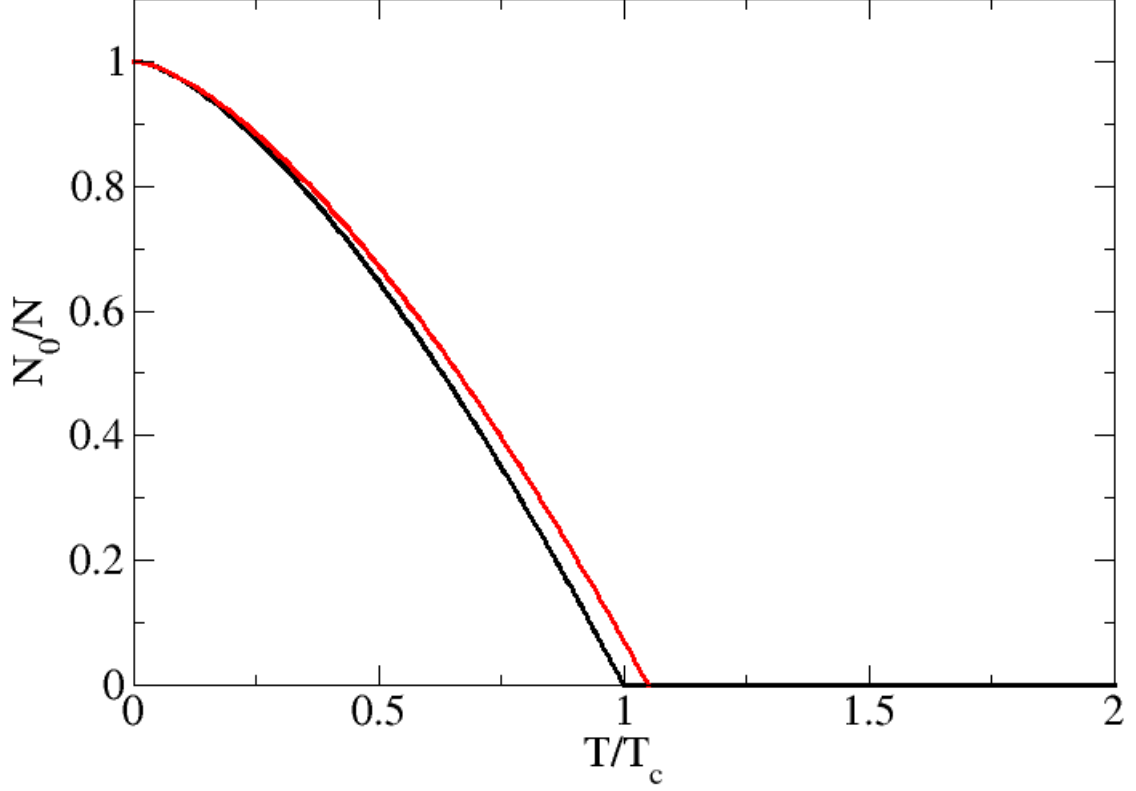
Figure 3.6: Condensate fraction of the isotropic three-dimensional finite box in the thermodynamic limit. The black line corresponds to the non-interacting curve while the red line is the interacting plot - here we have that the interaction decreases the curve behavior, following the prevision given by the critical temperature calculation.

So, we have that

$$\eta = \frac{N\beta_c^\alpha}{\zeta_\alpha(\hat{z}_c)} \left[1 - \beta_c\, E_G \frac{\zeta_{\alpha-1}(\hat{z}_c)}{\zeta_\alpha(\hat{z}_c)} + \frac{g}{\beta_c^{1/2}} \left(\frac{M}{2\pi\hbar^2} \right)^{3/2} \frac{\zeta\left(\frac{3}{2},\frac{3}{2},\alpha-\frac{5}{2}\right)}{\zeta_\alpha(\hat{z}_c)} \right] . \tag{3.97}$$

For simplicity, Eq. (3.96) can be written as

$$U(T < T_c) = U_1(T < T_c) + U_2(T < T_c) + U_3(T < T_c) , \tag{3.98}$$

where

$$U_1(T < T_c) = N\, k_B\, \beta_c^\alpha\, \beta^{-\alpha-1} \frac{\zeta_{\alpha+1}(\hat{z}_c)}{\zeta_\alpha(\hat{z}_c)} \left[1 - \beta_c\, E_G \frac{\zeta_{\alpha-1}(\hat{z}_c)}{\zeta_\alpha(\hat{z}_c)} + \frac{g}{\beta_c^{1/2}} \left(\frac{M}{2\pi\hbar^2} \right)^{3/2} \frac{\zeta\left(\frac{3}{2},\frac{3}{2},\alpha-\frac{5}{2}\right)}{\zeta_\alpha(\hat{z}_c)} \right] ,$$
$$\tag{3.99}$$

$$U_2(T < T_c) = N\, E_G\, (\alpha - 1) \left(\frac{T}{T_c} \right)^\alpha , \tag{3.100}$$

and

$$U_3(T < T_c) = -N\,\beta_c^\alpha\, g\left(\frac{M}{2\pi\hbar^2}\right)^{3/2}\frac{\zeta\left(\frac{3}{2},\frac{3}{2},\alpha-\frac{3}{2}\right)}{\zeta_\alpha(\hat{z}_c)}\left(\alpha+\frac{1}{2}\right)\beta^{-\alpha-3/2}\,. \qquad (3.101)$$

Now, we can calculate the heat capacity by Eq. (2.83) for each decomposition of $U(T \le T_c)$ such that

$$C(T < T_c) = C_1(T < T_c) + C_2(T < T_c) + C_3(T < T_c)\,, \qquad (3.102)$$

where,

$$C_1(T < T_c) = N\,k_B\,\alpha(\alpha+1)\frac{\zeta_{\alpha+1}(\hat{z}_c)}{\zeta_\alpha(\hat{z}_c)}\left(\frac{T}{T_c}\right)^\alpha\left[1-\beta_c\,E_G\frac{\zeta_{\alpha-1}(\hat{z}_c)}{\zeta_\alpha(\hat{z}_c)}+\frac{g}{\beta_c^{1/2}}\left(\frac{M}{2\pi\hbar^2}\right)^{3/2}\frac{\zeta\left(\frac{3}{2},\frac{3}{2},\alpha-\frac{5}{2}\right)}{\zeta_\alpha(\hat{z}_c)}\right],$$
$$(3.103)$$

$$C_2(T < T_c) = N\,k_B\,\alpha(\alpha-1)\,E_G\,\beta_c\left(\frac{T}{T_c}\right)^{\alpha-1}\,, \qquad (3.104)$$

$$C_3(T < T_c) = -N\,k_B\left(\alpha+\frac{1}{2}\right)\left(\alpha+\frac{3}{2}\right)\frac{g}{\beta_c^{1/2}}\left(\frac{M}{2\pi\hbar^2}\right)^{3/2}\frac{\zeta\left(\frac{3}{2},\frac{3}{2},\alpha-\frac{3}{2}\right)}{\zeta_\alpha(\hat{z}_c)}\left(\frac{T}{T_c}\right)^{\alpha+1/2}\,.$$
$$(3.105)$$

Now, the polylogarithm function in the critical point follows Eq. (3.65), and here as this expansion has two contributions, we have that to discard the terms that depend on $a_s E_G, E_G^2, a_s^2$.

To see the behavior of the heat capacity in the condensate phase, we study the two traps studied in the non-interacting case which are the harmonic trap and the finite box. By Eqs. (3.103), (3.104) and (3.105), we have that their only depend of α and the interaction parameter g.

Starting with the three-dimensional harmonic trap, that is, when $\alpha = 3$, we obtain that

$$C_{\max} = 12\,N\,k_B\,\frac{\zeta_4(\hat{z}_c)}{\zeta_3(\hat{z}_c)}\left[1-\beta_c\,E_G\frac{\zeta_2(\hat{z}_c)}{\zeta_3(\hat{z}_c)}+\frac{g}{\beta_c^{1/2}}\left(\frac{M}{2\pi\hbar^2}\right)^{3/2}\frac{\zeta\left(\frac{3}{2},\frac{3}{2},\frac{1}{2}\right)}{\zeta_3(\hat{z}_c)}\right]+6\,N\,k_B\,E_G\,\beta_c$$
$$-\frac{63}{4}\,N\,k_B\,\frac{g}{\beta_c^{1/2}}\left(\frac{M}{2\pi\hbar^2}\right)^{3/2}\frac{\zeta\left(\frac{3}{2},\frac{3}{2},\frac{3}{2}\right)}{\zeta_3(\hat{z}_c)}\,, \qquad (3.106)$$

and using Eq. (3.89), Eq. (3.106) becomes

$$C_{\max} = 12\,N\,k_B\,\frac{\zeta_4(\hat{z}_c)}{\zeta_3(\hat{z}_c)}\left[1-\beta_c\,E_G\frac{\zeta_2(\hat{z}_c)}{\zeta_3(\hat{z}_c)}+\frac{4a_s}{\lambda_0}\frac{\zeta\left(\frac{3}{2},\frac{3}{2},\frac{1}{2}\right)}{\zeta_3(\hat{z}_c)}\right]+6\,N\,k_B\,E_G\,\beta_c$$
$$-63\,N\,k_B\,\frac{a_s}{\lambda_0}\frac{\zeta\left(\frac{3}{2},\frac{3}{2},\frac{3}{2}\right)}{\zeta_3(\hat{z}_c)}\,. \qquad (3.107)$$

To compare its value with the non-interacting result given by Eq. (2.100) in the critical point when $T/T_c = 1$,

$$C_{\max}^{(0)} = N\,k_B\left[12\,\frac{\zeta(4)}{\zeta(3)}+6\,E_G\,\beta_c^{(0)}\right]\,, \qquad (3.108)$$

and is clear that Eq. (3.108) is less than Eq. (3.107). Therefore, the inclusion of the interaction increases the maximum point of the heat capacity. Now, let us see the box case looking only at perturbative contribution, thus now $\alpha = 3/2$. When we have this value for α, the last term in Eq. (3.103) does not contribute due to its divergence, therefore,

$$C_{\max} = N\,k_B \frac{15}{4} \frac{\zeta_{5/2}(\hat{z}_c)}{\zeta_{3/2}(\hat{z}_c)} - 24\,N\,k_B \frac{a_s}{\lambda_0} \frac{\zeta\left(\frac{3}{2},\frac{3}{2},0\right)}{\zeta_{3/2}(\hat{z}_c)}\,, \tag{3.109}$$

and clearly, this result is less than the homogeneous case which is given by

$$C_{\max}^{(0)} = N\,k_B \frac{15}{4} \frac{\zeta(5/2)}{\zeta(3/2)}\,. \tag{3.110}$$

When we studied the normal phase $(T > T_c)$, for high temperatures, shall have the Dulong-Petit limit as seen in the non-interacting case. As in the normal phase, the fugacity is different from the critical point, then the polylogarithm derivatives to β and $\hat{z}$ must be considered. Then in this case, we shall write this observable following the same procedure done in the non-interacting calculation Eq. (2.84). Here, we have the the internal energy is given by

$$U(T > T_c) = \alpha\eta\,\zeta_{\alpha+1}(\hat{z})\beta^{-\alpha-1} + \eta E_G(\alpha-1)\zeta_\alpha(\hat{z})\beta^{-\alpha} - \xi\left(\alpha + \frac{1}{2}\right)\beta^{-\alpha-3/2}\zeta_{3/2,3/2,\alpha-3/2}(\hat{z})\,, \tag{3.111}$$

and the number of particles N

$$N = \frac{\eta}{\beta^\alpha}\left[\zeta_\alpha(\hat{z}) + \beta E_G \zeta_{\alpha-1}(\hat{z})\right] - \frac{\xi}{\beta^{\alpha+1/2}}\zeta_{3/2,3/2,\alpha-5/2}(\hat{z})\,. \tag{3.112}$$

Applying the Jacobian technique to calculate the heat capacity as done in Eq. (2.84), we obtain that

$$\left(\frac{\partial U}{\partial \beta}\right)_{\hat{z}} = -\alpha(\alpha+1)\eta\,\zeta_{\alpha+1}(\hat{z})\beta^{-\alpha-2} - \alpha(\alpha-1)\eta E_G\,\zeta_\alpha(\hat{z})\beta^{-\alpha-1} + \xi\left(\alpha + \frac{3}{2}\right)\left(\alpha + \frac{1}{2}\right)\beta^{\alpha-5/2}\zeta_{3/2,3/2,\alpha-3/2}(\hat{z}) \tag{3.113}$$

$$\left(\frac{\partial N}{\partial \beta}\right)_{\hat{z}} = -\alpha\eta\beta^{-\alpha-1}\zeta_\alpha(\hat{z}) - \eta E_G\zeta_{\alpha-1}(\hat{z})(1-\alpha)\beta^{-\alpha} + \xi\left(\alpha + \frac{1}{2}\right)\zeta_{3/2,3/2,\alpha-5/2}(\hat{z})\,, \tag{3.114}$$

$$\left(\frac{\partial U}{\partial \hat{z}}\right)_\beta = \alpha\eta\beta^{-\alpha-1}\frac{1}{\hat{z}} + (\alpha-1)\eta E_G\frac{\beta^{-\alpha}}{\hat{z}}\zeta_{\alpha-1}(\hat{z}) - \xi\left(\alpha + \frac{1}{2}\right)\frac{\beta^{-\alpha-3/2}}{\hat{z}}\zeta_{3/2,3/2,\alpha-5/2}(\hat{z})\,, \tag{3.115}$$

$$\left(\frac{\partial N}{\partial \hat{z}}\right)_\beta = \eta\frac{\beta^{-\alpha}}{\hat{z}}\zeta_{\alpha-1}(\hat{z}) + \eta E_G\frac{\beta^{1-\alpha}}{\hat{z}}\zeta_{\alpha-2}(\hat{z}) - \frac{\xi}{\beta^{\alpha+1/2}\hat{z}}\zeta_{3/2,3/2,\alpha-7/2}(\hat{z})\,. \tag{3.116}$$

Now including Eqs. (3.113), (3.114), (3.115) and (3.116) in Eq. (2.83), we obtain that

$$\frac{C(T > T_c)}{Nk_B} = \left[\alpha(\alpha+1)\frac{\zeta_{\alpha+1}(\hat{z})}{\zeta_\alpha(\hat{z})} - \alpha^2\frac{\zeta_\alpha(\hat{z})}{\zeta_{\alpha-1}(\hat{z})}\right]\left[1 + \frac{\xi}{\eta}\beta^{-1/2}\frac{\zeta_{3/2,3/2,\alpha-5/2}(\hat{z})}{\zeta_\alpha(\hat{z})} - \beta E_G\frac{\zeta_{\alpha-1}(\hat{z})}{\zeta_\alpha(\hat{z})}\right]$$

$$+ \alpha(\alpha-1)\beta E_G - \frac{\xi}{\eta}\left(\alpha + \frac{3}{2}\right)\left(\alpha + \frac{1}{2}\right)\beta^{-1/2}\frac{\zeta_{3/2,3/2,\alpha-3/2}(\hat{z})}{\zeta_\alpha(\hat{z})}$$

$$- \alpha\beta^2 E_G\frac{\zeta_{\alpha-2}(\hat{z})}{\zeta_{\alpha-1}(\hat{z})} + \alpha\frac{\xi}{\eta}\beta^{1/2}\frac{\zeta_{3/2,3/2,\alpha-7/2}(\hat{z})}{\zeta_{\alpha-1}(\hat{z})} - 2\alpha\frac{\xi}{\eta}\beta^{1/2}\frac{\zeta_{3/2,3/2,\alpha-5/2}(\hat{z})}{\zeta_{\alpha-1}(\hat{z})}\,. \tag{3.117}$$

When we do not have interactions, this equation returns to the non-interacting result given by Eq. (2.101). Finally, checking the limit for the high temperature limit, $T \to \infty$, we have that

$$C(T \to \infty) = N\, k_B\, \alpha \,, \tag{3.118}$$

that is the Dulong-Petit law. Therefore, the inclusion of the interactions increases the maximum point of heat capacity for the harmonic trap and decreases for the finite box; moreover the classical limit is satisfied for high temperatures. The interesting here is that we have a semiclassical description of dilute Bose gases in the power law trap. Therefore, in a semiclassical description of the weakly interacting power law trap, the main thermodynamic properties are modified due to interactions but the magnitude of this modification depends of the size of the trap power. As these observables are functions of the polylogarithms and Riemann zeta functions, there are values where these functions diverge, is positive or negative, and this discussion was done with details in the section about the critical temperature, and this situation is reproduced in other quantities, as the condensed fraction and the heat capacity.

Chapter 4

Non-interacting canonical ensemble

The canonical ensemble consists of a statistical distribution in which the number of particles is fixed; besides the system exchanges heat with a bath reservoir at a fixed temperature T. But in general experiments with magnetic and optical traps, the system can be described theoretically using the canonical ensemble of a form more consistent compared with the grand canonical results, however, in the thermodynamic limit, these two ensembles are equivalent as shown in [13]. In this chapter, we present a recursive canonical theory for non-interacting Bose gas which was studied previously in [14, 15, 45] using different approaches: in [14, 45] used the classical counting statistics while in [15] by cycle decomposition.

First, we did the calculations to build a recursive non-interacting canonical theory using as a starting point, the grand canonical result developed in Chapter 2. After following [15, 36, 39], we connected these two ensembles to find the recursive formula for the N-particle partition function $Z_N(\beta)$. So, with the $Z_N(\beta)$-equation, we calculated the canonical probability and its moments: first which has a relation with the condensed fraction, and the second, with the ground-state fluctuations and to finalize, the other thermodynamic quantities: entropy, internal energy and heat capacity. As an application, we studied the homogeneous case, the gas confined in a three dimensional box, and in a harmonic trap.

4.1   Non-interacting canonical description

Our starting point is equation (2.17). It corresponds to grand canonical free energy for a non-interacting system, but as we want the partition function, let's use the connection between free energy and partition function, and so

$$\ln \Xi^{(0)} = -\sum_{\mathbf{k}} \ln \left(1 - e^{-\beta(E_{\mathbf{k}} - \mu)}\right). \tag{4.1}$$

To write a formula of $\Xi^{(0)}$ we shall expand the term which depends of quantum numbers $\mathbf{k}$ in a power series,

$$\ln \Xi^{(0)} = \sum_{n=1}^{\infty} \frac{z^n}{n} \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}} \tag{4.2}$$

then,

$$\Xi^{(0)} = \exp\left(\sum_{n=1}^{\infty} \frac{z^n}{n} \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}}\right). \qquad (4.3)$$

The summation over quantum numbers is a term that is very similar to a single particle partition function in the canonical ensemble by classical theory. The physical interpretation of this term is a single-particle partition function with total energy equal to n times single particle energy $E_{\mathbf{k}}$, therefore it term is denoted by $Z_1(n\beta)$,

$$Z_1(n\beta) \equiv \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}} \qquad (4.4)$$

hence, (4.3) becomes

$$\Xi^{(0)} = \exp\left(\sum_{n=1}^{\infty} \frac{z^n Z_1(n\beta)}{n}\right). \qquad (4.5)$$

The details about the development of this equation are in chapter 2 then here these passages were not shown. We are in a grand canonical ensemble yet, to build a canonical result must remember the connection between these two approaches[1]

$$\Xi^{(0)}(\beta, z) = \sum_{N=0}^{\infty} Z_N^B(\beta) z^N \qquad (4.6)$$

where B denotes a bosonic system throughout the dissertation. Here we follow [15], by Eq. (4.6), the N-particle partition function is a coefficient of fugacity series and it value can be calculated by equation

$$Z_N^B(\beta) = \frac{1}{N!} \left.\frac{\partial^N \Xi^{(0)}(\beta, z)}{\partial z^N}\right|_{z=0} \qquad (4.7)$$

and the N-th derivative of $\Xi^{(0)}$ involves chain rule and generalized Leibniz rule. In fact, by equation (4.5), the first derivative is given by

$$\frac{\partial \Xi^{(0)}}{\partial z} = \Xi^{(0)} \sum_{n=1}^{\infty} Z_1(n\beta) z^{n-1}, \qquad (4.8)$$

now we have a product of two functions and here will use the general Leibniz rule,

$$\frac{\partial^n}{\partial x^n}[f(x)g(x)] = \sum_{k=0}^{n} \frac{n!}{(n-k)!k!} \frac{\partial^{(n-k)} f(x)}{\partial x^{n-k}} \frac{\partial^k g(x)}{\partial x^k}. \qquad (4.9)$$

Using Eq. (4.9) in Eq. (4.8), we have that

$$\left.\frac{\partial^N \Xi^{(0)}}{\partial z^N}\right|_{z=0} = \sum_{k=0}^{N-1} \frac{(N-1)!}{(N-k-1)!k!} \left.\frac{\partial^{(N-1-k)} \Xi^{(0)}}{\partial z^{N-k-1}}\right|_{z=0} \left.\frac{\partial^k}{\partial z^k} \sum_{n=1}^{\infty} Z_1(n\beta) z^{n-1}\right|_{z=0} \qquad (4.10)$$

$$\left.\frac{\partial^N \Xi^{(0)}}{\partial z^N}\right|_{z=0} = \sum_{k=1}^{N} \frac{(N-1)!}{(N-k)!(k-1)!} \left.\frac{\partial^{(N-k)} \Xi^{(0)}}{\partial z^{N-k}}\right|_{z=0} \sum_{n=1}^{\infty} Z_1(n\beta) \left.\frac{\partial^k}{\partial z^k} z^{n-1}\right|_{z=0} \qquad (4.11)$$

---

[1]See, for instance, Ref. [37], p.178.

but

$$\left.\frac{\partial^k z^{n-1}}{\partial z^k}\right|_{z=0} = (n-1)!\,\delta_{n,k} \tag{4.12}$$

then inserting Eq. (4.12) in Eq. (4.11),

$$\left.\frac{\partial^N \Xi^{(0)}}{\partial z^N}\right|_{z=0} = \sum_{n=1}^{N} \frac{(N-1)!}{(N-n)!} \left.\frac{\partial^{(N-n)}\Xi^{(0)}}{\partial z^{N-n}}\right|_{z=0} Z_1(n\beta) \tag{4.13}$$

however by Eq. (4.7) definition,

$$\frac{1}{(N-n)!} \left.\frac{\partial^{(N-n)}\Xi^{(0)}}{\partial z^{N-n}}\right|_{z=0} = Z^B_{N-n}(\beta) \tag{4.14}$$

Therefore, putting Eq. (4.14) in Eq. (4.13) and after in (4.7), $Z^B_N(\beta)$ can be written in a recursive form,

$$Z^B_N(\beta) = \frac{1}{N} \sum_{n=1}^{N} Z_1(n\beta)\, Z^B_{N-n}(\beta). \tag{4.15}$$

This equation is the center of our theory and it is the same result obtained in [14, 15]. With it, we can calculate all thermodynamic quantities using the classical formulas of connection between the canonical approach and thermodynamics. But the two main quantities which are condensed fraction and ground-state fluctuations may be calculated using the general formula of canonical probability and we will see that these variables are also functions of Z^B_N. The average values are calculated by moments of grand canonical distribution and for this, we need canonical probability in the next section.

4.1.1 Canonical probability and mean values

Starting with Eq. (4.4), we can write it separating in two contributions: condensed phase (when $\mathbf{k} = 0$) - $\gamma_1(\beta)$ and normal phase (when $\mathbf{k} \neq 0$) - $\xi_n(\beta)$,

$$Z_1(n\beta) = \gamma_1^n(\beta) + \xi_n(\beta) \tag{4.16}$$

where

$$\gamma_1^n(\beta) \equiv e^{-n\beta E_G} \tag{4.17}$$

$$\xi_n(\beta) \equiv \sum_{\mathbf{k} \neq 0} e^{-n\beta E_{\mathbf{k}}} \tag{4.18}$$

and then, Eq. (4.16) can be used in Eq. (4.5),

$$\Xi^{(0)} = \exp\left(\sum_{n=1}^{\infty} \frac{z^n\,\left(\gamma_1^n(\beta) + \xi_n(\beta)\right)}{n}\right) \tag{4.19}$$

As we are interested in ground-state properties, then in Eq. (4.19) the first term that depends of γ_1 can be factored in a new form using Eq. (2.23),

$$\exp\left[\sum_{n=1}^{\infty} \frac{z^n\,\gamma_1^n(\beta)}{n}\right] = \exp\ln\left(1 - z\,\gamma_1(\beta)\right)^{-1} \tag{4.20}$$

and therefore,

$$\Xi^{(0)} = \frac{1}{1 - z\,\gamma_1(\beta)} \exp\left[\sum_{n=1}^{\infty} \frac{z^n\,\xi_n(\beta)}{n}\right]. \tag{4.21}$$

To find the canonical probability, let's remember the discussion about canonical ensemble - a system with temperature T in a thermal bath such that the number of particles N is fixed. This condition can be represented by formula

$$P_C(N,\beta) = \frac{1}{Z_N^B(\beta)} e^{-\beta H} \delta_{\sum n_k, N}. \tag{4.22}$$

developed in [14], where $P_C(N,\beta)$ represents the canonical probability for N particles with temperature T. Here the delta function fixes N is equal to the sum of all occupation numbers n_k. To calculate the average values of a statistical distribution, we need to remember the connection between the canonical and grand canonical ensembles, that is given by

$$\mathcal{A}(\beta, z) = \sum_{N=0}^{\infty} A_N(\beta)\, z^N \tag{4.23}$$

where $\mathcal{A}$ is any functional in GCE and A any functional in CE. As the probability is a functional, then Eq. (4.23) can be used to connect these two quantities, representing the grand canonical probability by $\mathcal{P}(n, \beta; z)$. In Eq. (4.22) H represents the non-interacting Hamiltonian in terms of occupation numbers,

$$H = \sum_{k=0}^{\infty} \varepsilon_k\, n_k. \tag{4.24}$$

The sum over n_k may be separated into ground-state and excited contributions. Making a decomposition of Eq. (4.22) using Eq. (4.24), we have that

$$P_C(N,\beta) = \frac{1}{Z_N^B(\beta)} e^{-\beta \sum_{k \neq 0} n_k \varepsilon_k} \left(e^{-\beta n_0 \varepsilon_0} \delta_{\sum_k n_k, N} \right) \tag{4.25}$$

but as the delta function is fixing n with respect to $\gamma_n(\beta)$, then the parenthesis in Eq. (4.25) can be written

$$e^{-\beta n_0 \varepsilon_0} \delta_{\sum_k n_k, N} = \gamma_1 \left(\frac{1}{N!} \frac{\partial^N}{\partial \gamma_1^N} \right) \gamma_1^N \tag{4.26}$$

then putting Eq. (4.26) in Eq. (4.25) and after in Eq. (4.23),

$$\mathcal{P}(N, \beta; z) = \gamma_1^N \left(\frac{1}{N!} \frac{\partial^N \Xi^{(0)}}{\partial \gamma_1^N} \right) \tag{4.27}$$

and finally, inserting Eq. (4.21) in Eq. (4.27), we have

$$\mathcal{P}(N, \beta; z) = \gamma_1^N(\beta)\, z^N \exp\left[\sum_{n=1}^{\infty} \frac{z^n\,\xi_n(\beta)}{n}\right] \tag{4.28}$$

but the last exponential term can be written in the function of Eq. (4.21) and so,

$$\mathcal{P}(N, \beta; z) = \gamma_1^N(\beta)\, z^N \left(1 - \gamma_1^N z^N\right) \Xi^{(0)} \tag{4.29}$$

and now returning in equation (4.23), the canonical result of probability is

$$P_C(n, \beta) = \gamma_1^n(\beta) \frac{Z_{N-n}^B(\beta)}{Z_N^B(\beta)} - \gamma_1^{n+1}(\beta) \frac{Z_{N-n-1}^B(\beta)}{Z_N^B(\beta)}. \tag{4.30}$$

Now we have a canonical probability to find n particles in the ground state. With it, we can calculate the moments of canonical distribution as the condensed fraction which corresponds to the first moment, and the variance which depends of the second moment. These quantities were also calculated using the cycle decomposition [15]. In the next underlines, we calculated the moments of a canonical distribution, specially the first which corresponds to the condensed fraction and the second which represents the variance following the idea introduced by [14].

First moment

By general probability theory when we have a probability distribution, the average value of any function f is

$$\langle f(n) \rangle = \sum_n f(n)\, P(n). \tag{4.31}$$

In case of condensed fraction, our purpose is to calculate the first moment of ground-state and for it, we shall compute the mean value of n occupation number,

$$\langle n \rangle = \sum_{n=1}^{N} n\, P_C(n, \beta) \tag{4.32}$$

and here inserting Eq. (4.30) in Eq. (4.32), we have

$$\langle n \rangle = \frac{1}{Z_N^B(\beta)} \sum_{n=1}^{N} \left[n\, \gamma_1^n(\beta)\, Z_{N-n}^B(\beta) - n\, \gamma_1^{n+1}(\beta)\, Z_{N-n-1}^B(\beta) \right] \tag{4.33}$$

making a transformation in last summation such that $n + 1 \equiv u$, we have that

$$\langle n \rangle = \sum_{n=1}^{N} n\, \gamma_1^n(\beta) \frac{Z_{N-n}^B(\beta)}{Z_N^B(\beta)}. \tag{4.34}$$

Finally, the condensed fraction is defined as Eq. (4.34) divided by total number of particles N,

$$\frac{\langle N_0 \rangle}{N} = \frac{1}{N} \sum_{n=1}^{N} \gamma_1^n(\beta) \frac{Z_{N-n}^B(\beta)}{Z_N^B(\beta)}. \tag{4.35}$$

Second moment

For the second moment, we have the same idea which was employed in first moment. In fact,

$$\langle n^2 \rangle = \sum_{n=1}^{N} n^2\, P_C(n, \beta) \tag{4.36}$$

and using the transformation $n + 1 \equiv u$ in Eq. (4.30) and Eq. (4.36), we have that

$$\langle n^2 \rangle = \sum_{n=1}^{N} (2n - 1)\, \gamma_1^n(\beta) \frac{Z_{N-n}^B(\beta)}{Z_N^B(\beta)}. \tag{4.37}$$

this formula was also obtained in Chapter 3 of [36]. Therefore, using the general formula of variance given by

$$\Delta n_0 \equiv \sqrt{\langle n^2 \rangle - \langle n \rangle^2} \tag{4.38}$$

and substituting Eqs. (4.34) and (4.37) in Eq. (4.38), we will have the ground-state fluctuations in the canonical ensemble,

$$\Delta n_0 = \frac{1}{N} \sqrt{\sum_{n=1}^{N} (2n - 1)\, \gamma_1^n(\beta) \frac{Z_{N-n}^B(\beta)}{Z_N^B(\beta)} - \left[\sum_{n=1}^{N} \gamma_1^n(\beta) \frac{Z_{N-n}^B(\beta)}{Z_N^B(\beta)} \right]^2}. \tag{4.39}$$

This last quantity corresponds to the ground-state fluctuation and its discussion will be made in Chapter 6 because about this topic there is an interesting theoretical discussion involving what are the better statistical ensemble to describe the Bose gases. Then in the next section, we have the application of this canonical theory of the main traps as the heat capacity and the condensed fraction. But also there are other quantities such as entropy, and internal energy which also can be calculated in a recursive formula. Besides, it is possible, approximately, to calculate the critical temperature from the maximum point of the heat capacity. So, we can compare our results with the literature and the large particle limit equivalent to the grand canonical results.

Other thermodynamic quantities

As said in the previous paragraph, the other thermodynamic quantities as entropy, internal energy, and heat capacity are calculated using $Z_N(\beta)$ as starting point. Following [37, 38], we have that the internal energy is given by

$$U_N(\beta) = -\frac{\partial}{\partial \beta} \ln Z_N(\beta), \tag{4.40}$$

but including our results as a function of T, Eq. (4.40) becomes

$$U_N(T) = k_B T^2 \frac{\partial}{\partial T} \ln Z_N(T). \tag{4.41}$$

To calculate the heat capacity, let us use Eq. (2.32) with energy now given by Eq. (4.41), and then we have that

$$C_N(T) = k_B T \frac{\partial^2}{\partial T^2} \ln Z_N(T). \tag{4.42}$$

With this equation, it is possible to determine the canonical critical temperature T_c by calculating the maximum point of Eq. (4.42),

$$\left(\frac{\partial C_N(T)}{\partial T} \right)_{T = T_c} = 0 \,. \tag{4.43}$$

The last important quantity is the entropy $S_N(T)$; for this, from Eq. (2.31) and that the canonical free energy $F_N(T)$ given by

$$F_N(T) = -k_B\, T\, \ln Z_N(T), \qquad (4.44)$$

we have that

$$S_N(T) = k_B\, \frac{\partial}{\partial T}\left(T \ln Z_N(T)\right). \qquad (4.45)$$

Now we have the complete quantities for a Bose gas described in a canonical ensemble. In the next section, we will study these observables in standard confinements.

4.2 Results for an ideal trapped systems

As an application of this non-interacting canonical theory, we will apply it to classical confinement Bose systems. First, to check the validity of the model we studied the homogeneous Bose gas after we studied two principal systems: the finite box and the harmonic trap. For each system, we calculated the heat capacity, condensed fraction, and ground-state fluctuations. This last quantity is significant in the context of the convergence of the statistical ensembles in studies of certain physical situations. One great vantage to using the recursive canonical description is that the finite-size condition is already included because we started of fact that N is fixed and the one-particle partition function is calculated in an exact form.

4.2.1 Homogeneous Bose gas

Let us consider a homogeneous non-interacting Bose gas in three dimensions. In this case, the spectrum of gas is a continuum, then when we will make the calculation of thermodynamic quantities, we shall use an integral representation in terms of phase-space. The reason for it will be shown now: the external potential $V(\mathbf{x})$ is zero in all space (because the homogeneous system does not have boundary conditions), then

$$V(\mathbf{x}) = 0, \qquad (4.46)$$

and writing the Schrödinger equation for Eq. (4.46),

$$\nabla^2 \psi(\mathbf{x}) + k^2\, \psi(\mathbf{x}) = 0, \qquad (4.47)$$

where

$$k^2 \equiv \frac{2ME}{\hbar^2}. \qquad (4.48)$$

Solving Eq. (4.47) in all space, we have that the wave function is written as a plane wave

$$\psi(\mathbf{x}) = \frac{1}{\sqrt{V}}\, e^{-i\mathbf{k}.\mathbf{x}}. \qquad (4.49)$$

where $\mathbf{k}$ is a real number. When we do not have the ground state, the thermodynamic limit is represented as a sum over all values of $\mathbf{k}$, $\sum_{\mathbf{k}}$, can be written as an integral in all space of moments k in the form

$$\sum_{\mathbf{k}} f(\mathbf{k}) \to f(\mathbf{0}) + \frac{V}{(2\pi)^3} \int d^3k\, f(\mathbf{k}), \qquad (4.50)$$

where V is the volume. Therefore using Eqs. (4.48), (4.50) in Eq. (4.4), we have that

$$Z_1(n\beta) = 1 + \frac{V}{(2\pi)^3} \int d^3k \, e^{-n\beta\hbar^2 k^2/2M} \tag{4.51}$$

and making this Gaussian integral, we have that

$$Z_1(n\beta) = 1 + \frac{V}{\lambda_T^3 \, n^{3/2}}, \tag{4.52}$$

where λ_T is the thermal wavelength

$$\lambda_T \equiv \sqrt{\frac{2\pi\hbar^2\beta}{M}}. \tag{4.53}$$

However, Eq. (4.52) can be written in function of dimensionless temperature t defined as the ratio of general temperature T of the critical temperature in thermodynamic limit $T_c^{(0)}$, in fact,

$$t \equiv \frac{T}{T_c^{(0)}}. \tag{4.54}$$

where

$$T_c^{(0)} = \frac{2\pi\hbar^2}{Mk_B} \left(\frac{N}{V\,\zeta(3/2)} \right)^{2/3}. \tag{4.55}$$

Then, looking Eqs. (4.52) and (4.53), we have that

$$\frac{V}{\lambda_T^3} = \tau^{3/2} \tag{4.56}$$

where τ is defined by Eq. (2.114) and now can be written as

$$\tau = \left(\frac{N}{\zeta(3/2)} \right)^{2/3} t. \tag{4.57}$$

Therefore, (4.52) can be written as

$$Z_1(n\tau) = 1 + \frac{\tau^{3/2}}{n^{3/2}}, \tag{4.58}$$

and now, we may calculate the all thermodynamic properties of this system in the function of the dimensionless temperature t using Eq. (4.15) as a starting point. Our homogeneous plots are in Fig. 4.1 for the condensed fraction and in Fig. 4.2 for the heat capacity.

4.2.2 Three dimensional Bose gas in a finite box

Now let us consider a more realistic case, that is a Bose gas confined in a box with length L, the same system shown in section (2.2). The external potential is given by

$$V(\mathbf{x}) = \begin{cases} 0 & |x_j| \leq L/2, \\ \infty & |x_j| \geq L/2. \end{cases}$$
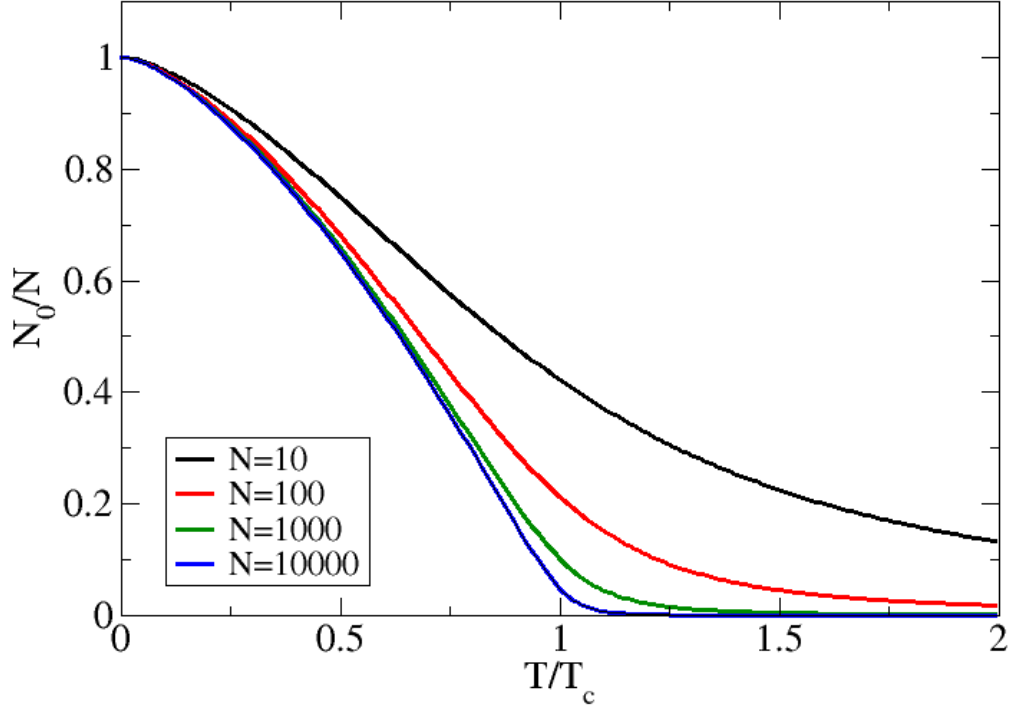
Figure 4.1: Condensed fraction of a homogeneous Bose gas as a function

Here, the difference between this case and the homogeneous system is that now we have boundary conditions and it will give that the energies eigenvalues are discrete. Seeing Chapter 2, the energies are given by Eqs. (2.106) and (2.111),

$$E_{k_1,k_2,k_3} = \frac{\hbar^2\pi^2(k_1^2 + k_2^2 + k_3^2)}{2ML^2},$$
(4.59)

and using Eq. (4.59) in Eq. (4.4), we have that

$$Z_1(n\beta) = \sum_{k_1,k_2,k_3} e^{-n\beta\hbar^2\pi^2(k_1^2+k_2^2+k_3^2)/(2ML^2)},$$
(4.60)

as each coordinate is independent, we can write Eq. (4.60) as a single summation, where now the letter m represents the general quantum number among k_1, k_2, k_3,

$$Z_1(n\beta) = \left[\sum_{m=1}^{\infty} e^{-n\beta\hbar^2\pi^2m^2/(2ML^2)}\right]^3.$$
(4.61)

Again, let's write $Z_1(n\beta)$ in terms of τ as made in the homogeneous case using the same dimensionless temperature τ given by Eq. (4.57) but now our volume is L^3, and then

$$\frac{\beta\hbar^2\pi^2}{2ML^2} = \frac{\pi}{4\tau},$$
(4.62)
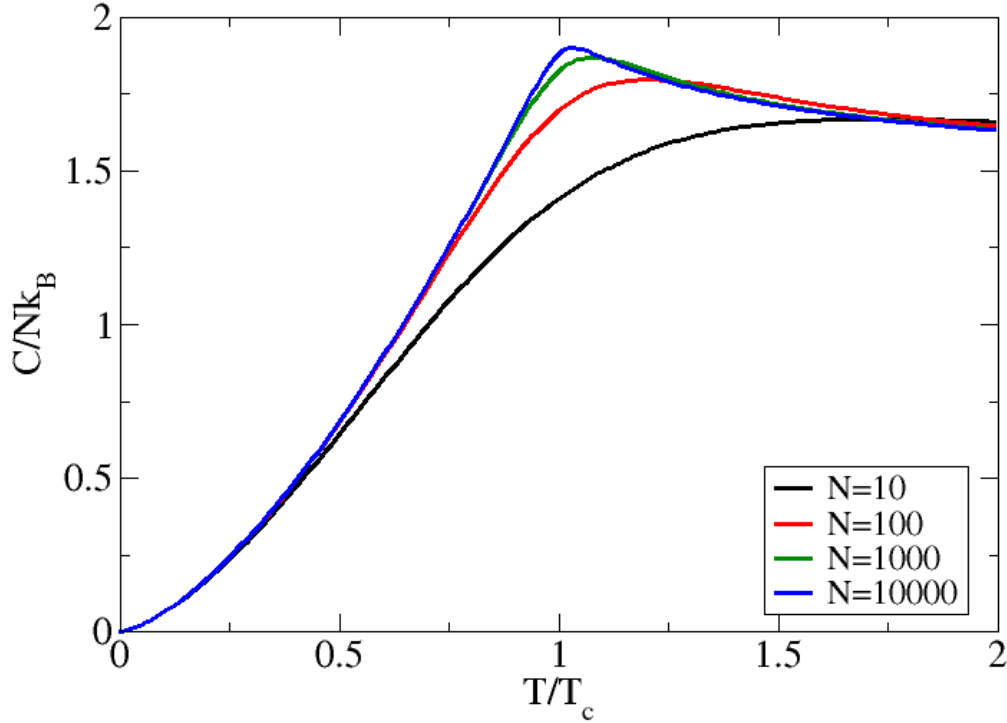
Figure 4.2: Heat capacity for a homogeneous 3D Bose gas as a function of the temperature in the canonical ensemble.

and including this result in Eq. (4.61), we have

$$Z_1(n\tau) = \left[\sum_{m=1}^{\infty} e^{-n\pi m^2/(4\tau)} \right]^3.$$ (4.63)

Given Eq. (4.63), we can plot the thermodynamic quantities following the same procedure done in the homogeneous case, the condensed fraction, ground-state fluctuation, and heat capacity given by Fig. 4.3, 4.5 and Fig. 4.4.

4.2.3   Bose gas in a three-dimensional harmonic trap

In this case, the potential $V(\mathbf{x})$ for a three dimensional harmonic trap with frequencies $\omega_1, \omega_2, \omega_3$ is given by Eq. (2.58) and the Hamiltonian by Eq. (2.59). We know that our analytical purpose is to calculate $Z_1(n\beta)$ Eq. (4.49). Then using Eq. (2.64) in Eq. (4.49),

$$Z_1(n\beta) = \sum_{k_1,k_2,k_3} e^{-n\beta(E_G + \hbar(k_1\,\omega_1 + k_2\,\omega_2 + k_3\,\omega_3))}$$ (4.64)
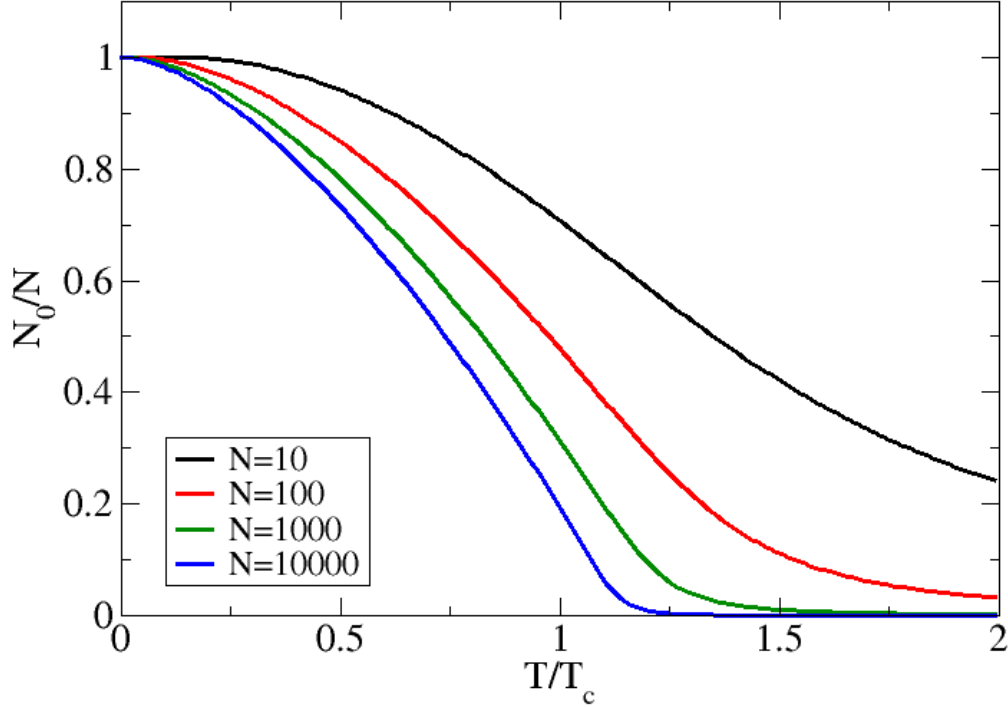
Figure 4.3: Condensed fraction of a 3D finite box as a function of the temperature in the canonical ensemble for different numbers of particles N.

as each coordinate is independent, then we can separate this summation for each quantum number k_i,

$$Z_1(n\beta) = e^{-n\beta E_G} \sum_{k_1=0}^{\infty} e^{-n\beta\hbar\omega_1 k_1} \sum_{k_2=0}^{\infty} e^{-n\beta\hbar\omega_2 k_2} \sum_{k_3=0}^{\infty} e^{-n\beta\hbar\omega_3 k_3}. \qquad (4.65)$$

The summation over n_i is a geometric series,

$$\sum_{m=0}^{\infty} x^m = \frac{1}{1-x}, \qquad (4.66)$$

where x is less than 1; so applying Eq. (4.66) in Eq. (4.65), we have a simple formula of $Z_1(n\beta)$,

$$Z_1(n\beta) = \frac{e^{-n\beta E_G}}{(1 - e^{-n\beta\hbar\omega_1})(1 - e^{-n\beta\hbar\omega_2})(1 - e^{-n\beta\hbar\omega_3})}. \qquad (4.67)$$

Again as made in other symmetries, let's put this result in terms of its respective dimensionless temperature τ. Looking the Chapter 2, this harmonic trap in a semiclassical approach was studied generically from power law trap potential because Eq. (2.58) is a type of power law potential Eq. (2.33). So is convenient to define τ as
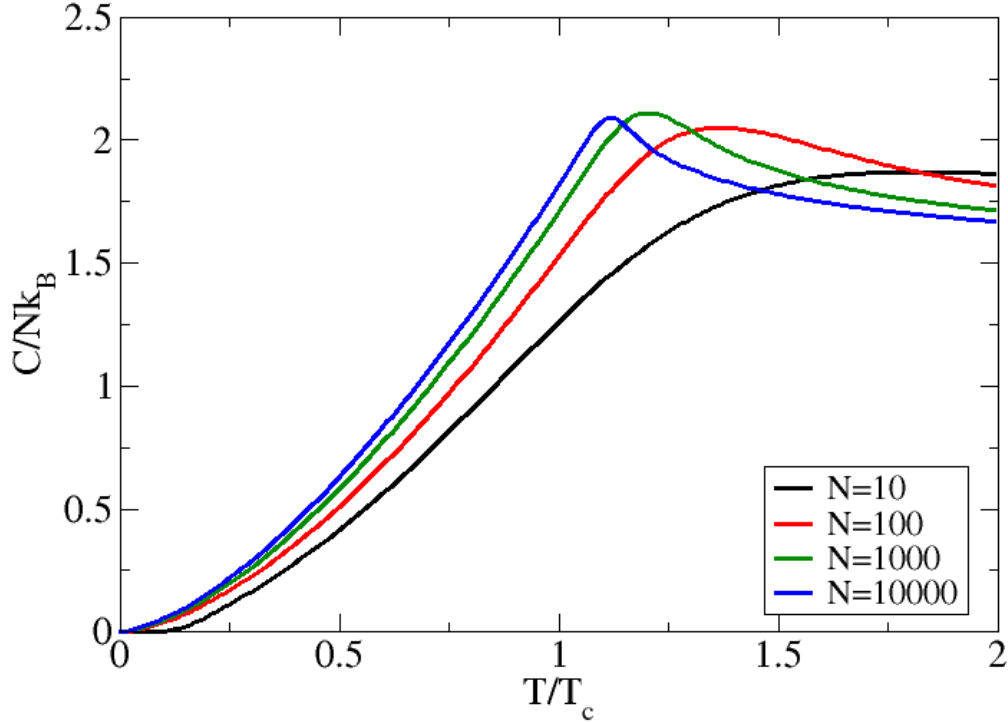
Figure 4.4: Heat capacity of a Bose gas in a 3D finite box as a function of the temperature in the canonical ensemble for different numbers of particles N.

done in Eq. (2.69), where $\tilde{\omega}$ is given by Eq. (2.61). Using the result of critical temperature $T_c^{(0)}$ given by (2.62). So, inserting Eq. (2.62) in (2.69), τ can be written as

$$\tau = \left[\frac{N}{\zeta(3)}\right]^{1/3} t, \tag{4.68}$$

with t given by Eq. (4.54). Therefore, Eq. (4.67) in function of τ is now

$$Z_1(n\tau) = \frac{e^{-3n\overline{\omega}/(2\tilde{\omega}\tau)}}{\left(1 - e^{-n\omega_1/(\tilde{\omega}\tau)}\right)\left(1 - e^{-n\omega_2/(\tilde{\omega}\tau)}\right)\left(1 - e^{-n\omega_1/(\tilde{\omega}\tau)}\right)}. \tag{4.69}$$

Given Eq. (4.69), we can plot the thermodynamic quantities following the same procedure done in homogeneous and finite box cases, the condensed fraction, ground-state fluctuation and heat capacity given by Figs. 4.7, 4.8 and 4.6.

4.3   Discussion of the results

By our plots for the canonical quantities, we see that in both cases when the number of particles increases, the critical dimensionless temperature nears one, and this situation is seen specially in the heat capacity plots Figs. 4.6, 4.4 and 4.2 - for 10 particles, the
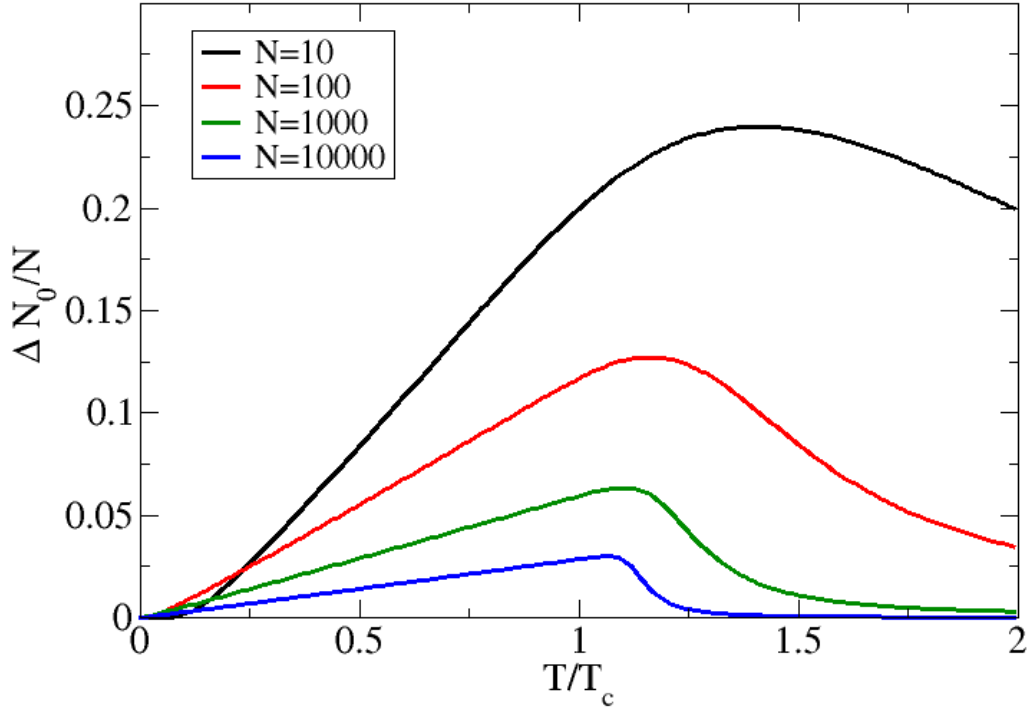
Figure 4.5: Ground-state fluctuation of a Bose gas in a 3D finite box as a function of the temperature in the canonical ensemble for different numbers of particles N.

dimensionless critical temperature is far to 1 but for 10000 this value converges to 1 following the grand canonical previews.

With the heat capacity plot, we can discover the canonical critical temperature by Eq. (4.43). To see better these temperatures, we have two tables for different values of N in two traps: the finite box (table 1) and the isotropic harmonic trap (table 2). The idea is to compare these values with their grand canonical results developed in Chapter 2, where the finite-size corrections were put.

N	Canonical	grand canonical
10	1.82	1.12
100	1.37	1.23
1000	1.20	1.19
10000	1.12	1.12

Table 4.1: Values of critical temperatures for a trapped Bose gas in a three-dimensional finite box calculated by two ensembles: canonical through Eq. (4.43) and grand canonical through Eq. (2.141).
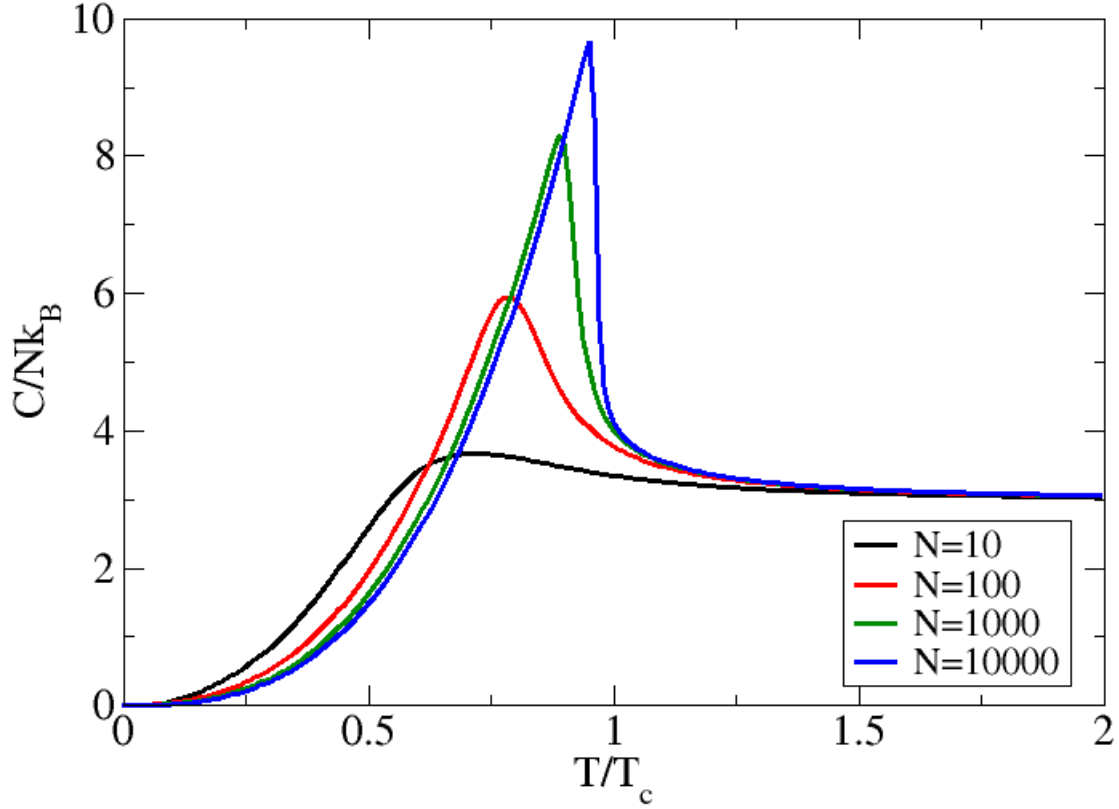
Figure 4.6: Heat capacity of a Bose gas in a 3D isotropic harmonic trap as a function of the temperature in the canonical ensemble for different numbers of particles N.

N	Canonical	grand canonical
10	0.72	0.66
100	0.78	0.84
1000	0.89	0.93
10000	0.95	0.97

Table 4.2: Values of critical temperatures for a trapped Bose gas in a three-dimensional isotropic harmonic trap calculated by two ensembles: canonical through Eq. (4.43) and grand canonical through Eq. (2.69).

With these tables, we see that when increases the number of particles, the canonical results converge into grand canonical results, which makes sense because, in the thermodynamic limit, the two ensembles are equivalents. For a few particles, in our case, for 10 and 100, the results have a greater difference that is explained by the fact that the grand canonical finite-size correction used here is up to first order. The result is closer when we consider more terms in our polylogarithm expansion - so, the inclusion of the finite-size correction is essential in the study of trapped Bose gases in the grand
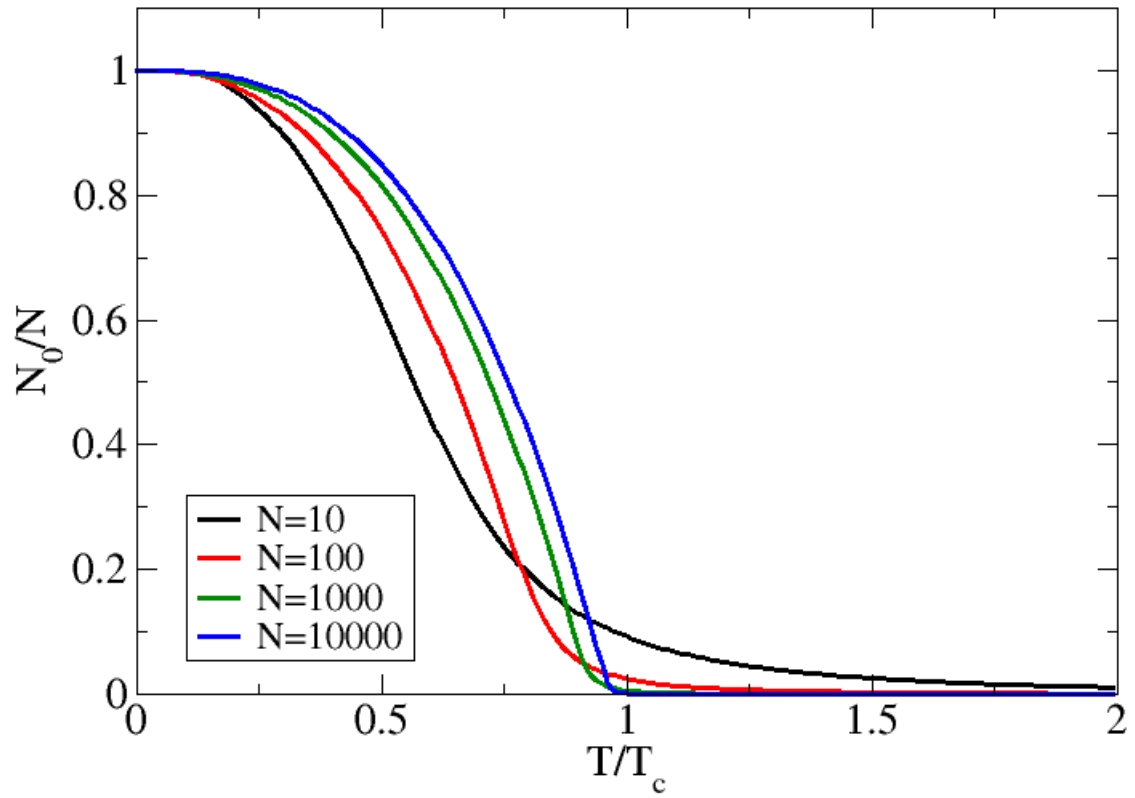
Figure 4.7: Condensed fraction of a Bose gas in a 3D isotropic harmonic trap as a function of the temperature in the canonical ensemble for different numbers of particles N.

canonical ensemble, but the canonical ensemble gives us a more precise value.
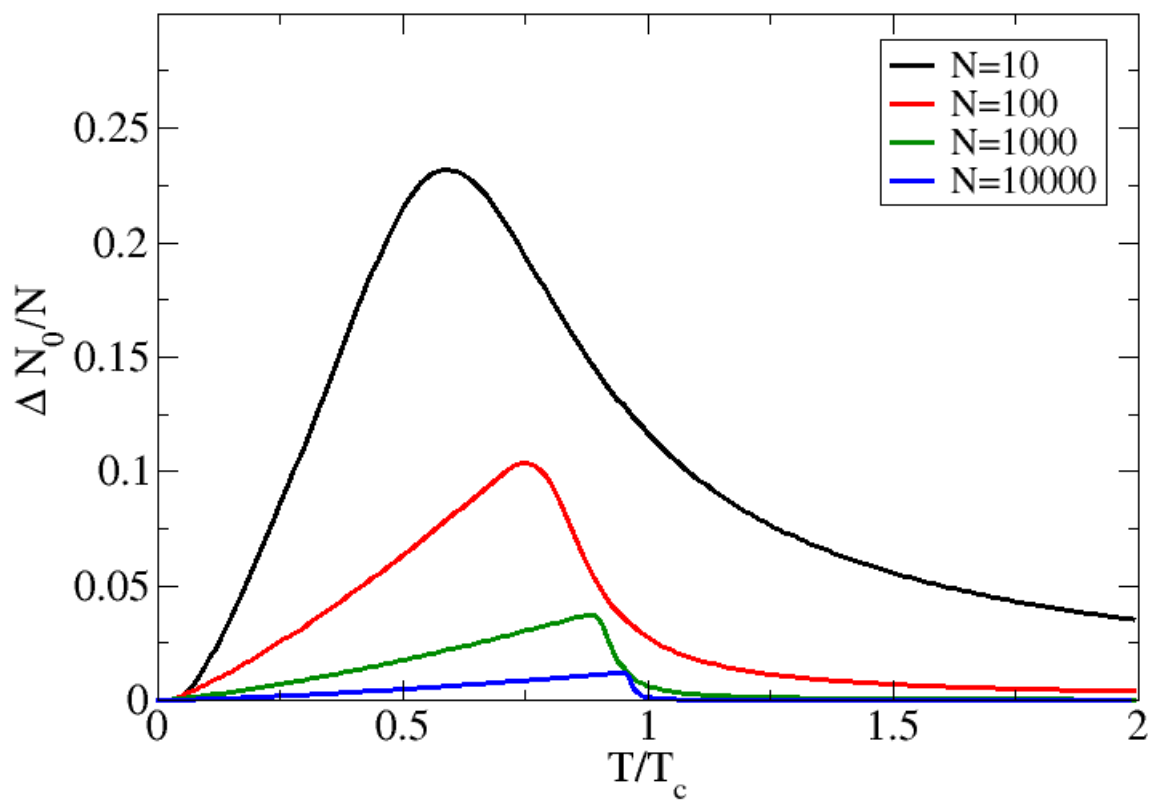
Figure 4.8: Ground-state fluctuation of a Bose gas in a 3D isotropic harmonic trap as a function of the temperature in the canonical ensemble for different numbers of particles N.

Chapter 5

Weakly interacting canonical theory

In some situations, we can approximate the physical system as a non-interacting gas and this condition in a canonical overview was described in chapter 4, however, in the majority of experiments, the interactions are very important in the physical behavior, and then its inclusion in the calculations is necessary for a better description. Here we continue studying a confined Bose gas in a canonical approach but now including interactions. To include these interactions, we started with a grand canonical idea writing the grand partition function Ξ and after extracting the N-particle partition function $Z_N(\beta)$ and we show through this chapter, the self-energies have to be included in one-quasiparticle partition function $Z_1(n\beta)$.

To study the interactions in quantum statistical mechanics, we can use the many possibilities depending on the interaction's type, and in our case, the interest is to calculate the thermodynamic properties for weakly interacting trapped Bose gases. As we have weak interactions, the perturbation theory up to the first order expands the interaction action in powers of the interacting potential.

5.1   Full N-particle partition function

5.1.1   General canonical formula

To get the canonical partition function, we shall start with the grand canonical ensemble as done in the non-interacting case, but now with the interacting grand partition function Ξ given by Eq. (3.7). So, for simplicity, we define a new notation for wave function as $\psi_x \equiv \psi(\mathbf{x}, \tau)$ and the term $\langle \psi^*(\mathbf{x}, \tau)\,\psi(\mathbf{x}, \tau)\,\psi^*(\mathbf{x}', \tau)\psi(\mathbf{x}', \tau)\rangle^{(0)}$ from Wick's theorem is given by

$$\langle \psi_x^*\,\psi_x\,\psi_{x'}^*\,\psi_{x'}\rangle^{(0)} = \langle \psi_x^*\,\psi_x\rangle^{(0)}\,\langle \psi_{x'}^*\,\psi_{x'}\rangle^{(0)} + \langle \psi_x^*\,\psi_{x'}\rangle^{(0)}\,\langle \psi_{x'}^*\,\psi_x\rangle^{(0)}. \qquad (5.1)$$

As seen here, in the first order, the interacting contribution has two terms: one which represents the direct product between each coordinate $\langle \psi_x^*\,\psi_x\rangle^{(0)}\,\langle \psi_{x'}^*\,\psi_{x'}\rangle^{(0)}$ called the Hartree channel and other which contains the product of exchange term $\langle \psi_x^*\,\psi_{x'}\rangle^{(0)}\,\langle \psi_{x'}^*\,\psi_x\rangle^{(0)}$ called the Fock channel and this results is known as the Hartree-Fock approximation.

Each two-body correlation term in Eq. (5.1) is the Green's function of the Schrödinger field calculated in non-interacting grand canonical system $G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau')$. However, in

$$\Xi = \Xi^{(0)} - \text{⬡} - \text{⬡} + ...$$

Figure 5.1: Diagrammatic representation of the grand partition function that mathematically is represented by Eq. (5.4). Here we have an important difference between the grand canonical free energy $\mathcal{F}$ diagrams described in Fig. 3.1 are only connected due to the logarithm function, while the partition function contains all diagrams: connected and disconnected as viewed in [3,4]. As we are doing the calculation until the first order, the diagrams are the same as viewed in Fig. 3.1 except by the dimensional constant $1/\beta$.

Eq. (5.1), we have the diagonal terms because these products are over the same imaginary time τ. Then, let us consider the limit of general formula of $G^{(0)}$ when τ' converges to τ,

$$G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau) = \lim_{\tau' \downarrow \tau} G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{x}) \psi_{\mathbf{k}}^*(\mathbf{x}') \frac{1}{e^{\beta(E_{\mathbf{k}} - \mu)} - 1}. \tag{5.2}$$

Putting Eq. (5.2) in Eq. (5.1) with $G_{\mathbf{x},\mathbf{x}'}^{(0)} \equiv G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau)$, we have that

$$\langle \psi_{\mathbf{x}}^* \psi_{\mathbf{x}} \psi_{\mathbf{x}'}^* \psi_{\mathbf{x}'} \rangle^{(0)} = G_{\mathbf{x},\mathbf{x}}^{(0)} G_{\mathbf{x}',\mathbf{x}'}^{(0)} + G_{\mathbf{x},\mathbf{x}'}^{(0)} G_{\mathbf{x}',\mathbf{x}}^{(0)}, \tag{5.3}$$

and inserting Eq. (5.3) in Eq. (3.7), we have that

$$\Xi = \Xi^{(0)} \left(1 - \frac{1}{2\hbar} \int_0^{\hbar\beta} d\tau \int d^3x \, d^3x' \, V^{(\text{int})}(\mathbf{x} - \mathbf{x}') \left(G_{\mathbf{x},\mathbf{x}}^{(0)} G_{\mathbf{x}',\mathbf{x}'}^{(0)} + G_{\mathbf{x},\mathbf{x}'}^{(0)} G_{\mathbf{x}',\mathbf{x}}^{(0)} \right) + ... \right). \tag{5.4}$$

With the equation Eq. (5.4), we have the grand canonical result for the first-order grand partition function because its formula depends on Green's function Eq. (5.2) and $\Xi^{(0)}$, and both expressions are functions of the chemical potential μ. But to build a canonical theory starting with this result, we must write Ξ as a power series of fugacity z whose coefficients will be the canonical quantities.

The grand partition function Ξ is a dimensionless quantity. To calculate the thermodynamic quantities, we need the grand canonical free energy given by Eq. (2.15) but now for any system. As discussed in Chapter 3, the free energy and consequently, the partition function can be represented in a pictorial representation, where the only difference between Ξ and $\mathcal{F}$ is the mathematical formulas. The expansion up to the first order is shown in Fig. 3.1.

First, we see that Green's function $G^{(0)}$ given by Eq. (5.2) can be written using a geometric series in Bose-Einstein distribution because, in general, Bose systems the chemical potential is smaller to energy eigenvalues, then is convenient to use this

representation,

$$\frac{1}{e^x - 1} = \sum_{n=1}^{\infty} e^{-nx}, \quad \text{when } |x| << 1 \tag{5.5}$$

and putting (5.5) in (5.2) where now $x \equiv \beta(E_{\mathbf{k}}^{(0)} - \mu)$ and then,

$$G^{(0)}(\mathbf{x}, \tau; \mathbf{x}', \tau) = \sum_{n=1}^{\infty} e^{n\beta\mu} (\mathbf{x}, n\hbar\beta; \mathbf{x}', 0)^{(0)}, \tag{5.6}$$

where $(\mathbf{x}, n\hbar\beta; \mathbf{x}', 0)^{(0)}$ is the spectral representation of Green's function of Schrödinger field (or the propagator) [39]

$$(\mathbf{x}, n\hbar\beta; \mathbf{x}', 0)^{(0)} = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^*(\mathbf{x}') \, \psi_{\mathbf{k}}(\mathbf{x}) \, e^{-n\beta E_{\mathbf{k}}}. \tag{5.7}$$

To do the canonical form of Green's functions, we must use its spectral representation given by Eq. (5.6) in Eq. (5.4), where the first term $G_{\mathbf{x},\mathbf{x}}^{(0)} G_{\mathbf{x}',\mathbf{x}'}^{(0)}$ corresponds to Hartree contribution and the second, $G_{\mathbf{x},\mathbf{x}'}^{(0)} G_{\mathbf{x}',\mathbf{x}}^{(0)}$, to the Fock contribution. This form, the first order perturbation term in equation (5.4) that will be denoted by $\Xi^{(1)}$ can be written as

$$\Xi^{(1)} = -\frac{1}{2\hbar} \int_0^{\hbar\beta} d\tau \int d^3x \, d^3x' \, V^{(\text{int})}(\mathbf{x} - \mathbf{x}') \sum_{k,l=1}^{\infty} z^{k+l}$$
$$\left[(\mathbf{x}, k\hbar\beta; \mathbf{x}, 0)^{(0)} \, (\mathbf{x}', l\hbar\beta; \mathbf{x}', 0)^{(0)} + (\mathbf{x}, k\hbar\beta; \mathbf{x}', 0)^{(0)} \, (\mathbf{x}', l\hbar\beta; \mathbf{x}, 0)^{(0)} \right] \Xi^{(0)} \tag{5.8}$$

where $z \equiv e^{\beta\mu}$ is the fugacity. As Eq. (5.8) is big, we'll write it in a small form separating the Hartree and Fock channels,

$$\Xi^{(1)} = -\frac{\beta}{2} \int d^3x \, d^3x' \, V^{(\text{int})}(\mathbf{x} - \mathbf{x}') \left([H] + [F] \right), \tag{5.9}$$

where,

$$[H] \equiv \sum_{k,l=1}^{\infty} z^{k+l} (\mathbf{x}, k\hbar\beta; \mathbf{x}, 0)^{(0)} \, (\mathbf{x}', l\hbar\beta; \mathbf{x}', 0)^{(0)} \, \Xi^{(0)} \tag{5.10}$$

and

$$[F] \equiv \sum_{k,l=1}^{\infty} z^{k+l} (\mathbf{x}, k\hbar\beta; \mathbf{x}', 0)^{(0)} \, (\mathbf{x}', l\hbar\beta; \mathbf{x}, 0)^{(0)} \, \Xi^{(0)}. \tag{5.11}$$

Now, to connect the grand canonical with canonical results we shall represent the non-interaction partition function $\Xi^{(0)}$ in the function of z but it is easy due to

$$\Xi^{(0)} = \sum_{N=0}^{\infty} Z_N^{(0)}(\beta) \, z^N, \tag{5.12}$$

then the Hartree and Fock terms can be written fully in function of z and as we know that the general connection between GC and C ensemble is given by formula

$$\Xi = \sum_{N=0}^{\infty} Z_N(\beta) \, z^N, \tag{5.13}$$

therefore, we may obtain the canonical partition function $Z_N(\beta)$ writing Eqs. (5.10) and (5.11) using Eq. (5.13), for simplicity, we'll make the details of the calculations for the Hartree term and after, we'll substitute for the Fock term. So, using Eq. (5.10) and substituting Eq. (5.13) in Eq. (5.9), we obtain that

$$\Xi_H^{(1)} = -\frac{\beta}{2} \sum_{N=0}^{\infty} Z_N^{(0)}(\beta) z^N \int d^3x\, d^3x'\, V^{(\text{int})}(\mathbf{x}-\mathbf{x}') \sum_{k,l=1}^{\infty} z^{k+l}\, (\mathbf{x}, k\hbar\beta; \mathbf{x}, 0)^{(0)}\, (\mathbf{x}', l\hbar\beta; \mathbf{x}', 0)^{(0)},$$

(5.14)

and then,

$$\Xi_H^{(1)} = -\frac{\beta}{2} \sum_{N=0}^{\infty} \sum_{k,l=1}^{\infty} Z_N^{(0)}(\beta) z^{N+k+l} \int d^3x\, d^3x'\, V^{(\text{int})}(\mathbf{x}-\mathbf{x}')\, (\mathbf{x}, k\hbar\beta; \mathbf{x}, 0)^{(0)}\, (\mathbf{x}', l\hbar\beta; \mathbf{x}', 0)^{(0)}.$$

(5.15)

The idea is to write it term in an equation of type-(5.13). For it, let's make a transformation of form $N' \equiv N + k + l$ and denoting the Hartree integral $I_{k,l}^{(H)}(\beta)$ by

$$I_{k,l}^{(H)}(\beta) \equiv \int d^3x\, d^3x'\, V^{(\text{int})}(\mathbf{x} - \mathbf{x}')\, (\mathbf{x}, k\hbar\beta; \mathbf{x}, 0)^{(0)}\, (\mathbf{x}', l\hbar\beta; \mathbf{x}', 0)^{(0)}, \qquad (5.16)$$

we put these results in Eq. (5.15) and then we see that this term can be written as a new sum over N' whose expression are be given by

$$\Xi_H^{(1)} = \sum_{N'=0}^{\infty} \left(-\frac{\beta}{2}\right) \sum_{k,l=1}^{N'} Z_{N'-k-l}^{(0)}(\beta)\, I_{k,l}^{(H)}(\beta) z^{N'}. \qquad (5.17)$$

By Eq. (5.17) we see that the sum over n and l is restricted by N' and using Eq. (5.13) as model, we can define the **first order Hartree term of canonical partition function** by

$$Z_{N'}^{(H)}(\beta) = -\frac{\beta}{2} \sum_{k,l=1}^{N'} Z_{N'-k-l}^{(0)}(\beta)\, I_{k,l}^{(H)}(\beta). \qquad (5.18)$$

The next step is to solve this restricted summation in Eq. (5.18). For it, we make explicit our restricted sum:

$$\sum_{k,l=1}^{N'} Z_{N'-k-l}^{(0)}(\beta)\, I_{k,l}^{(H)}(\beta) \qquad (5.19)$$

The question is: How do we make this summation? The idea is to decompose Eq. (5.19) in two sums, one to l and the other to a new variable α that corresponds to k and l and is defined as $\alpha \equiv k + l$. It implies that $N' - \alpha = N$ and $k = \alpha - l$. Substituting this in Eq. (5.19), we changed the variable n until α of form

$$\sum_{k,l}^{N'} Z_{N'-k-l}^{(0)}(\beta)\, I_{k,l}^{(H)}(\beta) = \sum_{\alpha=a}^{N'} \sum_{l=b}^{f(\alpha)} Z_{N'-\alpha}^{(0)}(\beta)\, I_{l,\alpha-l}^{(H)}(\beta). \qquad (5.20)$$

To evaluate the sum over α, we have to know its bounds. Its expression is restricted over N', so we have that the highest bound is equal to N', otherwise $\alpha = k + l$, and its lowest values are 1, and therefore, the lowest bound is equal to 2. So,

$$\sum_{\alpha=a}^{N'} = \sum_{\alpha=2}^{N'}. \qquad (5.21)$$

As $\min(l) = 1$, then the summation over l starts in 1 but it highest bound is a function of α and as k is included in α, we'll fix it in $k = 1$ and so, the lowest bound will be $\alpha - 1$. This consideration is corrected because its is self-consistency with initial bounds in infinite sums. Using the discuss about index l and Eq. (5.21) in Eq. (5.20) we have that

$$\sum_{n,l=1}^{N'} Z_{N'-n-l}^{(0)}(\beta)\, I_{n,l}^{(H)}(\beta) = \sum_{\alpha=2}^{N'} \sum_{l=1}^{\alpha-1} Z_{N'-\alpha}^{(0)}(\beta)\, I_{l,\alpha-l}^{(H)}(\beta). \tag{5.22}$$

The fraction $-\beta/2$ can be written as $-(1/2\hbar)(\hbar\beta)$ and therefore rewriting Eq. (5.18) we obtain that

$$Z_{N'}^{(H)}(\beta) = -\frac{1}{2\hbar} \sum_{\alpha=2}^{N'} \sum_{l=1}^{\alpha-1} \hbar\beta\, I_{l,\alpha-l}^{(H)}(\beta)\, Z_{N'-\alpha}^{(0)}(\beta). \tag{5.23}$$

The same for Fock term

$$Z_{N'}^{(F)}(\beta) = -\frac{1}{2\hbar} \sum_{\alpha=2}^{N'} \sum_{l=1}^{\alpha-1} \hbar\beta\, I_{l,\alpha-l}^{(F)}(\beta)\, Z_{N'-\alpha}^{(0)}(\beta), \tag{5.24}$$

with

$$\hbar\beta\, I_{l,\alpha-l}^{(H)}(\beta) \equiv I_{l,\alpha-l}^{(D)}(\beta) = \hbar\beta \int d^3x\, d^3x'\, V^{(\text{int})}(\mathbf{x}-\mathbf{x}')\, (\mathbf{x}, l\hbar\beta; \mathbf{x}, 0)^{(0)}\, (\mathbf{x}', (\alpha-l)\hbar\beta; \mathbf{x}', 0)^{(0)} \tag{5.25}$$

and

$$\hbar\beta\, I_{l,\alpha-l}^{(F)}(\beta) \equiv I_{l,\alpha-l}^{(E)}(\beta) = \hbar\beta \int d^3x\, d^3x'\, V^{(\text{int})}(\mathbf{x}-\mathbf{x}')\, (\mathbf{x}, n\hbar\beta; \mathbf{x}', 0)^{(0)}\, (\mathbf{x}', (\alpha-l)\hbar\beta; \mathbf{x}, 0)^{(0)}, \tag{5.26}$$

where D is the direct term and E is the exchange term.

Here, we have an interesting discussion about these integrals. The canonical representation of the Hartree and Fock contributions is given by Eqs. (5.25) and (5.26), as the connection between the two ensembles is measured by fugacity expansion and the grand canonical ensemble is the generating function of all canonical functions, we have that the canonical diagrams are the same as the grand canonical theory, but the difference is the Feynman rules. The canonical diagrams are shown in Fig. 5.2, where the canonical Feynman rules are described in Fig. 5.3. By Eq. (5.13) and its connection with the canonical ensemble, we can write the **total first order partition function** as [15]

$$Z_N^B(\beta) = Z_N^{(0)}(\beta) - \frac{1}{2\hbar} \sum_{k=2}^{N} \sum_{l=1}^{k-1} \left[I_{l,k-l}^{(D)}(\beta) + I_{l,k-l}^{(E)}(\beta) \right] Z_{N-k}^{(0)}(\beta). \tag{5.27}$$

5.1.2 Recursive N-particle partition function

By equation (5.27), we have that the fully N-particle partition function $Z_N(\beta)$ is in function of non-interacting result $Z_N^{(0)}(\beta)$. But from Eq. (4.15), the ideal result is written as a recursive equation; and following this idea we want to write Eq. (5.27) in a recursive

$$I_{n,m}^{(D)}(\beta) \equiv \quad (n) \quad \bigcirc\!\!-\!\!\bigcirc \quad (m) \qquad\qquad I_{n,m}^{(E)}(\beta) \equiv \quad \overset{(n)}{\underset{(m)}{\bigcirc}}$$

Figure 5.2: The diagrammatic representation of the canonical Hartree and Fock contributions of $Z_N^B(\beta)$. These diagrams are computed following the canonical Feynman rules given by Fig.5.3, where we have the same pictorial representation of the grand canonical ensemble but now with their respective canonical representations.

formula at the same form of Eq. (4.15) because we may use the same numerical methods to find the thermodynamic quantities.

To discover the recursive formula of $Z_N(\beta)$, first, by simplicity, let's denote the sum of Hartree and Fock integrals $I_{l,k-l}^{(D)}(\beta) + I_{l,k-l}^{(E)}$ by $f(k,l)$. Using $f(k,l)$ in Eq. (5.27), we have

$$Z_N^B(\beta) = \frac{1}{N}\sum_{n=1}^{N} Z_1(n\beta) Z_{N-n}^{(0)}(\beta) - \frac{1}{2\hbar}\sum_{k=2}^{N}\sum_{l=1}^{k-1} f(k,l)\, Z_{N-k}^{(0)}(\beta), \tag{5.28}$$

and can write it in terms of a single index n as

$$Z_N^B(\beta) = \frac{1}{N}\sum_{n=1}^{N}\left[Z_1(n\beta) - \frac{N}{2\hbar}\sum_{l=1}^{n-1} f(n,l)\right] Z_{N-n}^{(0)}(\beta). \tag{5.29}$$

The non-interacting term $Z_{N-n}^{(0)}(\beta)$ can be written using Eq. (5.27) and so, Eq. (5.29) will be a term in function of $Z_N^B(\beta)$,

$$Z_{N-n}^{(0)}(\beta) = Z_{N-n}^B(\beta) + \frac{1}{2\hbar}\sum_{k=2}^{N-n}\sum_{l=1}^{n-1} f(k,l)\, Z_{N-k-n}^{(0)}(\beta) \tag{5.30}$$

and hence,

$$Z_N^B(\beta) = \frac{1}{N}\sum_{n=1}^{N}\left[Z_1(n\beta) - \frac{N}{2\hbar}\sum_{l=1}^{n-1} f(n,l)\right]\left[Z_{N-n}^B(\beta) + \frac{1}{2\hbar}\sum_{k=2}^{N-n}\sum_{l=1}^{n-1} f(k,l)\, Z_{N-k-n}^{(0)}(\beta)\right] \tag{5.31}$$

the term which depends of $f(n,l)f(k,l)$ here is neglected since this product is of second order. Therefore, up to first order Eq. (5.31) is equal to

$$Z_N^B(\beta) = \frac{1}{N}\sum_{n=1}^{N}\left[Z_1(n\beta) - \frac{N}{2\hbar}\sum_{l=1}^{n-1} f(n,l)\right] Z_{N-n}^B(\beta)$$

$$+ \frac{1}{N}\sum_{n=1}^{N} Z_1(n\beta)\frac{1}{2\hbar}\sum_{k=2}^{N-n}\sum_{l=1}^{n-1} f(k,l)\, Z_{N-k-n}^{(0)}(\beta), \tag{5.32}$$

$$\mathbf{x},\tau \;\xrightarrow{\;(n)\;}\; \mathbf{x}',\tau \;\;\equiv\;\; (\mathbf{x}, n\hbar\beta; \mathbf{x}', 0)^{(0)}$$

$$\mathbf{x} \mathord{>}\!\!\!\mathrm{\sim}\!\!\!\mathord{<}\mathbf{x}' \;\equiv\; -\frac{1}{\hbar}\int_0^{\hbar\beta}\!\mathrm{d}\tau \int\!\mathrm{d}^3x \int\!\mathrm{d}^3x'\, V^{(\mathrm{int})}(\mathbf{x}-\mathbf{x}')$$

Figure 5.3: The canonical Feynman rules: the wiggly line is the interacting contribution represented by the interacting integral over the coordinates $\mathbf{x}$ and $\mathbf{x}'$, the circle around the same point $\mathbf{x}$ with length n is the one-particle propagator for the same coordinate, while the line corresponds to the one-particle propagator for two coordinates $\mathbf{x}$ and $\mathbf{x}'$. We see that we have the same diagrams but now the Green's function G is substituted by the propagator.

Note that the sum over k from 2 to $N-n$ is equal to sum over k between 1 and $N-n$ and the summations in the last term of Eq. (5.32) can be written as

$$\sum_{n=1}^{N} Z_1(n\beta) \sum_{k=1}^{N-n}\sum_{l=1}^{k-1} f(k,l)\, Z_{N-k-n}^{(0)}(\beta) = \sum_{n=1}^{N-1}\sum_{k=1}^{N-n} Z_1(n\beta) Z_{N-k-n}^{(0)}(\beta) \sum_{l=1}^{k-1} f(k,l)\,. \tag{5.33}$$

this nested sum on n and k can be changed by looking the terms is the (n,k). The nested summation corresponds to all points in the triangle in figure 5.4, and changing the order of the summation gives

$$\sum_{n=1}^{N-1}\sum_{k=1}^{N-n} Z_1(n\beta) Z_{N-k-n}^{(0)}(\beta) = \sum_{k=1}^{N-1}\sum_{n=1}^{N-k} Z_1(n\beta) Z_{N-k-n}^{(0)}(\beta) \tag{5.34}$$

but

$$\sum_{n=1}^{N-k} Z_1(n\beta) Z_{N-k-n}^{(0)}(\beta) = (N-k)\, Z_{N-k}^{(0)}(\beta) \tag{5.35}$$

and it is equal to

$$\sum_{n=1}^{N-k} Z_1(n\beta) Z_{N-k-n}^{(0)}(\beta) = (N-k)\, Z_{N-k}^{B}(\beta) \tag{5.36}$$

because in first order when let's substitute $Z_{N-k}^{(0)}(\beta)$ in terms of $Z_{N-k}^{B}(\beta)$ they are equal
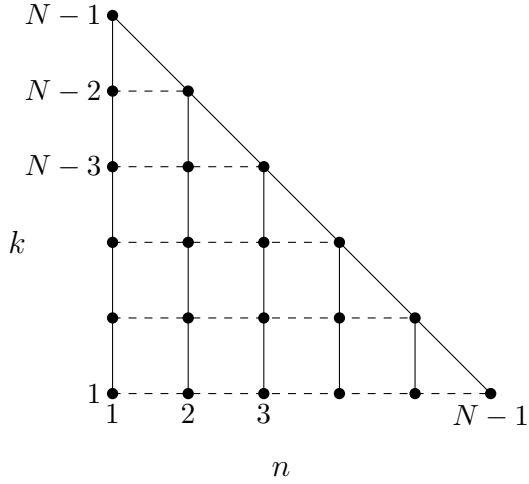
Figure 5.4: Triangle for nested summation in (n, k) plane. $\sum_{n=1}^{N-1} \sum_{k=1}^{N-n}$ corresponds to adding points following each vertical line and later summing all vertical lines. This is equivalent to sum all points along each horizontal line and later add all the horizontal lines, which corresponds to $\sum_{k=1}^{N-1} \sum_{n=1}^{N-k}$.

(remember that the second order terms are neglected) and so,

$$\sum_{n=1}^{N-1} Z_1(n\beta) \sum_{k=1}^{N-n} \sum_{l=1}^{k-1} f(k,l) Z_{N-k-n}^{(0)}(\beta) = \sum_{k=1}^{N-1} \sum_{l=1}^{k-1} f(k,l) (N-k) Z_{N-k}^{B}(\beta) \quad (5.37)$$

and inserting Eq. (5.36) in Eq. (5.34) and on Eq. (5.32), we obtain

$$Z_N^B(\beta) = \frac{1}{N} \sum_{n=1}^{N} \left[Z_1(n\beta) - \frac{N}{2\hbar} \sum_{l=1}^{n-1} f(n,l) \right] Z_{N-n}^B(\beta)$$

$$+ \frac{1}{N} \frac{1}{2\hbar} \sum_{k=1}^{N-1} \sum_{l=1}^{k-1} f(k,l)(N-k) Z_{N-k}^B(\beta)$$

$$(5.38)$$

and doing the simplifications, we obtain the recursive formula for interacting partition in the first order [15],

$$Z_N^B(\beta) = \frac{1}{N} \sum_{n=1}^{N} \left[Z_1(n\beta) - \frac{n}{2\hbar} \sum_{l=1}^{n-1} \left(I_{l,n-l}^{(D)}(\beta) + I_{l,n-l}^{(E)}(\beta) \right) \right] Z_{N-n}^B(\beta), \quad (5.39)$$

and now we have the recursive formula for fully N-particle partition function in the canonical ensemble.

5.1.3 Problem of recursive N-particle partition function

From Eq. (5.39), we have that the fully $Z_N(\beta)$ depends of $Z_1(n\beta)$ and of Hartree and Fock integrals. However it formula has a numerical/physical problem: by Eqs. (5.25) and (5.26), we have that both terms are proportional to β, therefore when we see the

limit for low temperatures ($\beta \to \infty$), the second term is major that $Z_1(n\beta)$ implying that our N-particle partition function will be negative, that is a physical problem.

One way to solve this problem is to renormalize Eq. (5.39). The general idea is to correct $Z_1(n\beta)$ so as it is greater than the sum of Hartree and Fock integrals and so, the interacting kernel will be always positive. For this, let us include the energy corrections $Z_1(n\beta)$ writing it as a new $\hat{Z}_1(n\beta)$, where

$$\hat{Z}_1(n\beta) = \sum_{\mathbf{k}} e^{-n\beta \hat{E}_{\mathbf{k}}^{(n)}}. \tag{5.40}$$

where the new energies $\hat{E}_{\mathbf{k}}^{(n)}$ are now shifted by self-energies which correspond to the interacting contribution of quasiparticle energy. However the discussion about self-energies comes from interacting Green's function and Dyson's equation are described in a grand canonical ensemble. Therefore, is necessary to write a canonical theory of these corrections because as we are studying a physical system in the canonical ensemble must eliminate the chemical potential of our results. In the next section, let us discuss this theory starting with the original grand canonical approach. With this new renormalization, we check that this new representation for the single particle partition $Z_1(n\beta)$ eliminates the problem for low temperatures.

5.2 Interacting Green's function and self-energy in canonical ensemble

As done in Chapter 3, we must start with the interacting Green's function in the grand canonical ensemble given by Eq. (3.35). With the same procedure of perturbation theory, we obtain that the full G can be written as an integral equation known as Dyson's equation (3.44), where the self-energy $\Sigma(\mathbf{x}, \tau; \mathbf{x}', \tau')$ up to first-order is equal to the summation of the Hartree and Fock contributions Eqs. (3.45) and (3.46) whose diagrammatic representation is given by Fig. 3.3. These self-energies depend of grand canonical non-interacting Green's function $G^{(0)}$ and this result is a function of the chemical potential μ. But as done in fully N-particle partition function calculation, $G^{(0)}$ can be written as a power series of fugacity from (5.6). So is more convenient to write $\Sigma^{(D),(E)}(\mathbf{x}, \tau; \mathbf{x}', \tau')$ in a new series with respect to fugacity,

$$\Sigma^{(D)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \sum_{n=0}^{\infty} \sigma_n^{(D)}(\mathbf{x}, \tau; \mathbf{x}', \tau') z^n \tag{5.41}$$

$$\Sigma^{(E)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \sum_{n=0}^{\infty} \sigma_n^{(E)}(\mathbf{x}, \tau; \mathbf{x}', \tau') z^n \tag{5.42}$$

where

$$\sigma_n^{(D)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = -\frac{1}{\hbar} \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau') \int d^3 x'' \, V^{(\text{int})}(\mathbf{x} - \mathbf{x}'') \, (\mathbf{x}'', n\hbar\beta; \mathbf{x}'', 0)^{(0)} \tag{5.43}$$

$$\sigma_n^{(E)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = -\frac{1}{\hbar} \delta(\tau - \tau') V^{(\text{int})}(\mathbf{x} - \mathbf{x}') \, (\mathbf{x}, n\hbar\beta; \mathbf{x}', 0)^{(0)}. \tag{5.44}$$

$$\sigma_n^{(D)}(\boldsymbol{x},\tau;\boldsymbol{x}',\tau') = \overset{(n)}{\underset{\boldsymbol{x}\,\tau\quad\boldsymbol{x}'\tau'}{\bigcirc}} \quad, \qquad \sigma_n^{(E)}(\boldsymbol{x},\tau;\boldsymbol{x}',\tau') = \overset{(n)}{\underset{\boldsymbol{x}\,\tau\qquad\qquad\boldsymbol{x}'\tau'}{\frown}}$$

Figure 5.5: The canonical representation of the Hartree and Fock self-energy following the Feynman rules shown in Fig. 5.3. The difference between the partition function and the self-energy diagrams is that for the self-energy we cut one line as done in the grand canonical case. Again, we have the same diagrams but with different mathematical formulas.

are the canonical representations of self-energies. The interesting here is that the canonical self-energies follow the same Feynman diagrams, but different mathematical formulas of grand canonical results Eqs. (3.45), (3.46). Still, the difference is that the canonical representation of non-interacting Green's function is the one-particle Schrödinger propagator.

As discussed in the final of the section about Green's function in the grand canonical ensemble of Chapter 3, by the Fourier-Matsubara representation of this function, we obtain the single particle Hamiltonian. For an interacting Bose gases, this function is shifted by the self-energies without Matsubara frequency dependence. Therefore our work will calculate the Fourier-Matsubara representation of the self-energy. By Eq. (3.56) follows the same transformation of G which is given by Eq. (3.47), then for Σ, we have that

$$\Sigma(\mathbf{k},i\omega_m) = \int_0^{\hbar\beta} d(\tau-\tau') \int d^3x\, d^3x'\, \Sigma(\mathbf{x},\tau;\mathbf{x}',\tau')\psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x}')\frac{e^{-i\omega_m(\tau-\tau')}}{\hbar\beta} \quad (5.45)$$

where the dependence of new Σ is over the quantum numbers and the Matsubara frequencies, in principle. This formula depends on the classical coordinate-Euclidean time dependence and by Eqs. (5.41) and (5.42), the Fourier representation of the Hartree and Fock results follow the same series,

$$\Sigma^{(D)}(\mathbf{k},i\omega_m) = \sum_{n=1}^{\infty} \sigma_n^{(D)}(\mathbf{k},i\omega_m)z^n \quad (5.46)$$

$$\Sigma^{(E)}(\mathbf{k},i\omega_m) = \sum_{n=1}^{\infty} \sigma_n^{(E)}(\mathbf{k},i\omega_m)z^n \quad (5.47)$$

such that

$$\sigma_n^{(D)}(\mathbf{k},i\omega_m) = \int_0^{\hbar\beta} d(\tau-\tau') \int d^3x\, d^3x'\, \psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x}')\sigma_n^{(D)}(\mathbf{x},\tau;\mathbf{x}',\tau')\frac{e^{-i\omega_m(\tau-\tau')}}{\hbar\beta} \quad (5.48)$$

$$\sigma_n^{(D)}(\boldsymbol{k}) = \quad\overset{(n)}{\bigcirc}\qquad\qquad \sigma_n^{(E)}(\boldsymbol{k}) = \quad\overset{(n)}{\frown}$$

Figure 5.6: The canonical representation of the Hartree and Fock self-energy in the Fourier space whose mathematical formulas are given by Eqs. (5.50) and (5.51). Now we have the vertices as a function of the quantum number vector **k**, and the dependence of the imaginary time disappeared because the Matsubara term is zero for the energy contribution.

$$\sigma_n^{(E)}(\mathbf{k}, i\omega_m) = \int_0^{\hbar\beta} d(\tau - \tau') \int d^3x \, d^3x' \, \psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x}')\sigma_n^{(E)}(\mathbf{x}', \tau; \mathbf{x}, \tau') \frac{e^{-i\omega_m(\tau-\tau')}}{\hbar\beta}$$
(5.49)

and inserting Eq. (5.43) in Eq. (5.48) and Eq. (5.44) in Eq. (5.49) for both contributions, the integral of the imaginary time difference is one because the delta function will give this result and with the symmetry of integral of the Matsubara exponential, don't have the Matsubara frequency dependence. This condition shows us that the energy eigenvalues do not depend on imaginary time contribution, and therefore, the final result is

$$\sigma_n^{(D)}(\mathbf{k}) = -\frac{1}{\hbar} \int d^3x \, d^3x' \, \psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x}')\delta(\mathbf{x} - \mathbf{x}') \int d^3x'' \, V^{(\text{int})}(\mathbf{x} - \mathbf{x}'') \, (\mathbf{x}'', n\hbar\beta; \mathbf{x}'', 0)^{(0)}$$
(5.50)

$$\sigma_n^{(E)}(\mathbf{k}) = -\frac{1}{\hbar} \int d^3x \, d^3x' \, \psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x}')V^{(\text{int})}(\mathbf{x} - \mathbf{x}') \, (\mathbf{x}, n\hbar\beta; \mathbf{x}', 0)^{(0)}.$$
(5.51)

From Eqs. (5.50) and (5.51), we have that the self-energy is a function of quantum numbers **k**. By Eq. (3.63), the correspondent eigenvalues of this Hamiltonian are given by

$$E_{\mathbf{k}}^{(n)} = E_{\mathbf{k}} - \hbar\sigma_n(\mathbf{k})$$
(5.52)

where

$$\sigma_n(\mathbf{k}) = \sigma_n^{(D)}(\mathbf{k}) + \sigma_n^{(E)}(\mathbf{k})$$
(5.53)

with each σ given by Eqs. (5.50) and (5.51). Therefore, we have a complete representation of a single quasiparticle energy and with this formula, we can renormalize our single-particle partition function $\tilde{Z}_1(n\beta)$ writing

$$\tilde{Z}_1(n\beta) = \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}^{(n)}}$$
(5.54)

where $E_{\mathbf{k}}^{(n)}$ given by Eq. (5.52). As an application of this formula, let's calculate the thermodynamic properties of interacting canonical systems with specific weak interactions, but before we have the final recursive formula inserting Eq. (5.54) in Eq. (5.39),

$$Z_N^B(\beta) = \frac{1}{N} \sum_{n=1}^{N} \left\{ \tilde{Z}_1(n\beta) - \frac{n}{2\hbar} \sum_{l=1}^{n-1} \left[I_{l,n-l}^{(D)}(\beta) + I_{l,n-l}^{(E)}(\beta) \right] \right\} Z_{N-n}^B(\beta).$$
(5.55)

Now, as a check, and finalizing our interacting canonical theory, let's show that when we include this correction in our $Z_1(n\beta)$, the canonical kernel becomes positive for all temperatures and so, the final formula is consistent.

Checking the consistency of the N-particle partition function

Starting with Eq. (5.55), the idea now is to show that $\tilde{Z}_1(n\beta)$ is greater than $n \sum_{l=1}^{n-1} (I_{l,n-l}^{(D)}(\beta) + I_{l,n-l}^{(E)}(\beta))/(2\hbar)$. Then, for this, remembering the definition of the Hartree and Fock integrals Eqs. (5.25), (5.26), we have that these integrals depend on the one-particle Schrödinger propagator $(\mathbf{x}, m\hbar\beta; \mathbf{x}', 0)_{(0)}$ given by Eq. (5.7). On the other hand, Eq. (5.80) depends of the canonical self-energies $\sigma_n(\mathbf{k})$ whose formulas are given in Eqs. (5.50) and (5.51). First, let's start with Hartree and Fock integrals, substituting Eq. (5.7) in Eqs. (5.25) and (5.26), we have that

$$
I_{l,n-l}^{(D)}(\beta) + I_{l,n-l}^{(E)}(\beta) = \hbar\beta \int d^3x\, d^3x'\, V^{(\mathrm{int})}(\mathbf{x} - \mathbf{x}') \sum_{\mathbf{k},\mathbf{k}'} e^{-l\beta E_\mathbf{k}}\, e^{-(n-l)\beta E_{\mathbf{k}'}}
$$

$$
\times \left[\psi_\mathbf{k}(\mathbf{x})\psi_\mathbf{k}^*(\mathbf{x})\psi_{\mathbf{k}'}(\mathbf{x}')\psi_{\mathbf{k}'}^*(\mathbf{x}') + \psi_\mathbf{k}(\mathbf{x})\psi_\mathbf{k}^*(\mathbf{x}')\psi_{\mathbf{k}'}(\mathbf{x}')\psi_{\mathbf{k}'}^*(\mathbf{x}) \right]. \quad (5.56)
$$

Now, let's see the $\tilde{Z}_1(n\beta)$, expanding the perturbative contribution:

$$
\tilde{Z}_1(n\beta) = \sum_\mathbf{k} e^{-n\beta E_\mathbf{k}} \left(1 - n\beta\sigma_n(\mathbf{k})\right) , \quad (5.57)
$$

here, inserting Eq. (5.53), after, in Eqs. (5.50) and (5.51), we obtain that

$$
\tilde{Z}_1(n\beta) = \sum_\mathbf{k} e^{-n\beta E_\mathbf{k}} + n\beta \sum_\mathbf{k} e^{-n\beta E_\mathbf{k}} \int d^3x\, d^3x'\, \psi_\mathbf{k}(\mathbf{x})\psi_\mathbf{k}^*(\mathbf{x}') V^{(\mathrm{int})}(\mathbf{x}-\mathbf{x}')(\mathbf{x}, n\hbar\beta; \mathbf{x}', 0)^{(0)}
$$

$$
+ n\beta \sum_\mathbf{k} e^{-n\beta E_\mathbf{k}} \int d^3x\, d^3x'\, \psi_\mathbf{k}(\mathbf{x})\psi_\mathbf{k}^*(\mathbf{x}') \int d^3x''\, V^{(\mathrm{int})}(\mathbf{x} - \mathbf{x}'')(\mathbf{x}'', n\hbar\beta; \mathbf{x}'', 0)^{(0)} .
$$

$$
(5.58)
$$

Now, substituting the propagators by its general formula Eq. (5.7), we have that

$$
\tilde{Z}_1(n\beta) = \sum_\mathbf{k} e^{-n\beta E_\mathbf{k}} + n\beta \sum_\mathbf{k} e^{-n\beta E_\mathbf{k}} \int d^3x\, d^3x'\, \psi_\mathbf{k}(\mathbf{x})\psi_\mathbf{k}^*(\mathbf{x}') V^{(\mathrm{int})}(\mathbf{x}-\mathbf{x}') \sum_{\mathbf{k}'} \psi_{\mathbf{k}'}(\mathbf{x})\psi_{\mathbf{k}'}^*(\mathbf{x}')\, e^{-n\beta E_{\mathbf{k}'}}
$$

$$
+ n\beta \sum_\mathbf{k} e^{-n\beta E_\mathbf{k}} \int d^3x\, d^3x'\, \psi_\mathbf{k}(\mathbf{x})\psi_\mathbf{k}^*(\mathbf{x}')\delta(\mathbf{x}-\mathbf{x}') \int d^3x''\, V^{(\mathrm{int})}(\mathbf{x}-\mathbf{x}'') \sum_{\mathbf{k}'} \psi_{\mathbf{k}'}(\mathbf{x}'')\psi_{\mathbf{k}'}^*(\mathbf{x}'')\, e^{-n\beta E_{\mathbf{k}'}} ,
$$

$$
(5.59)
$$

and putting Eqs. (5.59), (5.56) in our canonical kernel of equation Eq. (5.55),

$$\tilde{Z}_1(n\beta) - \frac{n}{2\hbar} \sum_{l=1}^{n-1} \left[I_{l,n-l}^{(D)}(\beta) + I_{l,n-l}^{(E)}(\beta) \right] = \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}}$$

$$+ n\beta \sum_{\mathbf{k},\mathbf{k}'} e^{-n\beta(E_{\mathbf{k}}+E_{\mathbf{k}'})} \int d^3x \, d^3x' \psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x}')\delta(\mathbf{x}-\mathbf{x}') \int d^3x'' \, V^{(\text{int})}(\mathbf{x}-\mathbf{x}'')\psi_{\mathbf{k}'}(\mathbf{x}'')\psi_{\mathbf{k}'}^*(\mathbf{x}'')$$

$$+ n\beta \sum_{\mathbf{k},\mathbf{k}'} e^{-n\beta(E_{\mathbf{k}}+E_{\mathbf{k}'})} \int d^3x \, d^3x' \psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x}')V^{(\text{int})}(\mathbf{x}-\mathbf{x}')\psi_{\mathbf{k}'}(\mathbf{x})\psi_{\mathbf{k}'}^*(\mathbf{x}')$$

$$- \frac{n\beta}{2} \sum_{l=1}^{n-1} \sum_{\mathbf{k},\mathbf{k}'} e^{-l\beta E_{\mathbf{k}}-(n-l)\beta E_{\mathbf{k}'}} \int d^3x \, d^3x' \, V^{(\text{int})}(\mathbf{x}-\mathbf{x}') \big[\psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x})\psi_{\mathbf{k}'}(\mathbf{x}')\psi_{\mathbf{k}'}^*(\mathbf{x}')$$

$$+ \psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x}')\psi_{\mathbf{k}'}(\mathbf{x}')\psi_{\mathbf{k}'}^*(\mathbf{x}) \big]. \quad (5.60)$$

Here, we have a good point: the terms that depend on the product of ψ are similar in Eqs. (5.59) and (5.56), and both are positive independently of β. Therefore, the integrals over $\mathbf{x}, \mathbf{x}'$ are always positive. The first line in Eq. (5.60) is the fully non-interacting partition function also always positive, so, the only check is to see the exponential term. Clearly, the exponential of $n\beta(E_{\mathbf{k}} + E_{\mathbf{k}'})$ is positive for any β, let's see for the last line of Eq. (5.60),

$$-\frac{n\beta}{2} \sum_{l=1}^{n-1} \sum_{\mathbf{k},\mathbf{k}'} e^{-l\beta E_{\mathbf{k}}-(n-l)\beta E_{\mathbf{k}'}} = -\frac{n\beta}{2} \sum_{\mathbf{k},\mathbf{k}'} \sum_{l=1}^{n-1} e^{-l\beta E_{\mathbf{k}}-(n-l)\beta E_{\mathbf{k}'}}$$

$$= -\frac{n\beta}{2} \sum_{\mathbf{k},\mathbf{k}'} \frac{e^{-(n-1)\beta E_{\mathbf{k}}} - e^{-(n-1)\beta E_{\mathbf{k}'}}}{e^{\beta E_{\mathbf{k}'}} - e^{\beta E_{\mathbf{k}}}}. \quad (5.61)$$

Therefore, we have that

$$\tilde{Z}_1(n\beta) - \frac{n}{2\hbar} \sum_{l=1}^{n-1} \left[I_{l,n-l}^{(D)}(\beta) + I_{l,n-l}^{(E)}(\beta) \right] \cong \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}} + 2\,n\beta \sum_{\mathbf{k},\mathbf{k}'} e^{-n\beta(E_{\mathbf{k}}+E_{\mathbf{k}'})}$$

$$- \frac{n\beta}{2} \sum_{\mathbf{k},\mathbf{k}'} \frac{e^{-(n-1)\beta E_{\mathbf{k}}} - e^{-(n-1)\beta E_{\mathbf{k}'}}}{e^{\beta E_{\mathbf{k}'}} - e^{\beta E_{\mathbf{k}}}}, \quad (5.62)$$

and solving the double summation,

$$\sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}} + n\beta \sum_{\mathbf{k},\mathbf{k}'} \frac{4e^{-n\beta(E_{\mathbf{k}}+E_{\mathbf{k}'})+\beta E_{\mathbf{k}'}} - 4e^{-n\beta(E_{\mathbf{k}}+E_{\mathbf{k}'})+\beta E_{\mathbf{k}}} + e^{-(n-1)\beta E_{\mathbf{k}'}} - e^{-(n-1)\beta E_{\mathbf{k}}}}{2(e^{\beta E_{\mathbf{k}'}} - e^{\beta E_{\mathbf{k}}})}.$$

$$(5.63)$$

To see the positivity of this formula, we can suppose that $E_{\mathbf{k}'} > E_{\mathbf{k}}$. And is clear that Eq. (5.63) is positive for any β, thus

$$\tilde{Z}_1(n\beta) - \frac{n}{2\hbar} \sum_{l=1}^{n-1} \left[I_{l,n-l}^{(D)}(\beta) + I_{l,n-l}^{(E)}(\beta) \right] > 0, \quad (5.64)$$

and finally, our recursive formula is consistent. Now, we can apply this approach to study the trapped interacting Bose gases.
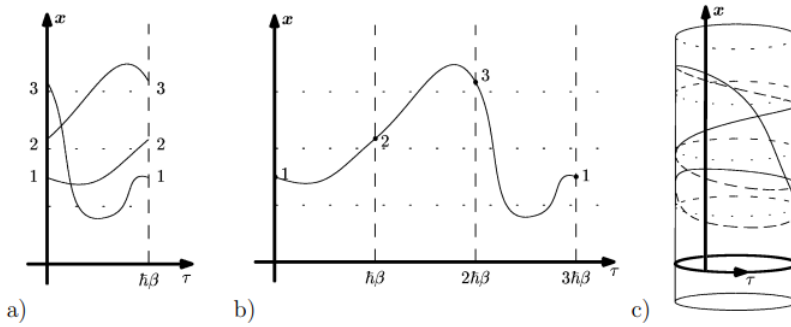
Figure 5.7: Representations of the possible paths for three non-interacting particles for different overviews: a) we have all possible paths and combinations in a period $\hbar\beta$, in b) we have the same paths but now with the three periods closing the cycle of length $3\hbar\beta$ and in c) the representation in a Feynman cylinder.

5.3 Thermodynamic quantities

As done in Chapter 4 about the canonical approach of the non-interacting gases, with the recursive formulas for $\tilde{Z}_1(n\beta)$ and $Z_N^B(\beta)$, we can calculate the main quantities to describe the condensate that are the heat capacity, condensate fraction and ground-state fluctuation. The interesting here is that the recursive formulas for the interacting systems follow the same recursive idea of the ideal case and this condition is proved in this section.

Remembering the discussion about the canonical probability done in 4.2.1, our idea is to show the same probability to find n particles in the ground state given a temperature β in the interacting case and in the non-interacting case. For this, we will use the cycle representation of $Z_N^B(\beta)$ following the procedure used in [15]. The integrals involving the propagators correspond to closed cycles that can be represented in Fig. 5.7. In the ideal case, each closed cycle corresponds to the single particle partition function whose formula is

$$Z_1(n\beta) \equiv \int d^3x_1...d^3x_n \, (\mathbf{x}_1, \hbar\beta; \mathbf{x}_n, 0)^{(0)}...(\mathbf{x}_2, \hbar\beta; \mathbf{x}_1, 0)^{(0)} \, . \tag{5.65}$$

and its illustrative representation in Fig. 5.8. As we have a bosonic system, our N-particle partition function must be proportional to the sums over all possible permutations of $Z_1(n\beta)$ as discussed in [36]. When we include interactions, these integrals have some differences due to the Hartree and Fock contributions derived in our perturbative expansions. But we can interpret the Hartree and Fock as the modified cycle representation and this is more clear in Fig. 5.9. In the case of interactions, Fig. 5.9 is a modified representation of Fig. 5.8, where our $Z_1(\beta) \, Z_1(2\beta)$ has two contributions: the direct cycles $I_{1,2}^{(D)}(\beta)$ and the exchange cycles $I_{1,2}^{(E)}(\beta)$. The cycles have the same behavior, however, for direct and exchange terms, we need the interacting wiggly line to represent the two-body interaction. Then, to see better this discussion, let's compare Eqs. (5.65), (5.25) and (5.26) for three particles. First, for (5.65):

$$Z_1(\beta) \equiv \int d^3x_1 \, (\mathbf{x}_1, \hbar\beta; \mathbf{x}_1, 0)^{(0)} \, , \tag{5.66}$$
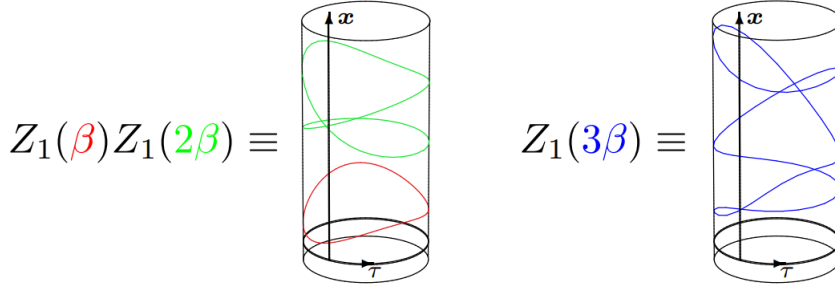
Figure 5.8: An illustrative representation of the non-interacting paths in the Feynman cylinder - in the left figure, we have the product of two cycles, one with length 1 (in red) and the other with length 2 (in green), in the right figure, one cycle with length 3 (in blue) - but all figures were done for a period $3\hbar\beta$.

$$Z_1(2\beta) \equiv \int d^3x_1 \, d^3x_2 \, (\mathbf{x}_1, \hbar\beta; \mathbf{x}_2, 0)^{(0)} \, (\mathbf{x}_2, \hbar\beta; \mathbf{x}_1, 0)^{(0)} \, , \qquad (5.67)$$

$$Z_1(3\beta) \equiv \int d^3x_1 \, d^3x_2 \, d^3x_3 \, (\mathbf{x}_1, \hbar\beta; \mathbf{x}_3, 0)^{(0)} \, (\mathbf{x}_3, \hbar\beta; \mathbf{x}_2, 0)^{(0)} (\mathbf{x}_2, \hbar\beta; \mathbf{x}_1, 0)^{(0)} \, . \quad (5.68)$$

Now for the Hartree and Fock terms,

$$I_{1,2}^{(D)}(\beta) = \hbar\beta \int d^3x_1 \, d^3x_2 \, V^{(int)}(\mathbf{x} - \mathbf{x}') \, (\mathbf{x}_1, \hbar\beta; \mathbf{x}_1, 0)^{(0)} \, (\mathbf{x}_2, 2\hbar\beta; \mathbf{x}_2, 0)^{(0)} \, , \quad (5.69)$$

$$I_{1,2}^{(E)}(\beta) = \hbar\beta \int d^3x_1 \, d^3x_2 \, V^{(int)}(\mathbf{x} - \mathbf{x}') \, (\mathbf{x}_1, \hbar\beta; \mathbf{x}_2, 0)^{(0)} \, (\mathbf{x}_2, 2\hbar\beta; \mathbf{x}_1, 0)^{(0)} \, . \quad (5.70)$$

Looking at these integrals, we see that Eqs. (5.69) and (5.70) are quite similar to $Z_1(2\beta)$ except by interacting potential. Therefore, we can interpret that the Hartree and Fock integrals are the cycle representation of the interactions; so, the formula Eq. (5.27) is the cycle decomposition of first-order N particle partition function, where now, the non-interacting result is actually, its cycle formula [36]

$$Z_N^{(0)B}(\beta) = \frac{1}{N!} \sum_P \prod_{n=1}^{N} [Z_1(n\beta)]^{C_n} \, , \qquad (5.71)$$

where P represents the permutations and C_n is the cycle numbers such that $N = \sum n \, C_n$. The interacting part of Eq. (5.27) can be written in the same form as Eq. (5.71) because the term $I_{l,k-l}^{(D)}(\beta) + I_{l,k-l}^{(E)}(\beta)$ is proportional to $Z_1(k\beta)$, the summations over k, l correspond to the possible permutations with respect to the non-interacting system. We see this result writing Eq. (5.71) in a cycle length formalism,

$$Z_N^B(\beta) = \sum_{C_1,\ldots,C_N} \prod_{n=1}^{N} \frac{1}{C_n!} \left(\frac{Z_1(n\beta)}{n}\right)^{C_n} - \frac{1}{2\hbar} \sum_{k=2}^{N} \sum_{l=1}^{k-1} \left[I_{l,k-l}^{(D)}(\beta) + I_{l,k-l}^{(E)}(\beta) \right]$$

$$\times \sum_{C_1,\ldots,C_{N-k}} \prod_{n=1}^{N-k} \frac{1}{C_n!} \left(\frac{Z_1(n\beta)}{n}\right)^{C_n} \, . \quad (5.72)$$
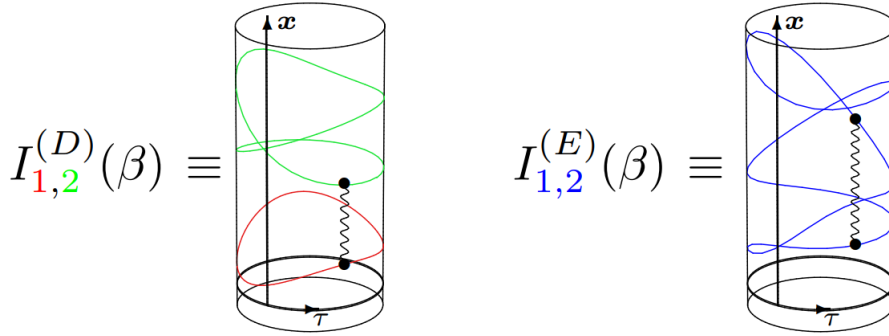
Figure 5.9: The Hartree and Fock integrals in their respective Feynman cylinder representations - the pictorial form is the same as the one shown in Fig. 5.8 but now we have the interacting contribution given by wiggly line connecting the two cycles.

This formula can be written as

$$Z_N^B(\beta) = \sum_{C_1,\dots,C_N} \prod_{n=1}^{N} \frac{1}{C_n!} \left(\frac{\overline{Z}_1(n\beta)}{n} \right)^{C_n}, \tag{5.73}$$

where

$$\overline{Z}_1(n\beta) = Z_1(n\beta) \left[1 - \frac{1}{2\hbar} \sum_{k=2}^{N} \sum_{l=1}^{k-1} \left(I_{l,k-l}^{(D)}(\beta) + I_{l,k-l}^{(E)}(\beta) \right) \right] \tag{5.74}$$

is a new single particle partition function including the corrections due to interactions. So, we have the same structure of founded in [36]. This means that we have the same cycle representation of the moments of the ground state canonical distribution, and therefore, we have the same formula of $P_C(n,\beta)$ given by Eq. (4.30), but now with $Z_N^B(\beta)$ given by Eq. (5.55). So, the condensate properties and their moments are given by Eqs. (4.35) and (4.39).

5.4 Results for trapped Bose gases with a contact interaction

Now, we have a complete theory of the canonical ensemble for an interacting system. To illustrate the application of this theory, we studied the dilute Bose gas in many trapped confinements: inside a box and in a harmonic trap, in general, the dilute interaction is represented by contact interacting potential given by [27]

$$V^{(\mathrm{int})}(\mathbf{x} - \mathbf{x}') = g\,\delta(\mathbf{x} - \mathbf{x}'), \tag{5.75}$$

where g is the coupling constant given by

$$g = \frac{4\pi\hbar^2 a_s}{M}. \tag{5.76}$$

Here, we must calculate the Hartree and Fock integrals by Eqs. (5.25) and (5.26) joint with the self-energies contributions in one-particle partition function $\tilde{Z}_1(n\beta)$ given by

Eq. (5.54). Finally, for each situation, we have to compute Eq. (5.39) using these previous quantities, but to calculate it we need the Schrödinger propagator $(x, n\hbar\beta|x', 0)_{(0)}$. However, for Eq. (5.75), the Hartree and Fock contributions are equal. So, the equations which will be used in this section are

$$I_{l,n-l}^{(D,E)}(\beta) = g\hbar\beta \int d^3x \, (\mathbf{x}, l\hbar\beta; \mathbf{x}, 0)^{(0)} \, (\mathbf{x}, (n-l)\hbar\beta; \mathbf{x}, 0)^{(0)}, \qquad (5.77)$$

and

$$\sigma_n^{(D,E)}(\mathbf{k}) = -\frac{g}{\hbar} \int d^3x \, \psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}^*(\mathbf{x}) \, (\mathbf{x}, n\hbar\beta; \mathbf{x}, 0)^{(0)}. \qquad (5.78)$$

In the case of a Bose gas with contact interaction, Eq. (5.53) becomes

$$\sigma_n(\mathbf{k}) = 2\,\sigma_n^{(D,E)}(\mathbf{k}), \qquad (5.79)$$

and

$$E_{\mathbf{k}}^{(n)} = E_{\mathbf{k}} - 2\,\hbar\,\sigma_n^{(D,E)}(\mathbf{k}). \qquad (5.80)$$

Therefore, our renormalized single-particle partition function $\tilde{Z}_1(n\beta)$ is written with Eq. (5.80) in Eq. (5.54). So, the fully N-particle partition function $Z_N^B(\beta)$ given by Eq. (5.39), now can be written as

$$Z_N^B(\beta) = \frac{1}{N}\sum_{n=1}^{N}\left[\tilde{Z}_1(n\beta) - \frac{n}{\hbar}\sum_{l=1}^{n-1} I_{l,n-l}^{(D,E)}(\beta)\right] Z_{N-n}^B(\beta), \qquad (5.81)$$

and it is the formula that will be calculated for two systems: the dilute Bose gas in a finite box and the dilute gas in a harmonic trap. The last quantity, the renormalized single-particle partition function can be written as

$$\tilde{Z}_1(n\beta) = \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}}\left(1 - 2n\hbar\beta\sigma_n^{(D,E)}(\mathbf{k})\right). \qquad (5.82)$$

At the end of the calculations, we will put the results in terms of the dimensionless temperature τ equivalent for each system. The numerical procedure is the same as done in the non-interacting case. The plots were done using the code shown in Appendix F.

5.4.1 Dilute Bose gas in a finite box

Following section 2.2 of Chapter 2, we have the expression of the wave function $\psi_{\mathbf{k}}(\mathbf{x})$ as a product of one-dimensional results Eqs. (2.105) and (2.109). The equation (2.109) can be written in other representations,

$$\psi_{k_j}(x_j) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi k_j x_j}{L}\right) \qquad (5.83)$$

and therefore, we can calculate the one-particle propagator for this system which is given by Eq. (5.7),

$$(\mathbf{x}, k\hbar\beta; \mathbf{x}', 0)^{(0)} = \prod_{j=1}^{3}\left(x_j, k\hbar\beta; x_j', 0\right)^{(0)}, \qquad (5.84)$$

where

$$\left(x_j, k\hbar\beta; x_j', 0\right)^{(0)} = \sum_{k_j=1}^{\infty} |\psi_{k_j}(x_j)|^2 \, e^{-k\beta E_{k_j}}, \qquad (5.85)$$

and

$$E_{k_j} = \frac{\hbar^2 \pi^2 k_j^2}{2ML^2}. \qquad (5.86)$$

So inserting Eqs. (5.86), (5.83) in Eq. (5.85) we have that

$$\left(x_j, k\hbar\beta; x_j', 0\right)^{(0)} = \sum_{k_j=1}^{\infty} \frac{2}{L} \sin^2\left(\frac{\pi k_j x_j}{L}\right) e^{-k\beta\hbar^2\pi^2 k_j^2/2ML^2} \qquad (5.87)$$

but

$$\sinh^2(x) = \frac{1}{2}(1 - \cosh(2x)), \qquad (5.88)$$

then Eq. (5.87) becomes

$$\left(x_j, k\hbar\beta; x_j', 0\right)^{(0)} = \frac{1}{L} \sum_{k_j=1}^{\infty} \left[1 - \cos\left(\frac{2\pi k_j x_j}{L}\right)\right] e^{-k\beta\hbar^2\pi^2 k_j^2/2ML^2} \qquad (5.89)$$

and now we have the propagator in one dimension. By Eq. (5.77 we can calculate them using a classical decomposition which follows Eq. (5.84),

$$I_{l,n-l}^{(D,E)}(\beta) = g\hbar\beta \prod_{j=1}^{3} X_{l,n-l}(\beta) \qquad (5.90)$$

where

$$X_{l,n-l}(\beta) = \int_0^L dx_j \, (x_j, l\hbar\beta; x_j, 0)^{(0)} \, (x_j, (n-l)\hbar\beta; x_j, 0)^{(0)}. \qquad (5.91)$$

Inserting Eq. (5.89) in Eq. (5.91),

$$X_{l,n-l}(\beta) = \frac{1}{L^2} \int_0^L dx_j \sum_{k_j=1}^{\infty} \left[1 - \cos\left(\frac{2\pi k_j x_j}{L}\right)\right] e^{-l\beta\hbar^2\pi^2 k_j^2/2ML^2}$$

$$\times \sum_{m_j=1}^{\infty} \left[1 - \cos\left(\frac{2\pi m_j x_j}{L}\right)\right] e^{-(n-l)\beta\hbar^2\pi^2 m_j^2/2ML^2} \qquad (5.92)$$

$$X_{l,n-l}(\beta) = \frac{1}{L^2} \sum_{k_j,m_j=1}^{\infty} e^{-l\beta\hbar^2\pi^2 k_j^2/2ML^2} \, e^{-(n-l)\beta\hbar^2\pi^2 m_j^2/2ML^2}$$

$$\times \int_0^L dx_j \left[1 - \cos\left(\frac{2\pi k_j x_j}{L}\right)\right] \left[1 - \cos\left(\frac{2\pi m_j x_j}{L}\right)\right]. \qquad (5.93)$$

Our problem now is to calculate the last integral over x_j. For this, let us consider the cosine integral:

$$\int_0^L dx \, \cos\left(\frac{2\pi k_j x_j}{L}\right) = \frac{L}{2\pi k_j} \sin(2\pi k_j) = L\delta_{k_j,0}, \qquad (5.94)$$

where here we used the Kronecker delta to resume the full possible results. Then applying this idea in our integral in Eq. (5.93), we have that

$$\int_0^L dx_j \left[1 - \cos\left(\frac{2\pi k_j x_j}{L}\right)\right]\left[1 - \cos\left(\frac{2\pi m_j x_j}{L}\right)\right] = L - L\delta_{k_j,0} - L\delta_{m_j,0} + \frac{L}{2}\left(\delta_{k_j+m_j,0} + \delta_{k_j-m_j,0}\right)$$

$$= L\left(1 + \frac{1}{2}\delta_{k_j,m_j}\right) , \quad (5.95)$$

and now inserting Eq. (5.95) in Eq. (5.93), we have that

$$X_{l,n-l}(\beta) = \frac{1}{L}\sum_{k_j,m_j=1}^{\infty} e^{-l\beta\hbar^2\pi^2 k_j^2/2ML^2}\, e^{-(n-l)\beta\hbar^2\pi^2 m_j^2/2ML^2}\left(1 + \frac{1}{2}\delta_{k_j,m_j}\right) . \quad (5.96)$$

Finally, substituting Eq. (5.96) in Eq. (5.90), we have that the Hartree-Fock integral is

$$I_{l,n-l}^{(D,E)}(\beta) = \frac{g\hbar\beta}{L^3}\prod_{j=1}^{3}\left[\sum_{k_j,m_j=1}^{\infty} e^{-l\beta\hbar^2\pi^2 k_j^2/2ML^2}\, e^{-(n-l)\beta\hbar^2\pi^2 m_j^2/2ML^2} + \frac{1}{2}\sum_{k_j=1}^{\infty} e^{-n\beta\hbar^2\pi^2 k_j^2/2ML^2}\right] .$$
$$(5.97)$$

The last quantity is the self-energy given by Eq. (5.78), using the same transformation which was used in Eq. (5.77). So,

$$\sigma_n^{(D,E)}(\mathbf{k}) = -\frac{g}{\hbar}\prod_{j=1}^{3}\sigma_n^{(D,E)}(k_j), \quad (5.98)$$

where $\sigma_n^{(D,E)}(k_j)$ is the one-dimensional result following Eq. (5.78),

$$\sigma_n^{(D,E)}(k_j) \equiv \int dx_j\, \psi_{k_j}(x_j)\psi_{k_j}^*(x_j)\,(x_j, n\hbar\beta; x_j, 0)^{(0)}. \quad (5.99)$$

As we see, the self-energy contribution results depend on quantum numbers n_j and particle number n. Then, in this calculation, it is more convenient to represent the wave function in terms of the exponential as done in Eq. (2.109), so using Eqs. (2.109) and (5.89), we obtain

$$\sigma_n^{(D,E)}(k_j) = \frac{2}{L^2}\sum_{m_j=1}^{\infty} e^{-n\beta\hbar^2\pi^2 m_j^2/2ML^2}\int_0^L dx_j\left[1 - \cos\left(\frac{2\pi m_j x_j}{L}\right)\right]\sin^2\left(\frac{\pi k_j x_j}{L}\right).$$
$$(5.100)$$

The result of this last integral is

$$\int_0^L dx_j\left[1 - \cos\left(\frac{2\pi m_j x_j}{L}\right)\right]\sin^2\left(\frac{\pi k_j x_j}{L}\right) = \frac{L}{2}\left(1 + \frac{1}{2}\delta_{k_j,m_j}\right) . \quad (5.101)$$

So inserting Eq. (5.101) in Eq.(5.100), we have

$$\sigma_n^{(D,E)}(k_j) = \frac{1}{L}\sum_{m_j=1}^{\infty} e^{-n\beta\hbar^2\pi^2 m_j^2/2ML^2}\left(1 + \frac{1}{2}\delta_{k_j,m_j}\right) , \quad (5.102)$$

and therefore, with Eq. (4.61) and Eq. (5.98)

$$\sigma_n^{(D,E)}(\mathbf{k}) = -\frac{g}{\hbar L^3} \prod_{j=1}^{3} \left(\sum_{m_j=1}^{\infty} e^{-n\beta\hbar^2\pi^2 m_j^2/2ML^2} + \frac{1}{2} e^{-n\beta\hbar^2\pi^2 k_j^2/2ML^2} \right). \qquad (5.103)$$

With the complete formulas, we can calculate the thermodynamic quantities for this system following the recursive formulas for the non-interacting case, but before we shall put the Hartree-Fock integrals and the self-energy as a function of the dimensionless temperature τ which in the box case is given by Eq. (4.57). To write $\tilde{Z}_1(n\beta)$ and $I_{l,n-l}^{(D,E)}(\beta)$ from Eqs. (5.56), (5.103) and (5.97) we know that

$$\frac{g\beta}{L^3} = \frac{2a_s}{L\tau}, \qquad (5.104)$$

where here was used that g is given by Eq. (5.76) and τ by Eq. (4.57). Therefore,

$$I_{l,n-l}^{(D,E)}(\tau) = \frac{2na_s}{L\tau} \prod_{j=1}^{3} \left[\sum_{k_j,m_j=1}^{\infty} e^{-l\beta\hbar^2\pi^2 k_j^2/2ML^2} e^{-(n-l)\beta\hbar^2\pi^2 m_j^2/2ML^2} + \frac{1}{2} \sum_{k_j=1}^{\infty} e^{-n\beta\hbar^2\pi^2 k_j^2/2ML^2} \right], \qquad (5.105)$$

and

$$\sigma_n^{(D,E)}(\mathbf{k}) = -\frac{2na_s}{L\hbar\tau\beta} \prod_{j=1}^{3} \left(\sum_{m_j=1}^{\infty} e^{-n\beta\hbar^2\pi^2 m_j^2/2ML^2} + \frac{1}{2} e^{-n\beta\hbar^2\pi^2 k_j^2/2ML^2} \right). \qquad (5.106)$$

So, we can write the renormalized one-particle partition function $\hat{Z}_1(n\beta)$ using Eqs. (5.56) and (5.106),

$$\tilde{Z}_1(n\beta) = \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}} \left[1 + \frac{4na_s}{L\tau} \prod_{j=1}^{3} \left(\sum_{m_j=1}^{\infty} e^{-n\beta\hbar^2\pi^2 m_j^2/2ML^2} + \frac{1}{2} e^{-n\beta\hbar^2\pi^2 k_j^2/2ML^2} \right) \right], \qquad (5.107)$$

where $E_{\mathbf{k}}$ is given by Eq. (4.59). Finally, with this equation and Eq. (5.105), we have the canonical formula,

$$Z_N^B(\beta) = \frac{1}{N} \sum_{n=1}^{N} \left[\tilde{Z}_1(n\tau) - \frac{na_s}{L\tau} \sum_{l=1}^{n-1} \prod_{j=1}^{3} \sum_{k_j,m_j=1}^{\infty} e^{-l\pi k_j^2/4\tau} e^{-(n-l)\pi m_j^2/4\tau} + \frac{1}{2} \sum_{k_j=1}^{\infty} e^{-n\pi k_j^2/4\tau} \right] Z_{N-n}^B(\beta). \qquad (5.108)$$

With this final formula, we can plot the thermodynamic quantities for this system for some values of the gas parameter $a_s n^{1/3}$. To illustrate the behavior for many particles, we fixed the gas parameter in $a_s n^{1/3} = 0.1$. Using the same formulas of Chapter 4: Eqs. (4.42), (4.35) and (4.39). First, in figure 5.10, we have the condensed fraction for various numbers of particles, $10, 100, 1000$ considering the gas parameter equal to 0.1; after we have the heat capacity plot for the same N's and interacting parameter in 5.11.

Figure 5.10: Condensed fraction for $10, 100, 1000$ particles in a weakly interacting finite box with gas parameter given by $a_s n^{1/3} = 0.1$.

5.4.2 Dilute Bose gas in a harmonic trap

From Eqs. (5.77) and (5.78), we need the propagators of the three-dimensional harmonic oscillator. Then, for to compute the imaginary-time evolution amplitude $(x, k\hbar\beta|x, 0)_{(0)}$ we start from the 1D path integral representation

$$(x, k\hbar\beta; x', 0)^{(0)} = \int_{x(0)=x'}^{x(k\hbar\beta)=x} Dx \exp\left[-\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \frac{M}{2}\left(\dot{x}^2 + \omega_j^2 x^2\right)\right]. \qquad (5.109)$$

In Appendix D we present the details of calculations of the formula Eq. (5.109), and it final result is

$$(x, k\hbar\beta; x', 0)^{(0)} = \left[\frac{M\omega_j}{2\pi\hbar \sinh(k\beta\hbar\omega_j)}\right]^{1/2} \exp\left[-\frac{M\omega_j}{2\hbar \sinh(k\beta\hbar\omega_j)}\left[\left(x^2 + x'^2\right)\cosh(k\beta\hbar\omega_j) - 2x\,x'\right]\right].$$
$$(5.110)$$

Generalizing Eq. (5.110) for three dimensions, and taking for simplicity

Figure 5.11: Heat capacity for $10, 100, 1000$ particles in a weakly interacting finite box with gas parameter given by $a_s n^{1/3} = 0.1$.

$\omega = \omega_x = \omega_y = \omega_z$, we obtain the one-particle harmonic propagator as

$$(\mathbf{x}, k\hbar\beta; \mathbf{x}', 0)^{(0)} = \left[\frac{M\omega}{2\pi\hbar \sinh(k\beta\hbar\omega)} \right]^{3/2} \exp\left[-\frac{M\omega}{2\hbar \sinh(k\beta\hbar\omega)} \left[\left(\mathbf{x}^2 + \mathbf{x}'^2\right) \cosh(k\beta\hbar\omega) - 2\mathbf{x} \cdot \mathbf{x}' \right] \right].$$
(5.111)

Now that we calculated the harmonic one-particle propagator, we can use the canonical formalism developed in the previous section to compute Eq. (5.77). Substituting Eq. (5.111) in Eq. (5.75), we have that

$$I_{l,n-l}^{(D,E)}(\beta) = \hbar\beta g \left[\frac{M\omega}{2\pi\hbar \sinh(l\beta\hbar\omega)} \right]^{3/2} \left[\frac{M\omega}{2\pi\hbar \sinh((n-l)\beta\hbar\omega)} \right]^{3/2}$$

$$\times \int d^3x \exp\left[-\frac{M\omega\mathbf{x}^2}{\hbar \sinh(l\beta\hbar\omega)} \left[\cosh(l\beta\hbar\omega) - 1\right] \right] \exp\left[-\frac{M\omega\mathbf{x}^2}{\hbar \sinh((n-l)\beta\hbar\omega)} \left[\cosh((n-l)\beta\hbar\omega) - 1\right] \right],$$
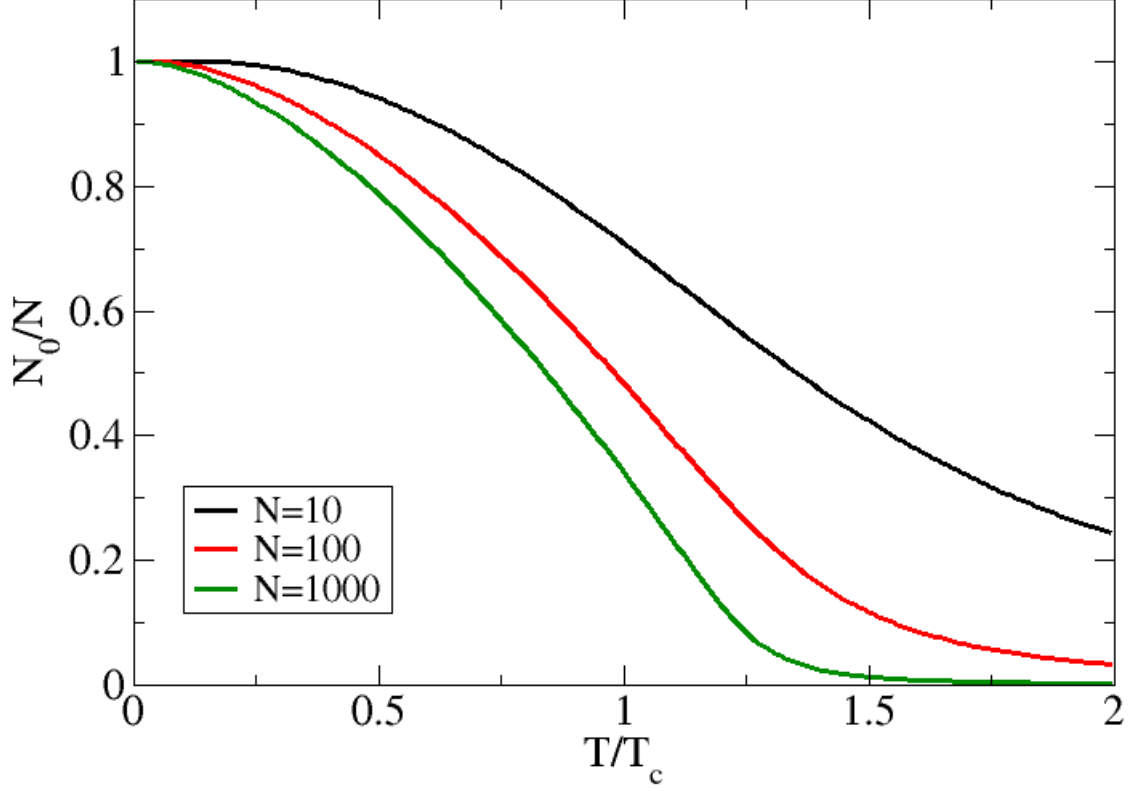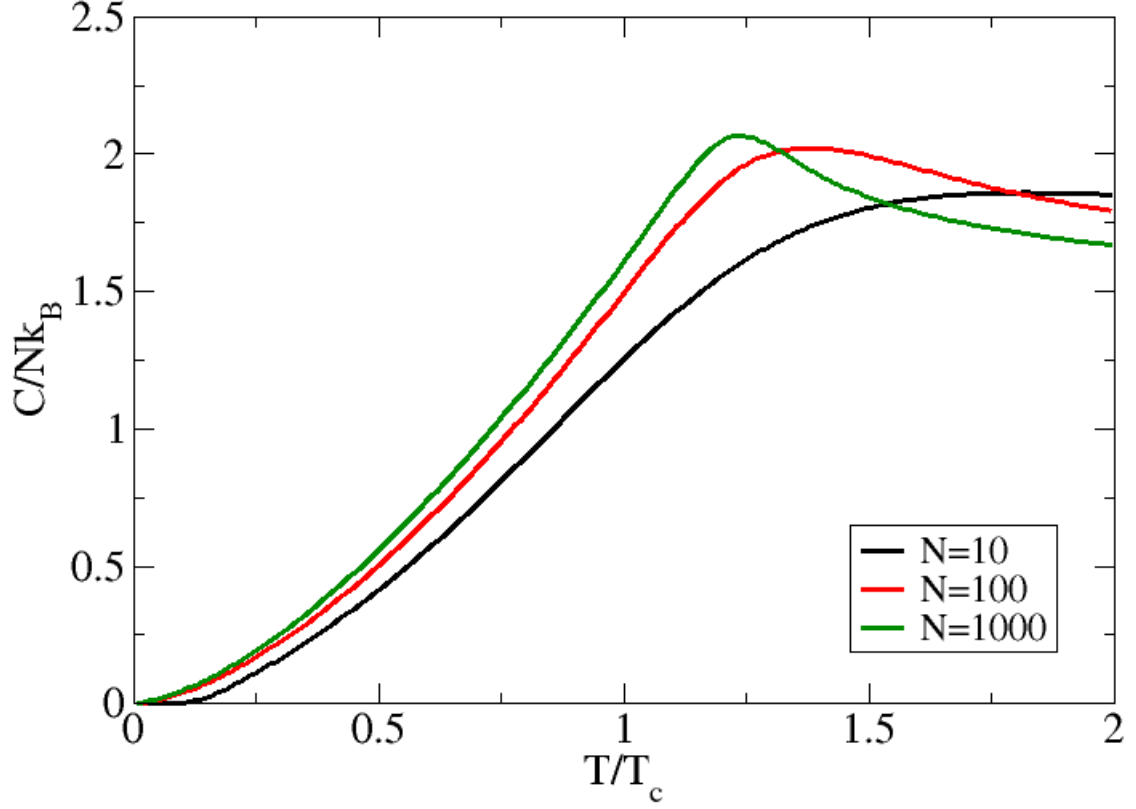(5.112)

Figure 5.12: Ground state fluctuation for $10, 100, 1000$ particles in a weakly interacting finite box with gas parameter given by $a_s n^{1/3} = 0.1$.

and solving the Gaussian integral we get

$$I_{l,n-l}^{(D,E)}(\beta) = g\hbar\beta \left[\frac{M\omega}{2\pi\hbar}\right]^3 \frac{1}{\sinh^{3/2}(l\beta\hbar\omega)\sinh^{3/2}((n-l)\beta\hbar\omega)}$$

$$\times \left[\frac{\pi\hbar}{M\omega}\left(\frac{\cosh(l\beta\hbar\omega)-1}{\sinh(l\beta\hbar\omega)} + \frac{\cosh((n-l)\beta\hbar\omega)-1}{\sinh((n-l)\hbar\beta\omega)}\right)^{-1}\right]^{3/2}. \quad (5.113)$$

But the hyperbolic trigonometric expression can be written as

$$\left(\frac{\cosh(l\beta\hbar\omega)-1}{\sinh(l\beta\hbar\omega)} + \frac{\cosh((n-l)\beta\hbar\omega)-1}{\sinh((n-l)\hbar\beta\omega)}\right)\sinh(l\beta\hbar\omega)\sinh((n-l)\beta\hbar\omega) =$$

$$4\sinh\left(\frac{l\beta\hbar\omega}{2}\right)\sinh\left(\frac{n\beta\hbar\omega}{2}\right)\sinh\left(\frac{(n-l)\beta\hbar\omega}{2}\right) \quad (5.114)$$

and inserting Eq. (2.56) in Eq. (2.55) gives

$$I_{l,n-l}^{(D,E)}(\beta) = g\hbar\beta \left[\frac{M\omega}{\pi\hbar}\right]^{3/2} \frac{1}{8 \times 4^{3/2}} \left[\sinh\left(\frac{l\beta\hbar\omega}{2}\right) \sinh\left(\frac{n\beta\hbar\omega}{2}\right) \sinh\left(\frac{(n-l)\beta\hbar\omega}{2}\right)\right]^{-3/2}.$$

(5.115)

Equation (5.115) is complicated, but can be simplified with a non-interacting partition function here by $Z_1^{(0)}(n\beta)$. Let's see how this is possible. The one-particle partition function $Z_1^{(0)}(n\beta)$ has another representation, that is by integral over diagonal terms in non-interacting time-evolution propagator $(\mathbf{x}, t; \mathbf{x}', 0)_{(0)}$:

$$Z_1(n\beta) = \int d^3x \ (\mathbf{x}, n\hbar\beta; \mathbf{x}, 0)^{(0)}.$$

(5.116)

According to Eq. (5.110), we have for Eq. (5.116):

$$Z_1(n\beta) = \int d^3x \left[\frac{M\omega}{2\pi\hbar \sinh(k\beta\hbar\omega)}\right]^{3/2} \exp\left[-\frac{M\omega\mathbf{x}^2}{\hbar \sinh(k\beta\hbar\omega)} [\cosh(k\beta\hbar\omega) - 1]\right]$$

(5.117)

and hence,

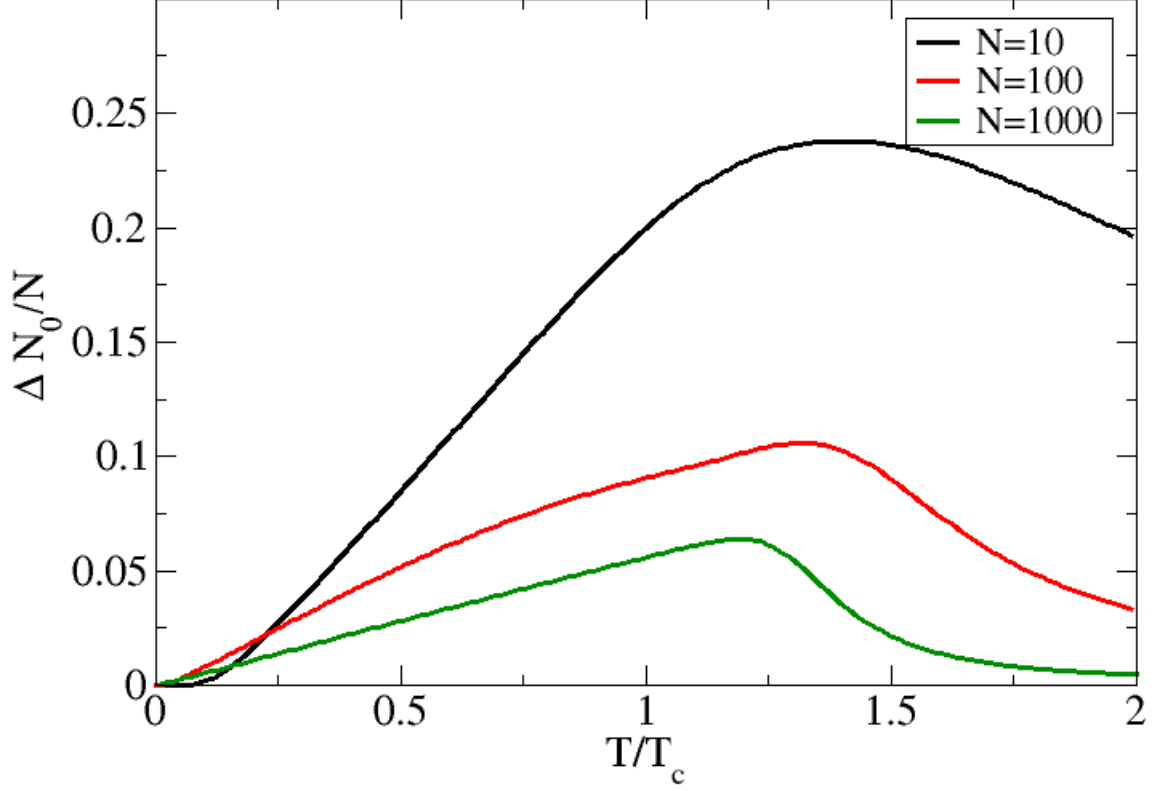$$Z_1(n\beta) = \frac{1}{8 \sinh^3\left(\frac{n\beta\hbar\omega}{2}\right)}.$$

(5.118)

By equation (2.2.1), we see that the hyperbolic sines in Eq. (2.70) can be written in terms of $Z_1^{(0)}(n\beta)$

$$\left[\sinh\left(\frac{l\beta\hbar\omega}{2}\right) \sinh\left(\frac{n\beta\hbar\omega}{2}\right) \sinh\left(\frac{(n-l)\beta\hbar\omega}{2}\right)\right]^{-3/2} = \left[\frac{1}{8 Z_1^{1/3}(n\beta) Z_1^{1/3}(l\beta) Z_1^{1/3}((n-l)\beta)}\right]^{-3/2}$$

$$= \frac{1}{2^{9/2} \left(Z_1(n\beta) Z_1(l\beta) Z_1((n-l)\beta)\right)^{1/2}}. \quad (5.119)$$

Therefore, equation (5.115) is equal to

$$I_{l,n-l}^{(D,E)}(\beta) = g\hbar\beta \left[\frac{M\omega}{2\pi\hbar}\right]^{3/2} \left(Z_1(n\beta) Z_1(l\beta) Z_1((n-l)\beta)\right)^{1/2}.$$

(5.120)

Now the next step is to calculate the self-energies contributions given by Eq. (5.78). We know that the quantum harmonic oscillator can be solved by two possibilities: using the matrix formula as made in non-interacting calculation. But here, we need of analytical formula of the wave functions because Eq. (5.78) is an integral. So, the three-dimensional wave function is given by

$$\psi_{\mathbf{k}}(\mathbf{x}) = \prod_{j=1}^{3} \left(\frac{M\omega_j}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^{k_j} k_j!}} e^{-M\omega_j x_j^2/2\hbar} H_{k_j}\left(\sqrt{\frac{M\omega_j}{\hbar}} x_j\right),$$

(5.121)

where $H_n(x)$ is the Hermite polynomial. The quantum number vector $\mathbf{k}$ is defined as (k_1, k_2, k_3). Due to the complicated formula of this wave function, is more convenient to write Eq. (5.78) as a product following Eqs. (5.98) and (5.98). So, we will solve Eq. (5.99) and after include this result in Eq. (5.98). Using the one-dimensional results of

Eqs. (5.111) and (5.121), (5.78) is written as an equation that depends on the Hermite-Gauss integral, then

$$\sigma_n^{(D,E)}(k_j) = \int_{-\infty}^{\infty} dx_j \left(\frac{M\omega_j}{\pi\hbar}\right)^{1/2} \frac{1}{2^{k_j}\, k_j!} e^{-M\omega_j x_j^2/\hbar}\, H_{k_j}^2 \left(\sqrt{\frac{M\omega_j}{\hbar}}\, x_j\right)$$
$$\times \left[\frac{M\omega_j}{2\pi\hbar \sinh(n\beta\hbar\omega_j)}\right]^{1/2} \exp\left[-\frac{M\omega_j x_j^2}{\hbar \sinh(n\beta\hbar\omega_j)} [\cosh(n\beta\hbar\omega_j) - 1]\right] \quad (5.122)$$

however,

$$\frac{\cosh(n\beta\hbar\omega_j) - 1}{\sinh(n\beta\hbar\omega_j)} = \tanh\left(\frac{n\beta\hbar\omega_j}{2}\right) \quad (5.123)$$

therefore,

$$\sigma_n^{(D,E)}(k_j) = \int_{-\infty}^{\infty} dx_j \left(\frac{M\omega_j}{\pi\hbar}\right)^{1/2} \frac{1}{2^{k_j}\, k_j!} e^{-M\omega_j x_j^2/\hbar}\, H_{k_j}^2 \left(\sqrt{\frac{M\omega_j}{\hbar}}\, x_j\right)$$
$$\times \left[\frac{M\omega_j}{2\pi\hbar \sinh(n\beta\hbar\omega_j)}\right]^{1/2} \exp\left[-\frac{M\omega_j x_j^2}{\hbar} \tanh\left(\frac{n\beta\hbar\omega_j}{2}\right)\right]. \quad (5.124)$$

$$\sigma_n^{(D,E)}(k_j) = \left(\frac{M\omega_j}{\pi\hbar}\right)^{1/2} \frac{1}{2^{k_j}\, k_j!} \left[\frac{M\omega_j}{2\pi\hbar \sinh(n\beta\hbar\omega_j)}\right]^{1/2}$$
$$\times \int_{-\infty}^{\infty} dx_j\, e^{-M\omega_j x_j^2/\hbar}\, H_{k_j}^2 \left(\sqrt{\frac{M\omega_j}{\hbar}}\, x_j\right) \exp\left[-\frac{M\omega_j x_j^2}{\hbar} \tanh\left(\frac{n\beta\hbar\omega_j}{2}\right)\right]. \quad (5.125)$$

Here our problem is the last integral in Eq. (5.125) because it is a complicated integral. In Appendix D we have the details of the solution to this integral. For simplicity, let us denote the integral in Eq. (5.125) as $X(n, k_j)$,

$$X(n, k_j) = \int_{-\infty}^{\infty} dx_j\, e^{-M\omega_j x_j^2/\hbar}\, H_{k_j}^2 \left(\sqrt{\frac{M\omega_j}{\hbar}}\, x_j\right) \exp\left[-\frac{M\omega_j x_j^2}{\hbar} \tanh\left(\frac{n\beta\hbar\omega_j}{2}\right)\right].$$
$$(5.126)$$

The Hermite-Gauss integral can be given by [46]

$$\int_{-\infty}^{\infty} H_m(x)\, H_n(x)\, e^{-a^2 x^2}\, dx = \frac{2^{m+n}}{a^{m+n+1}} \left(1 - a^2\right)^{(m+n)/2} \Gamma\left(\frac{1+m+n}{2}\right)$$
$$\times \sum_{\nu=0}^{\min(m,n)} \frac{(-m)_\nu (-n)_\nu}{\nu!\left(\frac{1-m-n}{2}\right)_\nu} \left(\frac{a^2}{2(a^2 - 1)}\right)^\nu, \quad (5.127)$$

where $(x)_\nu$ is the Pochhammer symbol [46, 47] defined as

$$(x)_\nu = \frac{\Gamma(x+\nu)}{\Gamma(x)}. \quad (5.128)$$

Then, applying Eq. (5.127) in Eq. (5.126), we have

$$X(n, k_j) = \left(\frac{\hbar}{M\omega_j}\right)^{1/2} \frac{2^{2k_j}}{a^{2k_j+1}} \left(1 - a^2\right)^{k_j} \Gamma\left(\frac{1 + 2k_j}{2}\right)$$
$$\times \sum_{\nu=0}^{k_j} \frac{(-k_j)_\nu (-k_j)_\nu}{\nu! \left(\frac{1-2k_j}{2}\right)_\nu} \left(\frac{a^2}{2(a^2-1)}\right)^\nu, \quad (5.129)$$

where

$$a^2 \equiv 1 + \tanh\left(\frac{n\beta\hbar\omega_j}{2}\right). \quad (5.130)$$

The Gamma function in Eq. (5.129) [47] is

$$\Gamma\left(\frac{1 + 2k_j}{2}\right) = \frac{(2k_j)! \pi^{1/2}}{4^{k_j} k_j!} \quad (5.131)$$

using Eq. (5.131) in Eq. (5.129),

$$X(n, k_j) = \left(\frac{\hbar\pi}{M\omega_j}\right)^{1/2} \frac{(2k_j)!}{k_j!} \frac{(1 - a^2)^{k_j}}{(a^2)^{k_j+1/2}} \sum_{\nu=0}^{k_j} \frac{(-k_j)_\nu (-k_j)_\nu}{\nu! \left(\frac{1-2k_j}{2}\right)_\nu} \left(\frac{a^2}{2(a^2-1)}\right)^\nu. \quad (5.132)$$

Then with Eq. (5.132), we can calculate Eq. (5.125) and we obtain that

$$\sigma_n^{(D,E)}(k_j) = \left[\frac{M\omega_j}{2\pi\hbar \sinh(n\beta\hbar\omega_j)}\right]^{1/2} \frac{(2k_j)!}{2^{k_j}(k_j!)^2} \frac{(1 - a^2)^{k_j}}{(a^2)^{k_j+1/2}} \sum_{\nu=0}^{k_j} \frac{(-k_j)_\nu (-k_j)_\nu}{\nu! \left(\frac{1-2k_j}{2}\right)_\nu} \left(\frac{a^2}{2(a^2-1)}\right)^\nu.$$
$$(5.133)$$

Now the next step is to substitute the values of a^2 in terms of n-dependence. As a^2 is given by Eq. (5.130), then

$$\frac{a^2}{a^2 - 1} = 2\frac{e^{n\beta\hbar\omega_j}}{e^{n\beta\hbar\omega_j} - 1}, \quad (5.134)$$

$$\frac{1 - a^2}{a^2} = -\frac{e^{n\beta\hbar\omega_j} - 1}{2\, e^{n\beta\hbar\omega_j}}. \quad (5.135)$$

Therefore putting Eqs. (5.135), (5.134) in Eq. (5.133), we have a complete formula of one-dimensional self-energy,

$$\sigma_n^{(D,E)}(k_j) = \left[\frac{M\omega_j}{2\pi\hbar \sinh(n\beta\hbar\omega_j)}\right]^{1/2} \frac{(2k_j)!}{2^{k_j}(k_j!)^2} \left(-\frac{e^{n\beta\hbar\omega_j} - 1}{2\, e^{n\beta\hbar\omega_j}}\right)^{k_j} \sum_{\nu=0}^{k_j} \frac{(-k_j)_\nu (-k_j)_\nu}{\nu! \left(\frac{1-2k_j}{2}\right)_\nu} \left(\frac{e^{n\beta\hbar\omega_j}}{e^{n\beta\hbar\omega_j} - 1}\right)^\nu.$$
$$(5.136)$$

The final result of three-dimensional self-energy is given by Eq. (5.78), that is,

$$\sigma_n^{(D,E)}(\mathbf{k}) = -\frac{g}{\hbar} \prod_{j=1}^{3} \left[\frac{M\omega_j}{2\pi\hbar \sinh(n\beta\hbar\omega_j)}\right]^{1/2} \frac{(2k_j)!}{2^{k_j}(k_j!)^2} \left(-\frac{e^{n\beta\hbar\omega_j} - 1}{2\, e^{n\beta\hbar\omega_j}}\right)^{k_j}$$
$$\times \sum_{\nu=0}^{k_j} \frac{(-k_j)_\nu (-k_j)_\nu}{\nu! \left(\frac{1-2k_j}{2}\right)_\nu} \left(\frac{e^{n\beta\hbar\omega_j}}{e^{n\beta\hbar\omega_j} - 1}\right)^\nu. \quad (5.137)$$

This formula can be simplified by developing the Pochhammmer symbols. As the numbers are integers, then the gamma function will reduce to factorials. First, we see that

$$\left(\frac{1}{2} - k_j\right)_\nu = \frac{\Gamma(1/2 + \nu - k_j)}{\Gamma(1/2 - k_j)},$$ (5.138)

where

$$\Gamma\left(\frac{1}{2} - k_j\right) = \frac{(-4)^{k_j} k_j! \sqrt{\pi}}{(2k_j)!}.$$ (5.139)

The other Pochhammer symbol $(-k_j)_\nu$ is

$$(-k_j)_\nu = \frac{\Gamma(\nu - k_j)}{\Gamma(-k_j)} = \frac{(-1)^\nu k_j!}{(k_j - \nu)!}.$$ (5.140)

Another simplification is over the exponentials,

$$\left(-\frac{e^{n\beta\hbar\omega_j} - 1}{2\, e^{n\beta\hbar\omega_j}}\right)^{k_j} \left(\frac{e^{n\beta\hbar\omega_j}}{e^{n\beta\hbar\omega_j} - 1}\right)^\nu = \left(\frac{-1}{2}\right)^{k_j} \left(\frac{e^{n\beta\hbar\omega_j} - 1}{e^{n\beta\hbar\omega_j}}\right)^{k_j - \nu},$$ (5.141)

and therefore inserting Eqs. (5.141), (5.140), (5.139), (5.138) in Eq. (5.137), we obtain that

$$\sigma_n^{(D,E)}(\mathbf{k}) = -\frac{g}{\hbar} \prod_{j=1}^3 \left[\frac{M\omega_j}{\pi\hbar}\right]^{1/2} \frac{k_j!}{(e^{n\beta\hbar\omega_j} - e^{-n\beta\hbar\omega_j})^{1/2}} \sum_{\nu=0}^{k_j} \left(\frac{e^{n\beta\hbar\omega_j} - 1}{e^{n\beta\hbar\omega_j}}\right)^{k_j - \nu} \frac{(2(k_j - \nu))!}{(-4)^{k_j - \nu} \nu!\, [(k_j - \nu)!]^3},$$ (5.142)

that is the self-energy contribution of a harmonic trap with contact interaction. Now, we have the complete formulas to build the N-particle partition function $Z_N^B(\beta)$. The same procedure used in the finite box case will be done here, writing Eqs. (5.142) and (5.120) in a function of τ using Eqs. (5.76) and (4.68). So, the constant is given by

$$g\hbar\beta\left(\frac{M\omega}{2\pi\hbar}\right)^{3/2} = \hbar\sqrt{\frac{2}{\pi}}\frac{a_s}{l\,\tau},$$ (5.143)

where l is the harmonic oscillator length,

$$l \equiv \sqrt{\frac{\hbar}{M\omega}}.$$ (5.144)

Then with this representation, Eq. (5.142) becomes

$$\sigma_n^{(D,E)}(\mathbf{k}) = -\sqrt{\frac{2}{\pi}}\frac{a_s}{l\hbar\beta\tau} \prod_{j=1}^3 \frac{k_j!}{(e^{n/\tau} - e^{-n/\tau})^{1/2}} \sum_{\nu=0}^{k_j} \left(\frac{e^{n/\tau} - 1}{e^{n/\tau}}\right)^{k_j - \nu} \frac{(2(k_j - \nu))!}{(-4)^{k_j - \nu} \nu!\, [(k_j - \nu)!]^3},$$ (5.145)

and therefore, Eq. (5.56) now is given by

$$\tilde{Z}_1(n\beta) = \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}} \left(1 + \sqrt{\frac{2}{\pi}}\frac{na_s}{l\tau} \prod_{j=1}^3 \frac{k_j!}{(e^{n/\tau} - e^{-n/\tau})^{1/2}} \sum_{\nu=0}^{k_j} \left(\frac{e^{n/\tau} - 1}{e^{n/\tau}}\right)^{k_j - \nu} \frac{(2(k_j - \nu))!}{(-4)^{k_j - \nu} \nu!\, [(k_j - \nu)!]^3}\right),$$ (5.146)
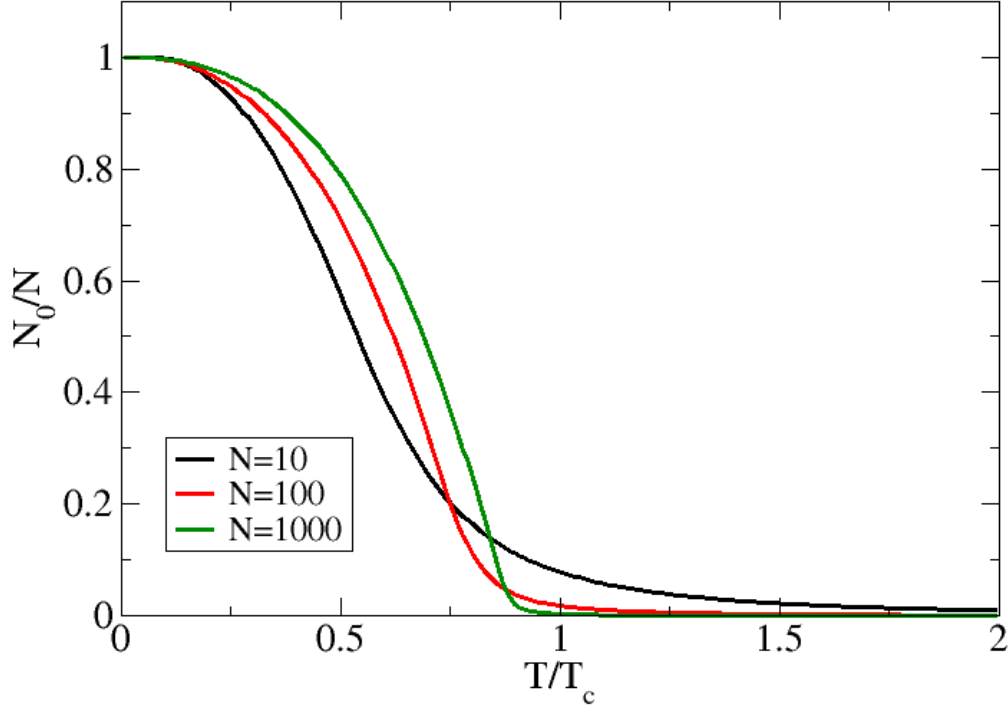
Figure 5.13: Condensed fraction for $10, 100, 1000$ particles in a weakly interacting harmonic trap with gas parameter given by $a_s n^{1/3} = 0.1$.

where $\mathbf{k}$ is the quantum number vectors and $E_{\mathbf{k}}$ given by Eq. (2.68). Then, the fully $Z_N^B(\beta)$ given by Eq. (5.55) for a three-dimensional harmonic trap is now,

$$Z_N^B(\beta) = \frac{1}{N} \sum_{n=1}^{N} \left[\tilde{Z}_1(n\beta) - \sqrt{\frac{2}{\pi}} \frac{na_s}{l\tau} \sum_{l=1}^{n-1} \left(Z_1^{(0)}(n\beta) Z_1^{(0)}(l\beta) Z_1^{(0)}((n-l)\beta) \right)^{1/2} \right] Z_{N-n}^B(\beta).$$

(5.147)

Now with the complete canonical scheme, we can compute the thermal properties of this system following the same parameters and different values of N as done in the finite box case. Then, by Eq. (4.35) we have the condensed fraction shown in Fig. 5.13, the heat capacity Eq. (4.6) in Fig. ; and finally, the comparison for the condensed fraction for 10 particles between ideal and interacting case as shown in 5.16.

5.5 Discussion of results

In the same form that was done in the previous chapter, we can do a table with the critical temperatures calculated by two ensembles to compare them. As seen in Chapter 3, the interacting corrections do not depend on the number of particles Eq. (3.74), its value is fixed and depends on scattering length. Therefore, now we are interested in comparing the values with and without interaction calculated in the canonical ensemble
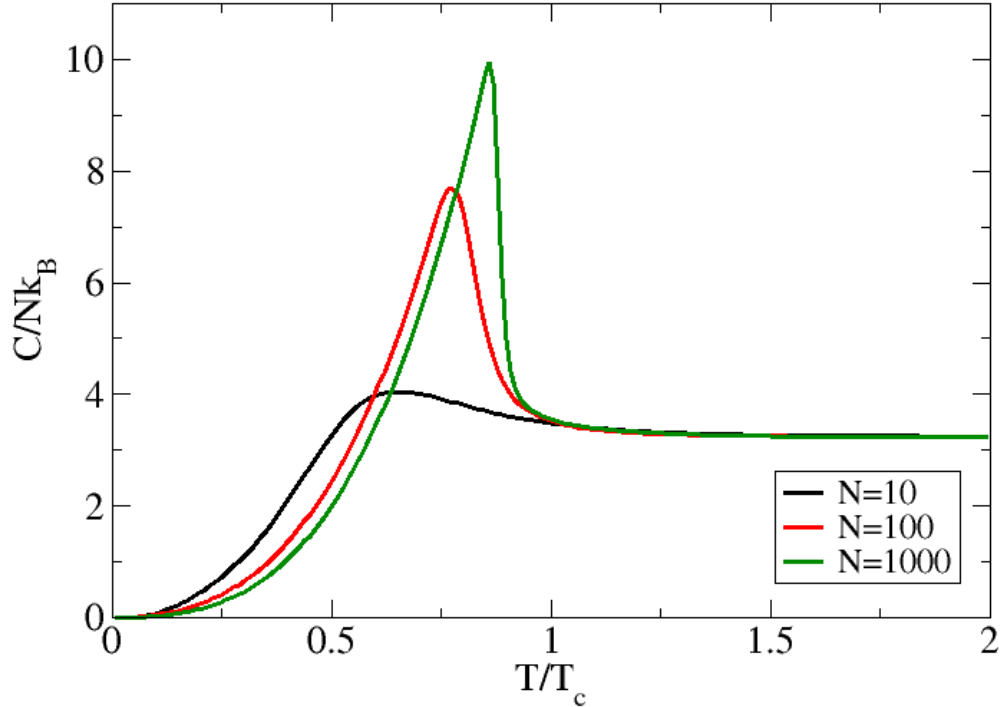
Figure 5.14: Heat capacity for $10, 100, 1000$ particles in a weakly interacting harmonic trap with gas parameter given by $a_s n^{1/3} = 0.1$.

and after, with the grand canonical preview. We did the plots for the heat capacity for 1000 particles, to check the consistency of our calculations for the harmonic trap and finite box given by Fig. 5.16 and Fig. 5.17. Each plot was done for two cases: the black line is the non-interacting case and the red line, is the interacting case done for a gas parameter given by $a_s n^{1/3} = 0.1$.

Here, we have the behavior of the traps due to interaction. For the harmonic trap, the interacting critical temperature is less than the non-interacting result, following the grand canonical preview. Another good point is the maximum point of the heat capacity in the critical point and by our grand canonical analysis, the prevision is that this maximum is greater than its ideal correspondent, and this behavior is seen in Fig. 5.16.

Of the same form as done in the non-interacting case, we have a table with the critical temperatures for each value of N, first for harmonic trap in Table 4.2 and second, for box trap in Table 5.1, but now the difference is that due to fact of the interacting shift do not depend of the number of particles, we compare the canonical non-interacting result given by Eq. () with the canonical interacting result Eq. ().

The good point of this weakly interacting canonical theory is that it has results agreeing with the grand canonical previews developed in Chapter 3. But when the number of particles increases, both calculations are similar. To see the difference between the
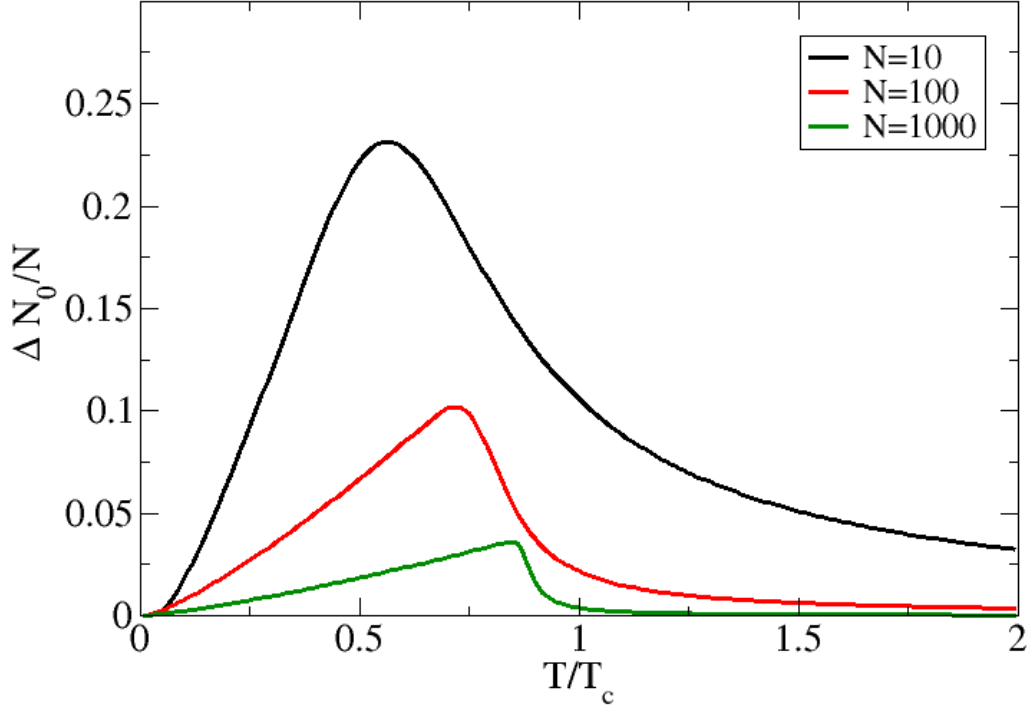
Figure 5.15: Ground state fluctuation for $10, 100, 1000$ particles in a weakly interacting harmonic trap with gas parameter given by $a_s n^{1/3} = 0.1$.

N	Canonical Interacting	Canonical Non-Interacting
10	1.82	1.82
100	1.38	1.37
1000	1.24	1.20

Table 5.1: Values of critical temperatures for a trapped Bose gas in a three-dimensional finite box calculated by two ensembles: canonical through Eq. (4.43) and grand canonical through Eq. (2.141).

N	Canonical Interacting	Canonical Non-Interacting
10	0.65	0.72
100	0.72	0.78
1000	0.85	0.89

Table 5.2: Values of critical temperatures for a trapped Bose gas in a three-dimensional isotropic harmonic trap calculated by two ensembles: canonical through Eq. (4.43) and grand canonical through Eq. (2.69).

Figure 5.16: Heat capacity for 1000 particles confined in a harmonic trap for two conditions: first, the black line representing the non-interacting case $a_s n^{1/3} = 0$ and in red, the weakly interacting situation with gas parameter given by $a_s n^{1/3} = 0.1$.

interacting and non-interacting canonical theory, we have the plots for the heat capacity, condensate fraction, and ground-state fluctuation for each system, finite box, and harmonic trap. The plots are in the Figs. 5.16, 5.17, 5.19, 5.18, 5.20 and 5.21. Clearly, the canonical interacting plots follow the grand canonical previews showing consistency with the previous theory developed in Chapter 3.
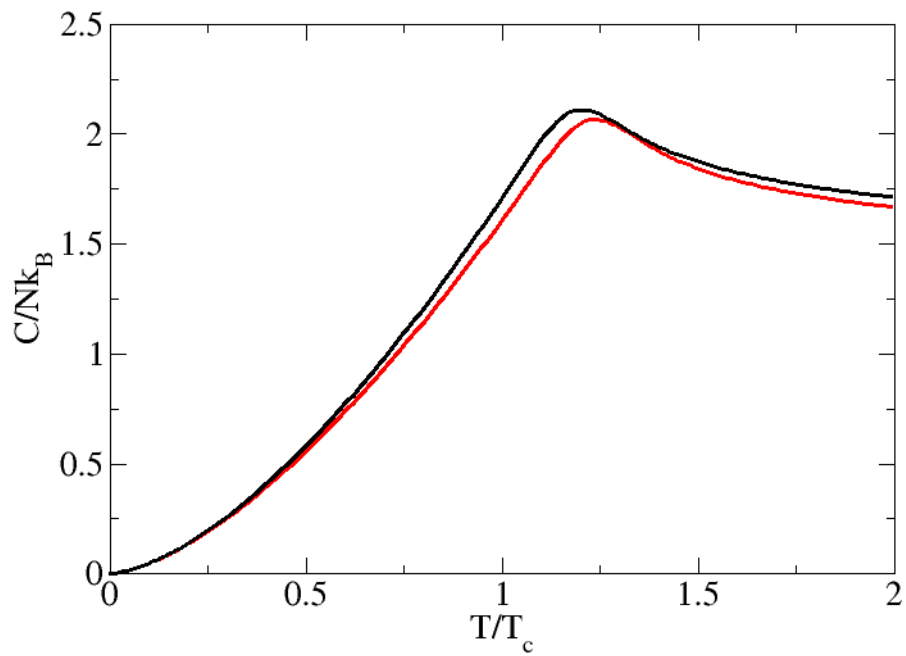
Figure 5.17: Heat capacity for 1000 particles confined in a finite box for two conditions: first, the black line representing the non-interacting case $a_s n^{1/3} = 0$ and in red, the weakly interacting situation with gas parameter given by $a_s n^{1/3} = 0.1$.
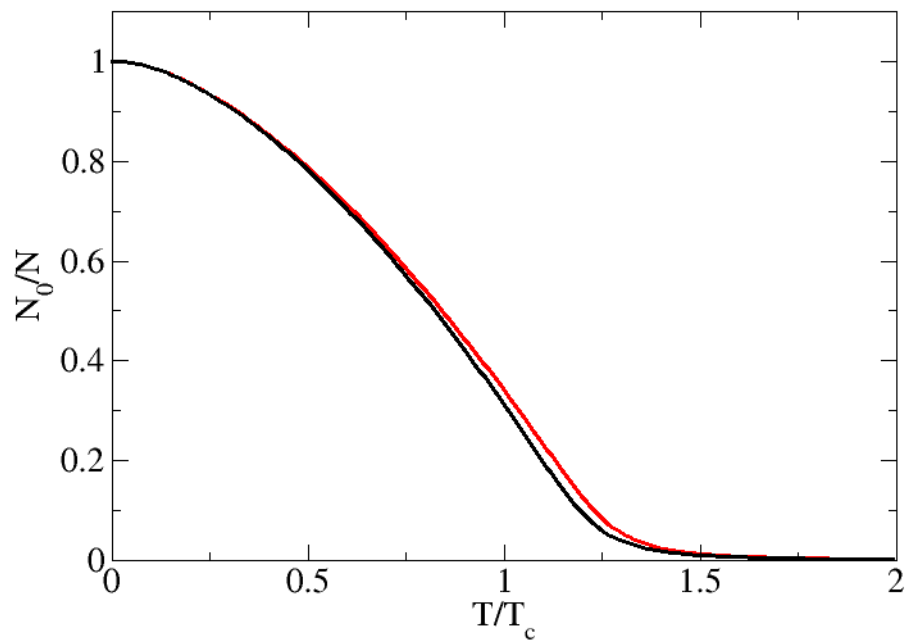
Figure 5.18: Condensed fraction for 1000 particles confined in a box trap for two conditions: first, the black line representing the non-interacting case $a_s n^{1/3} = 0$ and in red, the weakly interacting situation with gas parameter given by $a_s n^{1/3} = 0.1$.
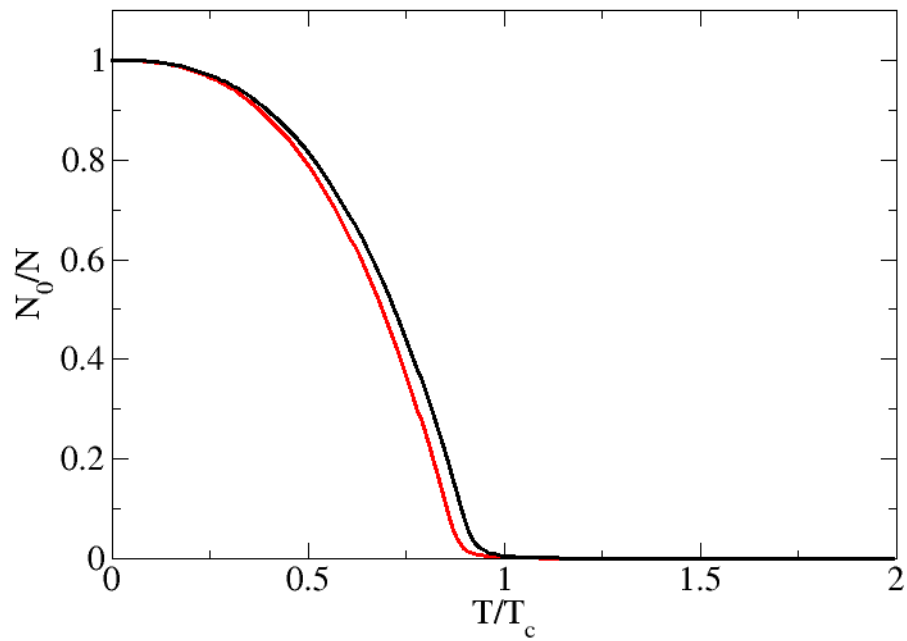
Figure 5.19: Condensed fraction for 1000 particles confined in a three-dimensional isotropic harmonic trap for two conditions: first, the black line representing the non-interacting case $a_s n^{1/3} = 0$ and in red, the weakly interacting situation with gas parameter given by $a_s n^{1/3} = 0.1$.

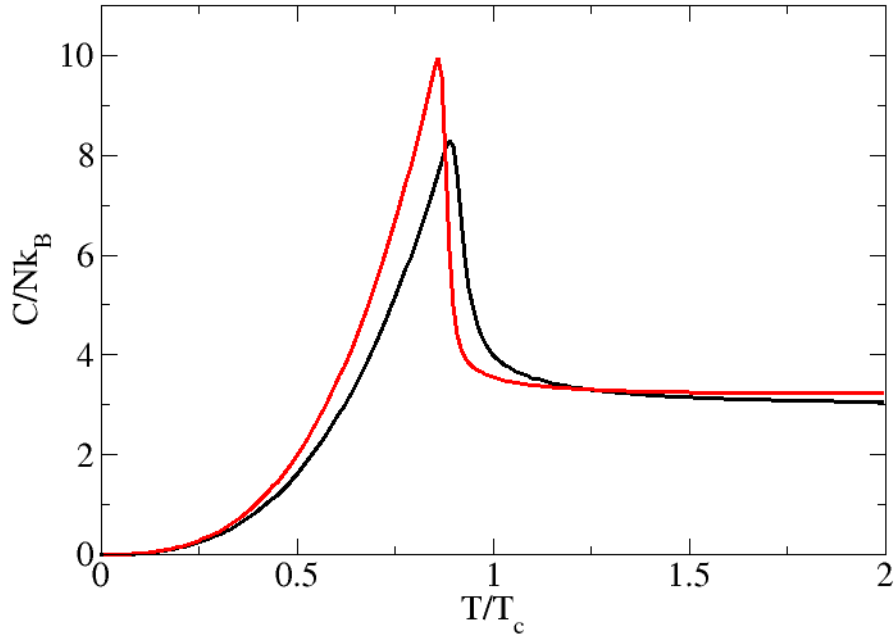Figure 5.20: Ground state fluctuation for 1000 particles confined in a box trap for two conditions: first, the black line representing the non-interacting case $a_s n^{1/3} = 0$ and in red, the weakly interacting situation with gas parameter given by $a_s n^{1/3} = 0.1$.

Figure 5.21: Ground state fluctuation for 1000 particles confined in a three-dimensional isotropic harmonic trap for two conditions: first, the black line representing the non-interacting case $a_s n^{1/3} = 0$ and in red, the weakly interacting situation with gas parameter given by $a_s n^{1/3} = 0.1$.
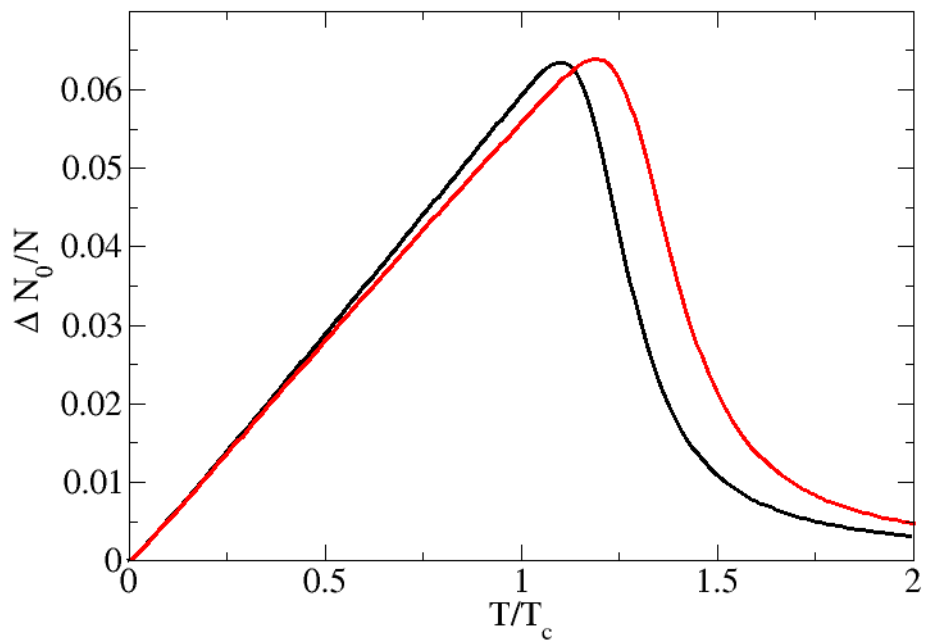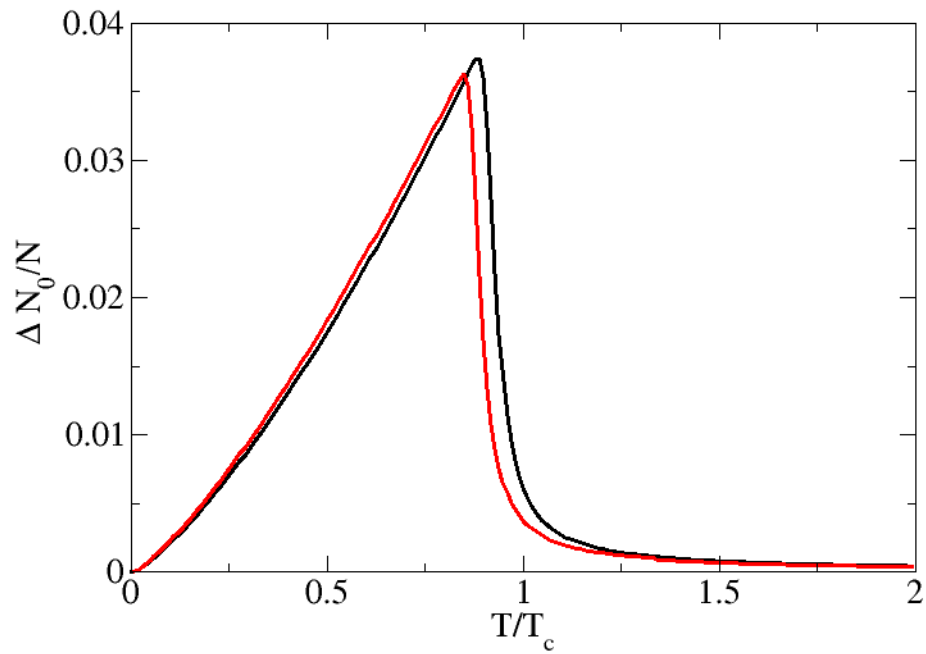
Chapter 6

Conclusions

This thesis studied the thermodynamics of the Bose gases using two different statistical ensembles, the grand canonical, and the canonical ensemble for two situations: the non-interacting and interacting case. The main idea was to describe the results for each ensemble and to check the validity of these in the thermodynamic limit when we have a large number of particles and we have one equivalence between them. We know that in the thermodynamic limit when the number of particles is very large, all statistical ensembles are equivalent.

By chapters 2 and 3, we saw that the inclusion of the interactions changes the critical temperature T_c. While in the finite box, the temperature increases, for the harmonic trap it decreases. The canonical results for these traps follow this idea as seen in Figs. 5.17 and 5.16 in the case of condensed fraction, clearly the plots follow the same grand canonical standard. The interesting here is that the critical temperatures have two corrections: first, the finite-size correction that is due to the new thermodynamic limit for confined Bose gas [13], and the perturbative correction due to interactions. The first shift depends on the number of particles when N is large, we have a small correction following the classical thermodynamic limit, and the second shift depends on the power interaction joined with the non-interacting critical temperature $T_c^{(0)}$. For the heat capacity, in the harmonic trap, the maximum point is greater than the non-interacting result while in the finite box is less than the non-interacting value. This behavior is seen in the canonical approach agreeing with our grand canonical one.

In Chapters 4 and 5, we developed the canonical theory, first with the classical non-interacting gas and later, with interactions. The results qualitatively agree with the grand canonical ones; this situation is described, first, in the ideal case when the plots for large N agree with the grand canonical ones with the finite-size correction as done in Figs. , while for interacting cases, we checked the critical temperatures with the grand canonical results. Again, we have that the canonical results agree with the grand canonical ones - and the same analysis method was employed for these two cases: with and without interaction. In Chapter 5 we developed the weakly interacting canonical theory where the Feynman diagrams are the same as the grand canonical theory but with different Feynman rules - and this is important to do a canonical perturbation theory for any order. We corrected the ground state due to interactions and could correctly obtain the heat capacity for low temperatures, and old problem finally solved.

Appendix A

Matsubara sums

The general calculations in the grand canonical ensemble use the summations over Matsubara frequencies called the Matsubara sums. As the dependence of these formulas on ω_m is complex, we shall use the techniques of complex calculus. Here let us use the residues theorem as made in [33], [47] joined with the classical techniques to solve the complex integrations.

Then, let us consider a general Matsubara sum

$$S \equiv \sum_{m=-\infty}^{\infty} F(\omega_m) \tag{A.1}$$

where $F(\omega_m)$ is any function of $\omega_m \equiv 2m\pi/\beta$ (bosons). The idea is to write this sum as a complex integral and, in fact, it is possible using an auxiliary function $g(z)$ that has a form of the Bose-Einstein distribution,

$$g(z) \equiv \frac{\beta}{e^{\beta z} - 1} \tag{A.2}$$

and the interesting here is that $g(z)$ has a simple pole for $z = i\hbar\omega_m$ because

$$e^{\beta z} = e^{i\beta\hbar\omega_m} = e^{2i\pi m} = 1 \tag{A.3}$$

and the denominator in (A.2) diverges in this case. We know that the complex integral over a contour can be calculated using the residues theorem [47]

$$\oint_C f(z)\,dz = 2\pi i \sum_{j=1}^{k} \mathrm{Res} f(z = z_j), \tag{A.4}$$

where

$$\mathrm{Res} f(z = z_0) = \frac{1}{(k-1)!} \lim_{z \to z_0} \left(\frac{d^{k-1}}{dz^{k-1}} \left[(z - z_0) f(z) \right] \right), \tag{A.5}$$

with pole order k. Then considering a new function $h(z)$ such that $h(z) = F(-iz)\,g(z)$ and applying (A.4), we have that

$$\oint_C h(z)\,dz = 2\pi i \sum_{m=-\infty}^{\infty} \mathrm{Res}\,h(z = i\hbar\omega_m), \tag{A.6}$$

114
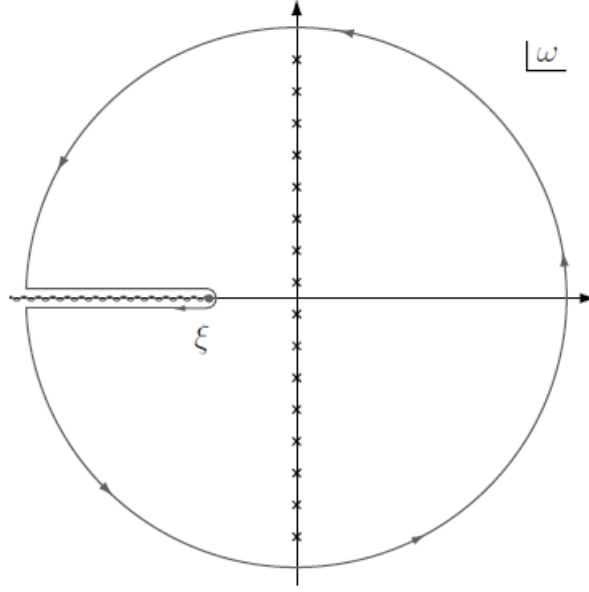
Figure A.1: Region of integration for complex logarithm, we need to exclude the real line such that $z > E_k$ and here, we will have two contributions: positive branch z^+ and negative branch z^-.

we see that our function has the same pole of $g(z)$ and this pole there is for $m \in (-\infty, \infty)$ and from (A.5),

$$\oint_C h(z)\, dz = 2\pi i \beta \sum_{m=-\infty}^{\infty} F(\omega_m) \lim_{z \to i\hbar\omega_m} \left(\frac{z - i\hbar\omega_m}{e^{\beta z} - 1} \right) \tag{A.7}$$

and this last limit is equal to 1. Then now, the Matsubara sum can be written as an integral,

$$\oint_C F(-iz)\, g(z)\, dz = 2\pi i \beta \sum_{m=-\infty}^{\infty} F(\omega_m). \tag{A.8}$$

As an example, let's calculate a classical Matsubara sum that appears in the calculation of the grand partition function Ξ in Chapter 2. Then,

$$\sum_{m=-\infty}^{\infty} \ln\left(\beta(-i\hbar\omega_m + E_k)\right) = \frac{1}{2\pi i \beta} \oint_C F(-iz)\, g(z)\, dz. \tag{A.9}$$

where

$$F(-iz) = \ln(z - E_k) \tag{A.10}$$

and $g(z)$ given by (A.2). But we know that there is the logarithm $\ln(x)$ when $x > 1$, so we have that $F(-iz)$ has a branch cut along $z \in (-\infty, E_k)$ implying on $z > E_k$ and therefore, we can use the contour C as a circumference given by Fig. A.1 to make the complex integral. Then (A.9) for (A.10) becomes

$$\sum_{m=-\infty}^{\infty} \ln\left(\beta(-i\hbar\omega_m + E_k)\right) = \frac{1}{2\pi i\beta} \int_{-\infty}^{\infty} dz\, g(z) \left[\ln(z^+ - E_k) - \ln(z^- - E_k)\right] = \frac{1}{2\pi i\beta}(I_1 - I_2),$$

(A.11)

where

$$z^{\pm} \equiv z \pm i\eta$$

(A.12)

$$I_1 \equiv \int_{-\infty}^{E_k} dz\, g(z)\, \ln(z^+ - E_k),$$

(A.13)

and

$$I_2 \equiv \int_{E_k}^{\infty} dz\, g(z)\, \ln(z^- - E_k).$$

(A.14)

Each integral can be solved using the partial integration and here we see that $g(z)$ can be written as a differential form [33]

$$g(z) = \frac{\beta}{e^{\beta z} - 1} = \frac{\partial}{\partial z} \ln(1 - e^{-\beta z})$$

(A.15)

As example, solving (A.13) with (A.15), we will obtain a other integral form of I_1,

$$I_1 = -\int_{-\infty}^{E_k} dz\, \ln(1 - e^{-\beta z}) \frac{1}{z^+ - E_k},$$

(A.16)

and hence,

$$I_2 = -\int_{E_k}^{\infty} dz\, \ln(1 - e^{-\beta z}) \frac{1}{z^- - E_k}.$$

(A.17)

So, with (A.17), (A.16) in (A.11),

$$\sum_{m=-\infty}^{\infty} \ln\left(\beta(-i\hbar\omega_m + E_k)\right) = \frac{-1}{2\pi i\beta} \left(\int_{-\infty}^{E_k} dz\, \ln(1 - e^{-\beta z}) \frac{1}{z^+ - E_k} - \int_{E_k}^{\infty} dz\, \ln(1 - e^{-\beta z}) \frac{1}{z^- - E_k}\right).$$

(A.18)

and finally, using the Dirac identity for (A.12)-terms,

$$\lim_{\eta \to 0} \frac{1}{x \pm i\eta} = -i\pi\delta(x).$$

(A.19)

Therefore,

$$\sum_{m=-\infty}^{\infty} \ln\left(\beta(-i\hbar\omega_m + E_k)\right) = \frac{1}{\beta} \ln(1 - e^{-\beta E_k}).$$

(A.20)

Appendix B

Robinson's formula

The polylogarithm function $\zeta_a(z)$, in general, has a series representation,

$$\zeta_a(e^x) = \sum_{n=1}^{\infty} \frac{e^{nx}}{n^a} \tag{B.1}$$

where our interest is to calculate the polylogarithm for an exponential function because its result appears in the grand canonical calculations. Then starting from (B.1), let us use a trick following [44] adding 0 in (B.1),

$$\zeta_a(e^x) = \int_0^{\infty} dn \, \frac{e^{nx}}{n^a} + \left(\sum_{n=1}^{\infty} - \int_0^{\infty} dn \right) \frac{e^{nx}}{n^a}. \tag{B.2}$$

but here, we have a finesse: the first integral can be solved by the gamma function, and the rest, can be made by expanding the exponential in a Taylor series. Then, let's do the first part. Remembering the definition of the gamma function

$$\Gamma(z) = \int_0^{\infty} dt \, e^{-t} \, t^{z-1}, \tag{B.3}$$

and doing a transformation of variables, $nx \equiv -t$, we have that

$$\zeta_a(e^x) = (-x)^{a-1} \int_0^{\infty} dt \, e^{-t} t^{-a} + \left(\sum_{n=1}^{\infty} - \int_0^{\infty} dn \right) \frac{e^{nx}}{n^a}. \tag{B.4}$$

where the integral over t is equal to $\Gamma(1-a)$ from (B.3). Therefore,

$$\zeta_a(e^x) = (-x)^{a-1} \, \Gamma(1-a) + \left(\sum_{n=1}^{\infty} - \int_0^{\infty} dn \right) \frac{e^{nx}}{n^a}. \tag{B.5}$$

The second part is to expand the exponential in a Taylor series,

$$e^{nx} = \sum_{k=0}^{\infty} \frac{(nx)^k}{k!} \tag{B.6}$$

and inserting (B.6) in (B.5), we have that

$$\zeta_a(e^x) = (-x)^{a-1}\,\Gamma(1-a) + \sum_{k=0}^{\infty} \frac{x^k}{k!}\left(\sum_{n=1}^{\infty} - \int_0^{\infty} dn\right)\frac{1}{n^{a-k}}. \tag{B.7}$$

Here, the summation over n is equal to the Riemann zeta function $\zeta(a-k)$ but the integral is zero because $a < 1$. Therefore, we have the called Robinson's formula,

$$\zeta_a(e^x) = (-x)^{a-1}\,\Gamma(1-a) + \sum_{k=0}^{\infty} \frac{x^k}{k!}\,\zeta(a-k). \tag{B.8}$$

This formula is valid for $a < 1$, but for $a = 1$, we need to do a new calculation.

Appendix C

Fourier-Matsubara transform of the non-interacting Green's function

Let's make the details of these calculations for the non-interacting case, By [4,15,39,40] we know that

$$G^{(0)}\left(\mathbf{X} + \frac{\Delta\mathbf{x}}{2}, \tau; \mathbf{X} - \frac{\Delta\mathbf{x}}{2}, \tau'\right) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar} \theta(\tau - \tau') \frac{e^{-H(\mathbf{p},\mathbf{X})(\tau-\tau'-\hbar\beta/2)/\hbar}}{2\sinh\left(\frac{\beta H(\mathbf{p},\mathbf{X})}{2}\right)}$$
(C.1)

Expanding the hyperbolic sine in the denominator of (3.55), we have that

$$G^{(0)}\left(\mathbf{X} + \frac{\Delta\mathbf{x}}{2}, \tau; \mathbf{X} - \frac{\Delta\mathbf{x}}{2}, \tau'\right) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar} \theta(\tau - \tau') e^{-(\mathbf{p},\mathbf{X})\tau/\hbar} \frac{1}{1 - e^{-\beta H(\mathbf{p},\mathbf{X})}}$$
(C.2)

but this last result is equal to the geometric series,

$$\frac{1}{1 - e^{-\beta H(\mathbf{p},\mathbf{X})}} = \sum_{n=0}^{\infty} e^{-n\beta H(\mathbf{p},\mathbf{X})}$$
(C.3)

then (C.2) becomes

$$G^{(0)}\left(\mathbf{X} + \frac{\Delta\mathbf{x}}{2}, \tau; \mathbf{X} - \frac{\Delta\mathbf{x}}{2}, \tau'\right) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar} \theta(\tau-\tau') e^{-H(\mathbf{p},\mathbf{X})\tau/\hbar} \sum_{n=0}^{\infty} e^{-n\beta H(\mathbf{p},\mathbf{X})},$$
(C.4)

where $H(\mathbf{p}, \mathbf{X})$ is the grand canonical Hamiltonian,

$$H(\mathbf{p}, \mathbf{X}) = \frac{p^2}{2M} + V(\mathbf{X}) - \hat{\mu} \equiv \frac{p^2}{2M} + \mathcal{V}(\mathbf{X}, \hat{\mu}).$$
(C.5)

Inserting (C.5) in (C.4), we have that

$$G^{(0)}\left(\mathbf{X} + \frac{\Delta\mathbf{x}}{2}, \tau; \mathbf{X} - \frac{\Delta\mathbf{x}}{2}, \tau'\right) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar} \theta(\tau-\tau') e^{-(\mathbf{p}^2/2M+\mathcal{V})(\tau-\tau')/\hbar} \sum_{n=0}^{\infty} e^{-n\beta(\mathbf{p}^2/2M+\mathcal{V})}.$$
(C.6)

We know that the complete Fourier-Matsubara transform is

$$G^{(0)}(\mathbf{p}, \omega_m; \mathbf{X}) = \int_0^{\hbar\beta} d\Delta\tau\, e^{i\omega_m\Delta\tau} \int d^3\Delta\mathbf{x}\, e^{-\mathbf{p}\cdot\Delta\mathbf{x}/\hbar}\, G^{(0)}\left(\mathbf{X} + \frac{\Delta\mathbf{x}}{2}, \tau; \mathbf{X} - \frac{\Delta\mathbf{x}}{2}, \tau'\right),$$
(C.7)

then inserting (C.6) in (C.7),

$$G^{(0)}(\mathbf{p}, \omega_m; \mathbf{X}) = \int_0^{\hbar\beta} d\Delta\tau\, e^{i\omega_m\Delta\tau} \int d^3\Delta\mathbf{x}\, e^{-i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar}$$

$$\times \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar}\, \theta(\Delta\tau)\, e^{-(\mathbf{p}^2/2M+\mathcal{V})\Delta\tau/\hbar} \sum_{n=0}^{\infty} e^{-n\beta(\mathbf{p}^2/2M+\mathcal{V})}. \quad \text{(C.8)}$$

$$G^{(0)}(\mathbf{p}, \omega_m; \mathbf{X}) = \int_0^{\hbar\beta} d\Delta\tau\, e^{i\omega_m\Delta\tau}\, \theta(\Delta\tau) \sum_{n=0}^{\infty} e^{-n\beta\mathcal{V}-\Delta\tau\mathcal{V}/\hbar} \int d^3\Delta\mathbf{x}\, e^{-i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar}$$

$$\times \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar}\, e^{-\tau\mathbf{p}^2/2M-n\beta\mathbf{p}^2/2M}. \quad \text{(C.9)}$$

The integrals over relative coordinates and momentum form a pair of Fourier transform and inverse Fourier transform. Therefore, this last result is equal to the same exponential without the Fourier kernel, in other words,

$$\int d\Delta\mathbf{x}\, e^{-i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar} \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{i\mathbf{p}\cdot\Delta\mathbf{x}/\hbar}\, e^{-\tau\mathbf{p}^2/2M-n\beta\mathbf{p}^2/2M} = e^{-\tau\mathbf{p}^2/2M-n\beta\mathbf{p}^2/2M}. \quad \text{(C.10)}$$

Putting (C.10) in (C.9), we obtain that

$$G^{(0)}(\mathbf{p}, \omega_m; \mathbf{X}) = \sum_{n=0}^{\infty} e^{-n\beta(\mathbf{p}^2/2M+\mathcal{V})} \int_0^{\hbar\beta} d\Delta\tau\, e^{i\omega_m\Delta\tau}\, \theta(\Delta\tau)\, e^{-\tau(\mathbf{p}^2/2M+\mathcal{V})/\hbar}, \quad \text{(C.11)}$$

making the summation over n we have the geometric series,

$$\sum_{n=0}^{\infty} e^{-n\beta(\mathbf{p}^2/2M+\mathcal{V})} = \frac{1}{1 - e^{-\beta(\mathbf{p}^2/2M+\mathcal{V})}}, \quad \text{(C.12)}$$

the integral over $\Delta\tau$,

$$\int_0^{\hbar\beta} d\Delta\tau\, e^{i\omega_m\Delta\tau}\, \theta(\Delta\tau)\, e^{-\tau(\mathbf{p}^2/2M+\mathcal{V})/\hbar} = \hbar\, \frac{1 - e^{-\beta(\mathbf{p}^2/2M+\mathcal{V}-i\hbar\omega_m)}}{\frac{\mathbf{p}^2}{2M} + \mathcal{V} - i\hbar\omega_m} \quad \text{(C.13)}$$

and looking that the exponential of the Matsubara frequency is 1 because

$$\omega_m = \frac{2\pi m}{\hbar\beta} \Rightarrow e^{i\beta\hbar\omega_m} = 1; \quad \text{(C.14)}$$

therefore, by putting (C.12), (C.13) and (C.14) in (C.11), we have the complete formula of the Fourier-Matsubara representation of $G^{(0)}$,

$$G^{(0)}(\mathbf{p}, \omega_m; \mathbf{X}) = \frac{\hbar}{-i\hbar\omega_m + \frac{\mathbf{p}^2}{2M} + V(\mathbf{X}) - \hat{\mu}}. \quad \text{(C.15)}$$

Appendix D

Imaginary time propagator for a quantum harmonic oscillator

In the section about dilute Bose gas in a harmonic trap, we need the one-particle Schrödinger propagator $(x, k\hbar\beta|x', 0)_{(0)}$. In particular, for this system, the exact formula coincides with the semiclassical approximation, then let's use the Feynman representation for the propagator. To compute the imaginary-time evolution amplitude $(x, k\hbar\beta|x, 0)_{(0)}$ we must use the path integral representation

$$(x, k\hbar\beta; x', 0)_{(0)} = \int_{x(0)=x'}^{x(k\hbar\beta)=x} Dx \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \frac{M}{2}\left(\dot{x}^2 + \omega^2 x^2\right)\right], \quad \text{(D.1)}$$

where the $\dot{x}$ represents the derivative with respect to the imaginary time τ. The solution of this path integral is obtained using the semiclassical approximation (or Van Vleck-Pauli-Morette formula) in real time:

$$\int_{x(0)=x'}^{x(\mathrm{t})=x} Dx \exp\left[\frac{i}{\hbar}\int_0^{\mathrm{t}} d\mathrm{t}' L(x, \dot{x}; \mathrm{t}')\right] = \sqrt{\frac{1}{2i\pi\hbar} \det\left(-\frac{\partial^2 S[x_{cl}]}{\partial x \, \partial x'}\right)} \, e^{i\,S[x_{cl}]/\hbar}, \quad \text{(D.2)}$$

where $S[x_{cl}]$ is the classical action for quantum harmonic oscillator whose form is given by

$$S[x_{cl}] = \int_0^{\mathrm{t}} d\mathrm{t}' \frac{M}{2}\left(\dot{x}_{cl}^2 - \omega^2 x_{cl}^2\right), \quad \text{(D.3)}$$

and x_{cl} is obtained through Euler-Lagrange equation for it classical path with $x_{cl}(0) = x'$ and $x_{cl}(\mathrm{t}) = x$, i.e.,

$$\frac{\partial L}{\partial x_{cl}} - \frac{d}{d\mathrm{t}}\left(\frac{\partial L}{\partial \dot{x}_{cl}}\right) = 0. \quad \text{(D.4)}$$

Solving (D.4) with boundary conditions cited by the previous paragraph, we obtain

$$x_{cl}(\mathrm{t}') = x' \cos(\omega \mathrm{t}') + \left[\frac{x}{\sin(\omega \mathrm{t}')} - x' \cot(\omega \mathrm{t}')\right]\sin(\omega \mathrm{t}') \quad \text{(D.5)}$$

and putting this path in (D.3),

$$S[x_{cl}] = \frac{M\omega}{2}\left[\left(x^2 + x'^2\right)\cot(\omega \mathrm{t}) - \frac{2x\,x'}{\sin(\omega \mathrm{t})}\right]. \quad \text{(D.6)}$$

Finally, including this result in (D.2) remembering that the determinant of function depends of its eigenvalues, we obtain[1]

$$(x, \mathrm{t}; x', 0)_{(0)} = \sqrt{\frac{-iM\omega}{2\pi\hbar \sin(\omega\mathrm{t})}} \exp\left[\frac{iM\omega}{2\hbar}\left(\left(x^2 + x'^2\right)\cot(\omega\mathrm{t}) - \frac{2x\,x'}{\sin(\omega\mathrm{t})}\right)\right]. \quad \text{(D.7)}$$

going back to imaginary time with $\tau = i\mathrm{t}$, we finally get

$$(x, k\hbar\beta; x', 0)_{(0)} = \left[\frac{M\omega}{2\pi\hbar \sinh(k\beta\hbar\omega)}\right]^{1/2} \exp\left[-\frac{M\omega}{2\hbar \sinh(k\beta\hbar\omega)}\left[\left(x^2 + x'^2\right)\cosh(k\beta\hbar\omega) - 2x\,x'\right]\right].$$
$$\text{(D.8)}$$

---

[1]Alternative derivations can be found in Ref. [48].

Appendix E

Integrals with Hermite polynomials

The calculation of the Hermite-Gauss integrals is a good challenge to solve because we have the classical Gaussian function joined the Hermite functions, that are one class of special functions. There are many possible integrals to calculate including these two functions, however in this dissertation, the purpose is to find the quadratic dependence in the Hermite polynomials. Therefore, we need to solve

$$\int_{-\infty}^{\infty} dx \, H_m(x) \, H_n(x) \, e^{-a^2 x^2} \equiv I(m, n; a) \,. \tag{E.1}$$

The first step for this is to represent the Hermite polynomial from generating function $g(x, t)$ [47, 49] as

$$g(x, t) = e^{2xt - t^2} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \,, \tag{E.2}$$

then we can represent the product of two Hermite polynomials following

$$e^{2xt - t^2} e^{2xs - s^2} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \sum_{m=0}^{\infty} H_m(x) \frac{s^m}{m!} \,, \tag{E.3}$$

but to compare the all sides of (E.3), we shall expand the left side in a power series, before we showed that

$$e^{2xt - t^2} e^{2xs - s^2} = e^{2x(s+t) - (s+t)^2} e^{2st} = \sum_{p=0}^{\infty} H_p(x) \frac{(s+t)^p}{p!} \sum_{\nu=0}^{\infty} \frac{(2st)^\nu}{\nu!} \,, \tag{E.4}$$

and here, the factor $(s + t)^p$ can be written using the binomial expansion,

$$(s + t)^p = \sum_{j=0}^{p} \binom{p}{j} s^j t^{p-j} \,, \tag{E.5}$$

where,

$$\binom{p}{j} = \frac{p!}{(p - j)! j!} \,, \tag{E.6}$$

is the combinatory. Therefore,

$$\sum_{p=0}^{\infty} H_p(x) \frac{1}{p!} \sum_{j=0}^{p} \binom{p}{j} s^j t^{p-j} \sum_{\nu=0}^{\infty} \frac{(2st)^\nu}{\nu!} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \sum_{m=0}^{\infty} H_m(x) \frac{s^m}{m!} \,, \tag{E.7}$$

doing the transformations $p \to m + n - 2\nu$ and $j \to m - \nu$, we have

$$\sum_{m,n=0}^{\infty} H_n(x) H_m(x) \frac{t^n s^m}{n! m!} = \sum_{n,m=0}^{\infty} \frac{t^n s^m}{n! m!} \sum_{\nu=0}^{\min(m,n)} H_{m+n-2\nu}(x) \frac{2^\nu m! n!}{\nu!(m+n-2\nu)!} \binom{m+n-2\nu}{m-\nu},$$
(E.8)

and finally,

$$H_n(x) H_m(x) = \sum_{\nu=0}^{\min(m,n)} H_{m+n-2\nu}(x) \frac{2^\nu m! n!}{\nu!(m+n-2\nu)!} \binom{m+n-2\nu}{m-\nu}.$$
(E.9)

Our purpose is to solve (E.1). With (E.9), we can represent now our integral in a function of one Hermite polynomial,

$$I(n.m; a) = \int_{-\infty}^{\infty} dx \, e^{-a^2 x^2} \sum_{\nu=0}^{\min(m,n)} H_{m+n-2\nu}(x) \frac{2^\nu m! n!}{\nu!(m+n-2\nu)!} \binom{m+n-2\nu}{m-\nu},$$
(E.10)

This form, we have

$$I(n, m; a) = \sum_{\nu=0}^{\min(m,n)} \frac{2^\nu m! n!}{\nu!(m+n-2\nu)} \binom{m+n-2\nu}{m-\nu} \int_{-\infty}^{\infty} dx \, e^{-a^2 x^2} H_{m+n-2\nu}(x) .$$
(E.11)

However this last integral can be calculated by [46]

$$\int_{-\infty}^{\infty} e^{-x^2} H_{2n}(xy) \, dx = \pi^{1/2} \frac{(2n)!}{n!} (y^2 - 1)^n = 2^{2n} \Gamma\left(n + \frac{1}{2}\right) (y^2 - 1)^n ,$$
(E.12)

putting $x' \to xa$, $y \to 1/a$ and $m + n - 2\nu \to 2(\alpha - \nu) \equiv 2n'$, (E.11) becomes

$$I(n, m; a) = \sum_{\nu=0}^{\min(m,n)} \frac{2^\nu m! n!}{\nu!(m+n-2\nu)!} \binom{m+n-2\nu}{m-\nu} \frac{2^{m+n-2\nu}}{a} \Gamma\left(\frac{m+n+1}{2} - \nu\right) \left(\frac{1-a^2}{a^2}\right)^{\frac{m+n}{2}-\nu},$$
(E.13)

however, this Gamma function and the other factorials can be written as Pochhammer symbols $(x)_n$ defined in (5.128). Here, let's remember that as m, n, ν are integer numbers, the factorials have a relationship with the Gamma functions and therefore, with the Pochhammer symbols. Then, with this approach, we can write (E.13) in an elegant form, that is our final result,

$$\int_{-\infty}^{\infty} dx \, H_m(x) H_n(x) e^{-a^2 x^2} = \frac{2^{m+n}}{a^{m+n+1}} (1-a^2)^{\frac{m+n}{2}} \Gamma\left(\frac{m+n+1}{2}\right) \sum_{\nu=0}^{\infty} \frac{(-m)_\nu (-n)_\nu}{\nu!(\frac{1-m-n}{2})_\nu} \left(\frac{a^2}{2(a^2-1)}\right)^\nu .$$
(E.14)

Appendix F

Code for numerical calculation of the canonical approach

In this section, we have the code used in our interacting canonical calculations. The structure of the program to calculate the N particle partition function is the same for any trap, but the kernel is different depending on the trap. Here, we show the code for the heat capacity calculated for a weakly interacting Bose gas confined in a three-dimensional harmonic trap; the interesting here is that the non-interacting case is obtained when we put $a_s = 0$, then we have a general code for these two possibilities. Then, the idea to do this recursive N particle partition function is, first, to calculate the single particle partition function $\tilde{Z}_1(n\beta)$, that in the harmonic case is given by Eq. (5.146); after, to write the N particle function $Z_N^B(\beta)$ complementing with the fully perturbative result in our single-particle canonical kernel, and finally, with a recursive scheme to do a complete N particle partition function using one auxiliar function $\eta_k(\beta)$ of form

$$Z_N^B(\beta) \equiv \prod_{k=1}^{N} \eta_k(\beta) \, , \tag{F.1}$$

where $\eta_k(\beta)$ is given by [36]

$$\eta_k(\beta) \equiv \frac{1}{k} \left[\overline{Z}_1(\beta) + \sum_{m=2}^{k} \overline{Z}_1(m\beta) \prod_{n=1}^{m-1} \frac{1}{\eta_{k-n}(\beta)} \right] \, , \tag{F.2}$$

with $\overline{Z}_1(n\beta)$ is the reduced single particle partition function defined as

$$\overline{Z}_1(n\beta) \equiv e^{n\beta E_G} \left[\tilde{Z}_1(n\beta) - \frac{n}{2\hbar} \sum_{l=1}^{n-1} \left(I_{l,n-l}^{(D)}(\beta) + I_{l,n-l}^{(E)}(\beta) \right) \right] \, . \tag{F.3}$$

The Hartree and Fock integrals, the renormalized $Z_1(n\beta)$ are given by Eqs. (5.120) and (5.146). Finally, to obtain the heat capacity by Eq. (4.42).
Below, we have the code in C++ utilized in our calculations, where some lines were divided into two or three lines to fit on the page.

```
#include <stdio.h>
```

```c
#include <math.h>
#include <stdlib.h>

const int N = 1000 ;
const double eps = 0.01 ;
const double zeta = 1.0201 ;
const double Pi = 3.14159 ;
const double c = pow(N/zeta ,0.33333) ;

int main()
{
double t, sd;
double Soma(double) ;
FILE *fptr;


fptr=fopen("Kond1000kast-mat.dat","w");

for ( t = 0.01 ; t <= 2.00 ; t = t + eps )
    {
       sd = t*((t+0.001)*Soma(t+0.001)-2*t*Soma(t)+(t-0.001)*
       Soma(t-0.001))/(0.001*0.001) ;
       fprintf(fptr ,"%7.4f %7.4f\n",t, sd/N);
     }
    fclose(fptr);
}

double Soma(double t)
{ int k,m,l,n,fact(int n) ;
double tau, fakt, expo, sum, prod, N0 ;
double Z1[N+1],eta[N+1],Z01[N+1],f[N+1] ;


tau = t*c ;
for ( k = 1 ; k <= N ; k++ )
    {
        f[k] = 1/(pow(1-exp(-k/tau),3)) ;
     }

tau = t*c ;
for ( k = 1 ; k <= N ; k++)
  for ( m = 0 ; m <= 30 ; m++)
        for ( n = 0 ; n <= m ; n++)
          { fakt = 0.0 ;
                { expo = exp(-k*m/tau)*fact(2*(m-n))*
  pow(-0.25,m-n)/(fact(n)*pow(fact(m-n),3)) ; fakt = fakt + expo
```

```
   *pow((exp(k/tau)-1)/exp(k/tau),m-n)  ; }
         Z01[k] = f[k]  -  0.79*(0.2/pow(1000,0.3333333))*(k/tau)
 *(fakt*fakt*fakt -1)*pow(exp(k/tau)-exp(-k/tau),-1.5)  ;
                   }


tau = t*c  ;
for ( k = 1 ; k <= N ; k++)
    { fakt = 0.0  ;
        for ( l = 1 ; l <= k-1 ; l++ )
            { sum = f[l]*f[k-l]*f[k] ; fakt = fakt + pow(sum,0.5)  ; }
        Z1[k] = Z01[k]*pow(1 + 0.79*(0.1/pow(1000,0.3333333))
        *(k/(Z01[k]*tau))*fakt,-1)  ;
    }

for ( k = 1 ; k <= N ; k++ )
    {   sum = 0.0 ; prod = 1.0  ;
        for ( m = 2 ; m <= k ; m++ )
            { prod = prod/eta[k+1-m] ; sum = sum + Z1[m]*prod  ; }
        eta[k] = (Z1[1] + sum)/k  ;
    }

for ( k = 1 ; k <= N ; k++ )
    {   N0 = N0 + log(eta[k])  ; }
return N0  ;
}

int fact(int n) {
  if(n > 1)
    return exp(log(n) + log(factorial(n - 1)))  ;
  else
    return 1;
}
```

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