

ASPECTS OF FINITE SIZE EFFECTS ON BOSE EINSTEIN CONDENSATION

by

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B.S. , Physics Engineering, Istanbul Technical University, 2011

Submitted to the Institute for Graduate Studies in
Science and Engineering in partial fulfillment of
the requirements for the degree of
Master of Science

Graduate Program in Physics

Boğaziçi University

2015

ACKNOWLEDGEMENTS

First of all, I would like to express my gratitude to my thesis advisor, Prof. Teoman Turgut, for sharing his time, experience and immense knowledge, for his tremendous support and concern since the beginning of my education at Bogazici University. It is impossible to describe how important to me to have the chance to work with him. I will take him as a role model for the rest of my life.

I also would like to thank all professors and friends at the Department of Physics, especially Haci Akbas for the scientific discussions and moral support during this thesis.

Lastly, I would like to thank my friends and family for all their never ending support and understanding.

ABSTRACT

ASPECTS OF FINITE SIZE EFFECTS ON BOSE EINSTEIN CONDENSATION

In this thesis, the number of particles calculations of Pathria for a 3 dimensional box is shortly reviewed. After that, the works of Toms and Kirsten which use the Mellin Barnes integral representation and heat kernel approximation to calculate the partition function summation is reviewed. Toms and Kirsten's approach is worked out in d dimension to calculate some thermodynamic quantities such as the number of particles, internal energy, heat capacity at constant volume and constant pressure, isothermal compressibility, adiabatic compressibility etc. The discontinuity of the heat capacity and the derivative of the heat capacity around the critical temperature is investigated. The results are checked at the bulk level to see that at $d = 3$ they are consistent with the ones given in Pathria. Lastly, the results are generalized to p^s for $s = 2k$ case and also an expression for the discontinuity of the heat capacity at constant volume is written.

ÖZET

BOSE EINSTEIN YOĞUŞMASINDA SONLU BOY ETKİLERİNE YAKLAŞIMLAR

Bu tezde, üç boyutta kübik kovuk için toplam parçacık sayısı ifadesi kısaca yazıldı. Sonrasında keyfi şekilli bir kovukta Bose-Einstein Yoğuşması hesapları yapıldı. Bu hesaplarda Mellin-Barnes integral gösterimi kullanıldı. Çeşitli termodinamik büyüklükler hesaplandı ve hacimsel ölçekte ve üç boyutta bilinen cevaplarla tutarlılığı kontrol edildi. Sabit hacimli ısı kapasitesinde bir süreksizlik olduğu gözlemlendi. Hesaplar p^s durumuna genellendi ve bazı termodinamik büyüklükler hesaplandı.

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LIST OF SYMBOLS

| | |
|-----------|------------------------------------|
| b | Boundary parameter |
| d | Dimension of the domain |
| f | Particle fraction coefficient |
| p | Momentum operator |
| V | Volume of the cavity |
| z | Fugacity |
| β | Temperature parameter |
| Γ | Gamma function |
| κ | Boundary parameter |
| ξ | Dimensionless expansion parameter |
| v | Volume per particle |
| ζ | Zeta function |
| \hbar | Reduced Planck constant |
| a_l | Heat kernel expansion coefficients |
| d_0 | Degeneracy |
| E_N | Energy at state N |
| k_B | Boltzman constant |
| Li_n | Polylogarithmic function |
| ζ_R | Riemann zeta function |

1. INTRODUCTION

For many reasons Bose Einstein Condensation had been very interesting to physicists since the first statistical studies of Satyendra Nath Bose and Albert Einstein in early 1900s. Because it is essential to understand first the Bose-Einstein Condensation concept to explain some recently developed studies on superfluidity and superconductivity, it will be a very important problem to study also in future.

The fundamental studies on Bose-Einstein condensation based on an idealized case which the Bose gas is dilute which means that the number of particles are very small comparing to the volume of the container and individual volume of each particle is neglected. Also, the particles are not interacting with each other and there is no external potential energy. Under these circumstances, what happens to the number of particles at condensation can be observed clearly and the thermodynamic calculations can be found explicitly. However, improvements in the experimental aspects of Bose Einstein Condensation leads physicist to make the calculations in a more realistic matter. The first adjustment to earlier calculations is to take the container volume as a finite volume which makes necessary the boundary conditions and brings boundary contributions with itself.

There are some approaches studied to see the finite size effects on Bose Einstein condensation. In this thesis, we will shortly review the calculations of Pathria for a 3 dimensional box using the Poisson summation method. After that, we will review the works of Toms and Kirsten which use the Mellin Barnes integral representation and heat kernel approximation to calculate the partition function summation. We will use Toms and Kirsten's approach in d dimension to calculate some thermodynamic quantities such as the number of particles, internal energy, heat capacity at constant volume and constant pressure, isothermal compressibility, adiabatic compressibility etc. The discontinuity of the heat capacity and the derivative of the heat capacity around the critical temperature will be investigated. We will check these results at the bulk level to see that at $d = 3$ they are consistent with the ones given in Pathria. Lastly, we

will generalize our results that we calculate for p^2 case to p^s for $s = 2k$ case and use the multiplication theorem of gamma functions to reach an explicit result of partition summation. We will also write an expression for the discontinuity of the heat capacity at constant volume.

2. STATISTICAL CALCULATIONS OF AN IDEAL BOSE GAS IN CUBIC CAVITY

2.1. General Concepts

An ideal Bose gas consists of identical bosons that the potential energy caused by their interaction with each other is negligible compared to the kinetic energy of the particles. This as a quantum system of ideal Bose gas, satisfies the Schrödinger equation[1]:

$$\hbar i \frac{\partial}{\partial t} \psi(\vec{r}^i, t) = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} \psi(\vec{r}^i, t) \quad (2.1)$$

where \hbar is the Planck constant, \mathbf{p}_i is the momentum operator and $\psi(\vec{r}^i, t)$ is the total wave function of the gas. Since the particles are non-interacting it is in product form. This product should be symmetrized to get a totally symmetric wave function.

In statistical mechanics, one of the most fundamental concepts is the partition function. For a Bosonic system the more natural choice is the grand canonical ensemble. For non-interacting , grand canonical q function is

$$q = \ln \sum_{r,s} e^{\beta \mu N_r - \beta \epsilon_s} \quad (2.2)$$

where ϵ_s is the energy and N_r is the number of particles in the state r . Various thermodynamic quantity is calculated in terms of q such as equation of state

$$q \equiv \frac{PV}{kT} \quad (2.3)$$

the total number of particles

$$N = kT \frac{\partial q}{\partial \mu} \Big|_{V,T} \quad (2.4)$$

and internal energy of the system

$$U = kT^2 \frac{\partial q}{\partial T} \Big|_{\mu,V} \quad (2.5)$$

2.2. Bose Einstein Condensation

Bose Einstein condensation is a very interesting subject to physicists. Liquid helium and cold alkali gases observations are some examples of Bose Einstein Condensation phenomenon as real physical systems.

Mathematical physicists want to see the effect of the geometry of the domain to the quantum statistical calculations as of order of volume and boundary separately. There are some articles in the literature addressing this subject which we will partially review.

Before describing our main approach for Bose-Einstein condensation in arbitrarily shaped cavities, we will make a very brief review of Pathria's work on the quantum statistics of an ideal, non-relativistic, free Bose gas of N particles in a cubic cavity [2-7].

First, we specify the geometry, that it will turn out to be the main reason we can use the Poisson summation technique. Cubic cavity geometry can be simply described as a 3 dimensional cubic box which has the volume element

$$V = L^3 \quad (2.6)$$

where L is the typical dimension of the boundary. The total number of particles is

$$N = \frac{1}{\sum_{\epsilon} e^{\beta(\epsilon-\mu)} - 1} \quad (2.7)$$

where the energy expression is

$$\epsilon = \frac{\hbar^2 \pi^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2) \quad , \quad n_1, n_2, n_3 = 0, \pm 1, \pm 2, \pm 3 \dots \quad (2.8)$$

under periodic boundary conditions. We rearrange the N expression as

$$\begin{aligned} N &= \sum_{\epsilon} \frac{1}{e^{\beta(\epsilon-\mu)} (1 - e^{-\beta(\epsilon-\mu)})} = \sum_{\epsilon} \frac{\sum_{j=0}^{\infty} e^{-\beta(\epsilon-\mu)j}}{e^{\beta(\epsilon-\mu)j}} \\ &= \sum_{\epsilon} e^{-\beta(\epsilon-\mu)} \sum_{j=0}^{\infty} e^{-\beta(\epsilon-\mu)j} = \sum_{\epsilon} \sum_{j=0}^{\infty} e^{-\beta(\epsilon-\mu)(j+1)} \end{aligned} \quad (2.9)$$

$$= \sum_{\epsilon} \sum_{j=1}^{\infty} e^{-\beta(\epsilon-\mu)j} \quad (2.10)$$

by using the approximation

$$\frac{1}{1-x} \simeq 1 + x + x^2 + \dots = \sum_{j=0}^{\infty} x^j, \quad \text{for small } x \quad (2.11)$$

Inserting (2.8) back in N expression we get

$$\begin{aligned} N &= \sum_{n_1, n_2, n_3} \sum_{j=1}^{\infty} e^{\beta \mu j} e^{-\beta \frac{\hbar^2 \pi^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2) j} \\ &= \sum_{j=1}^{\infty} e^{\beta \mu j} \sum_{n_1=-\infty}^{\infty} e^{-\beta \frac{\hbar^2 \pi^2}{2mL^2} n_1^2 j} \sum_{n_2=-\infty}^{\infty} e^{-\beta \frac{\hbar^2 \pi^2}{2mL^2} n_2^2 j} \sum_{n_3=-\infty}^{\infty} e^{-\beta \frac{\hbar^2 \pi^2}{2mL^2} n_3^2 j} \\ &= \sum_{j=1}^{\infty} e^{\beta \mu j} \prod_{i=1}^3 \sum_{n_i=-\infty}^{\infty} e^{-\beta \frac{\hbar^2 \pi^2}{2mL^2} n_i^2 j} \end{aligned} \quad (2.12)$$

At this point, Poisson summation formula,

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \tilde{f}(q) \quad (2.13)$$

where $\tilde{f}(q)$ is the Fourier transform of $f(n)$, will be used to work out the n_i -sums.

$$\sum_{n_i=-\infty}^{\infty} e^{-\beta \frac{\hbar^2 \pi^2}{2mL^2} n_i^2 j} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \sum_{k_i=-\infty}^{\infty} e^{-\beta \frac{\hbar^2 \pi^2}{2mL^2} k_i^2 j} e^{i2\pi k_i q_i} dk_i \quad (2.14)$$

For simplicity, here we drop the i index and set $\beta \frac{\hbar^2 \pi^2}{2mL^2}$ as w^2 . We calculate the integral and get

$$\begin{aligned} \sum_{n=-\infty}^{\infty} e^{-\beta \frac{\hbar^2 \pi^2}{2mL^2} n^2 j} &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \sum_{q=-\infty}^{\infty} e^{-(jwk+q\frac{i\pi}{wj})^2 - \frac{q^2 \pi^2}{w^2 j^2}} dk \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \sum_{q=-\infty}^{\infty} e^{-w^2 k^2 j} e^{i2\pi k q} dk \\ &= \frac{1}{2\pi} \sum_{q=-\infty}^{\infty} e^{-\frac{q^2 \pi^2}{w^2 j}} \int_{-\infty}^{\infty} e^{-w^2 j(k-q\frac{i\pi}{w^2 j})^2} dk \\ &= \frac{1}{2\pi} \sum_{q=-\infty}^{\infty} e^{-\frac{q^2 \pi^2}{w^2 j}} \sqrt{\frac{\pi}{w^2 j}} \end{aligned} \quad (2.15)$$

Putting (2.15) back in N expression, we get the bulk result of number of particles.

$$N = \sum_{j=1}^{\infty} e^{\beta \mu j} \prod_{i=1}^3 \left(\sqrt{\frac{1}{\pi j} \frac{1}{2w}} \right)^3 \sum_{q=-\infty}^{\infty} e^{-\frac{q^2 \pi^2}{w^2 j}} \quad (2.16)$$

To get rid of the j -sum Pathria uses another identity such that

$$\frac{1}{2}(f(a) + f(b)) + \sum_{n=a+1}^{b-1} f(n) = \lim_{L \rightarrow \infty} \sum_{|l| \leq L} \int_a^b f(t) e^{2\pi i l t} dt \quad (2.17)$$

If we write the j -sum accordingly we get

$$\sum_{j=0}^{\infty} j^{-\frac{3}{2}} e^{j\beta \mu} e^{\gamma(q)j} = \sum_{l=-\infty}^{\infty} \int_0^{\infty} \frac{e^{x\beta \mu}}{x^{3/2}} e^{-\frac{\gamma}{x}} e^{2\pi i l x} dx \quad (2.18)$$

where $\gamma(q) = \frac{\pi q^2 L^2}{\lambda^2}$ and $\lambda = \frac{\hbar^2}{\sqrt{2\pi m k T}}$. The integral in (2.18) can be calculated as it is an incomplete Bessel function of second kind. After the integration and some

arrangements, the number of particles becomes

$$N = \underbrace{\frac{L^3}{\lambda^3} \sum_{j=1}^{\infty} \frac{e^{\beta\mu j}}{j^{\frac{3}{2}}}}_{\text{Bulk term}} + \underbrace{\sum_q' \sum_{-\infty}^{\infty} \sqrt{\frac{\pi}{\gamma}} e^{-2\sqrt{\gamma}(-\beta\mu - 2\pi i l)^{1/2}}}_{\text{Higher order term}} \quad (2.19)$$

where the prime indicates that $q = 0$ term is excluded from the summation. Since the contribution coming from the $l = 0$ term will be much larger than the other terms[8], the total number of particles will be approximately written as below.

$$N \approx \frac{L^3}{\lambda^3} \sum_{j=1}^{\infty} \frac{e^{\beta\mu j}}{j^{\frac{3}{2}}} + \frac{L^3}{\lambda^3} \sum_q' \sqrt{\frac{\pi}{\gamma}} e^{-2\sqrt{\gamma}(-\beta\mu)^{1/2}} \quad (2.20)$$

After some algebra,

$$N \approx \frac{L^3}{\lambda^3} \left[Li_{\frac{3}{2}}(e^{\beta\mu}) + \pi^{1/2}(-\beta\mu)^{1/2} \frac{1}{\pi y} \left(2\pi y + \frac{\pi^2}{y^2} + C_3 - \sum_q' \frac{y^2}{q^2(y^2 + \pi^2 q^2)} \right) \right] \quad (2.21)$$

where

$$y = \pi^{1/2}(-\beta\mu)^{1/2} \frac{L}{\lambda} \quad (2.22)$$

$$Li_l(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^l} \quad (2.23)$$

$$C_3 = \lim_{y \rightarrow 0} \left(\sum_{i=1,2,\dots}' \frac{1}{Q_i^2} e^{\beta\mu Q_i^2 - \frac{2\pi^3/2}{(2y)^{1/2}}} \right), \quad Q_i^2 = q_1^2 + q_2^2 + \dots + q_i^2 \quad (2.24)$$

Now, looking at this expression at $d = 3$, using

$$-\beta\mu \approx \frac{1}{N_0} \quad \text{and} \quad \lim_{\beta\mu \rightarrow 0} Li_{\frac{3}{2}}(e^{\beta\mu}) = \zeta\left(\frac{3}{2}\right) \quad (2.25)$$

we get

$$N \approx N_0 + \frac{L^3}{\lambda^3} \zeta\left(\frac{3}{2}\right) + \frac{L^2}{\lambda^2} \left[\frac{C_3}{\pi} - \frac{y^2}{\pi} \sum'_q \frac{1}{q^2(y^2 + \pi^2 q^2)} \right] \quad (2.26)$$

at condensation. Lastly, we write this result in terms of the critical temperature as below.

$$N_0 \approx N \left[1 - \left(\frac{T}{T_C} \right)^{\frac{3}{2}} \right] - \frac{L^2}{\lambda^2} \left[\frac{C_3}{\pi} - \frac{y^2}{\pi} \sum'_q \frac{1}{q^2(y^2 + \pi^2 q^2)} \right] \quad (2.27)$$

This approach can be pursued further to find finite size corrections to various other thermodynamic functions such as S , C_V , κ_T etc. We will not continue in this direction, since a seemingly more powerful approach is proposed by Toms and Kirsten utilizing the asymptotic expansion of heat kernel.

We turn our attention to developing this approach further in the next section of our thesis.

3. REVIEW OF BEC IN ARBITRARILY SHAPED CAVITIES

There are two fundamental approaches on the phenomenon of Bose Einstein Condensation as discussed in the paper of Toms and Kirsten[9]. First, combining heat kernel techniques with partition function summation over energy levels which uses a Mellin-Barnes integral representation to reach the asymptotic expressions and secondly another integral representation of partition function summation using a suitable density of states function. The effect of the boundary and its shape on some thermodynamic quantities is investigated. In this thesis, we worked on the first approach.

In the next section, the first method of Toms and Kirsten to calculate the partition function summation will be reviewed.

3.1. Partition Function Calculation

Toms and Kirsten start to study the quantum statistics of a free Bose Gas in a d-Dimensional finite cavity by the calculating of the partition function to the next order.

Let us consider a non-interacting ideal gas system of N bosons, with energy levels of E_N which can be determined as the eigenvalues of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi_N(x) = E_N\phi_N(x) \quad (3.1)$$

where $\phi_N(x)$ is the energy eigenstate. The gas is contained in an arbitrarily shaped finite cavity with volume V and the boundary of this volume is ∂V . We are not specifying the boundary conditions since both Neumann or Dirichlet are equally acceptable at this stage. The fixed number of particles and grand canonical partition function of

this system is

$$N = \sum_i n_i = \sum_N \frac{1}{(e^{(\beta E_N - \beta \mu)} - 1)} \quad (3.2)$$

$$q = \frac{PV}{kT} = - \sum_N \ln(1 - ze^{-\beta E_N}) \quad (3.3)$$

respectively, where n_i 's are average number of particles at the state i with energy E_i , $\beta = \frac{1}{k_B T}$ where k_B is Boltzmann constant, $z = e^{\beta \mu}$ is fugacity and μ is chemical potential of this gas.

We can write the ground state of the partition sum separately as

$$q = q_0 - \sum'_N \ln(1 - ze^{(-\beta E_N)}) \quad , \quad \text{where} \quad q_0 = -d_0 \ln(1 - ze^{\beta E_0}) \quad (3.4)$$

Here d_0 is the degeneracy and E_0 is the energy of the ground state and the prime of the summation indicates that the ground state contribution is not included. In general ground state contribution is of a smaller order, except in case of condensation it becomes essential.

The series expansion of logarithmic function

$$-\ln(1 - x) = \sum_{n=1}^{\infty} \frac{x^n}{n} \quad , \quad |x| < 1 \quad (3.5)$$

will be used to calculate the partition function and the $\ln(1 - ze^{(-\beta E_N)})$ will be expanded in an infinite summation as below.

$$q = q_0 + \sum_{n=1}^{\infty} \sum'_N \frac{1}{n} e^{-\beta n(E_N - \mu)} \quad (3.6)$$

To evaluate this summation, we typically take the continuum limit. However, to see the effects of the boundary, Toms and Kirsten use the Mellin-Barnes integral:

$$e^{-\nu} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) \nu^{-\alpha} \quad (3.7)$$

which is true for any ν with a positive real part and $c \in \mathbb{R}$, greater than zero. Let us state a very brief proof of this. Definition of a gamma function is basically given by the integral representation

$$\Gamma(s) = \int_0^{\infty} x^{s-1} e^{-x} dx \quad \text{for } \text{Re}(s) > 0 \quad (3.8)$$

which then is analytically continued to its largest domain.

Also, Mellin transform of a function and the related inversion formula can be respectively noted as:

$$F(y) = \int_0^{\infty} x^{y-1} f(x) dx \quad (3.9)$$

$$f(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} x^{-y} F(y) dy \quad , \quad c > 0 \quad (3.10)$$

Let us calculate the integral and indeed we will see the result equals to e^{-x} . We will use the residue theorem, so we need to look at the poles of the gamma function in the complex plane. Gamma function satisfies the identity

$$\Gamma(t+n) = (t+n-1)(t+n-2)\dots(t+2)(t+1)t\Gamma(t) \quad (3.11)$$

$$\Rightarrow \Gamma(t) = \frac{\Gamma(t+n)}{t(t+1)\dots(t+n-1)} \quad (3.12)$$

As it seems, gamma function has poles at $n = 0, -1, -2, \dots$. If we take a contour \mathbf{C} enclosed by points $c \pm iR$ and $-(N + \frac{1}{2}) \pm iR$ the poles of gamma function stays inside

of the contour and the integral becomes equal to

$$\frac{1}{2\pi i} \int_{\mathbf{C}} x^{-s} \Gamma(s) ds = \sum_{n=0}^N \frac{(-1)^n}{n!} x^n \quad (3.13)$$

Now, we let $R \rightarrow \infty$ and $N \rightarrow \infty$, then Stirling's asymptotic formula for gamma function implies that the integral on \mathbf{C} minus the line joining $c - iR$ and $c + iR$ vanishes and the integral becomes equal to e^{-x} :

$$\begin{aligned} \Rightarrow \quad \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} x^{-s} \Gamma(s) ds &= \sum_i \text{Res}(f = n_i) \\ &= \lim_{N \rightarrow \infty} \sum_{n=0}^N \frac{(-1)^n}{n!} x^n = \sum_{n=0}^{\infty} \frac{(-x)^n}{n!} = e^{-x} \end{aligned} \quad (3.14)$$

If we go back our partition function calculation, we rewrite the N -sum replacing the exponential with the Mellin Barnes integral as

$$q = q_0 + \sum_{n=1}^{\infty} \frac{1}{n} e^{-n\beta(\mu_c - \mu)} \sum_N' e^{-\beta n(E_N - \mu_c)} \quad (3.15)$$

where $\mu_c = E_0$. We make the definition $\nu = \beta n(E_N - E_0)$ and put ν back in the partition function.

$$q = q_0 + \sum_{n=1}^{\infty} \frac{1}{n} e^{-n\beta(\mu_c - \mu)} \sum_N' \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) (\beta n)^{-\alpha} (E_N - E_0)^{-\alpha} \quad (3.16)$$

$$= q_0 + \sum_N' \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \sum_{n=1}^{\infty} \frac{1}{n^{\alpha+1}} e^{-n\beta(\mu_c - \mu)} \Gamma(\alpha) \beta^{-\alpha} (E_N - E_0)^{-\alpha} \quad (3.17)$$

The n -sum will be written as a polylogarithmic function;

$$Li_n(x) = \sum_{l=1}^{\infty} \frac{x^l}{l^n} \quad (3.18)$$

which satisfies the derivation relation

$$Li'_n(x) = \frac{1}{x} Li_{n-1}(x) \quad (3.19)$$

We insert the polylogarithmic function inside the equation and the partition function takes the form below.

$$q = q_0 + \sum'_N \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) Li_{\alpha+1}(e^{-\beta(\mu_c-\mu)}) \beta^{-\alpha} (E_N - E_0)^{-\alpha} \quad (3.20)$$

Now, this time we will interchange the N sum with the zeta function, $\zeta(s)$, associated with the energy eigenvalues (E_N) of the Schrödinger equation.

$$\zeta(s) = \sum'_N (E_N - \mu_c)^{-s} \quad (3.21)$$

Again, the prime above the summation implies that the ground state is not included and we write q as

$$q = q_0 + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) \beta^{-\alpha} Li_{\alpha+1}(e^{-\beta(\mu_c-\mu)}) \zeta(\alpha) \quad (3.22)$$

where the real part of \mathbf{c} is greater than $d/2$ (the rightmost pole of the zeta function). Now we insert the integral form of the ζ function

$$\zeta(\alpha) = \frac{1}{\Gamma(\alpha)} \sum'_N \int_0^\infty dt t^{\alpha-1} e^{-t(E_N-\mu_c)} \quad (3.23)$$

into the q equation.

$$q = q_0 + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) \beta^{-\alpha} Li_{\alpha+1}(e^{-\beta(\mu_c-\mu)}) \frac{1}{\Gamma(\alpha)} \sum'_N \int_0^\infty dt t^{\alpha-1} e^{-t(E_N-\mu_c)} \quad (3.24)$$

We will continue with the connection between the diagonal heat kernel and the

zeta function. It is essential to note that heat kernel has an asymptotic expansion:

$$K(t) = \sum_N e^{-t(E_N - \mu_c)} \approx \frac{1}{(4\pi t)^{\frac{d}{2}}} \sum_{l=0,1/2,1,\dots}^{\infty} a_l t^l \quad , \text{ for small } t \quad (3.25)$$

According to a theorem in ΨDE (Gilkey) $\zeta(\alpha)$ has poles at $\alpha = \frac{d}{m}, \frac{d-1}{m}, \dots, \frac{1}{m}, \dots, \frac{-(2l+1)}{m}$ where m is the degree of the elliptic differential operator, d is the dimension of the space and $l \in \mathbb{N}$. Here, the $\alpha = \frac{d}{m}$ is the right most pole and in our case, $m = 2$. We note that d can be an arbitrary positive number.

Since we want to calculate the residue of the α integral, we are interested in only the range of the integral which contains poles in α coming from the zeta function. We will take the zeta function integral limits similar with Toms and Kirsten. We separate the limits as $[0, \delta]$ and $[\delta, \infty)$ where δ is small and we will not calculate the latter since its contribution is an analytic function in α .

Let us explain more about this integral limits. Even though in [9] the upper limit of the integral is taken as 1, we want to take the upper limit more general as some small δ . The condition we choose δ such that as $V \rightarrow \infty$ goes to zero. It turns out that it does not matter what we take the upper limit of the integral since after the asymptotic expansion and integration terms of the form $\delta^{\alpha-d/2+l}$ will be analytic in α and not contribute anything as we will see.

Now, we will calculate the integral by taking the residues of only the leading two poles of zeta function which are $\alpha = \frac{d}{2}$ and $\alpha = \frac{d-1}{2}$ for $d > 1$. The N -sum in the integral will be replaced by the l -sum after we insert the heat kernel expansion. Let us write the partition function rearranged accordingly.

$$\begin{aligned} q &= q_0 + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \beta^{-\alpha} Li_{\alpha+1}(e^{-\beta(\mu_c - \mu)}) \frac{1}{(4\pi)^{d/2}} \sum_{l=0,1/2,1,\dots}^{\infty} a_l \int_0^{\delta} dt t^{\alpha-1-d/2+l} \\ &= q_0 + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \beta^{-\alpha} Li_{\alpha+1}(e^{-\beta(\mu_c - \mu)}) \frac{1}{(4\pi)^{d/2}} \sum_{l=0,1/2,1,\dots}^{\infty} a_l \frac{\delta^{\alpha-d/2+l}}{\alpha - \frac{d}{2} + l} \end{aligned} \quad (3.26)$$

We remark that usually in the literature, this asymptotic expansion is done in the small β approximation. This usually means $\lambda_T = \frac{h}{\sqrt{2\pi mkT}}$ is small compared to $V^{\frac{1}{d}}$. Small β (large T) behaviour of the partition function will be more accurate, since the asymptotic expansion of the heat kernel approximation is more reliable. Accordingly, partition function can be expressed as below.

$$q = q_0 + Res(f; \alpha = \frac{d}{2}) + Res(f; \alpha = \frac{d-1}{2}) \quad (3.27)$$

As it can be seen, (3.26) expression has two poles for $l = 0$ and $l = 1/2$ terms, which are our concern, as $\alpha = d/2$ and $\alpha = (d-1)/2$ respectively. We write the residues as

$$Res(f; \alpha = \frac{d}{2}) = \frac{a_0}{(4\pi)^{\frac{d}{2}}} \beta^{-\frac{d}{2}} Li_{\frac{d+2}{2}}(e^{-\beta(\mu_c - \mu)}) \quad (3.28)$$

$$Res(f; \alpha = \frac{d-1}{2}) = \frac{a_{1/2}}{(4\pi)^{\frac{d}{2}}} \beta^{-\frac{d-1}{2}} Li_{\frac{d+1}{2}}(e^{-\beta(\mu_c - \mu)}) \quad (3.29)$$

where

$$f = \frac{1}{2\pi i} \beta^{-\alpha} Li_{\alpha+1}(e^{-\beta(\mu_c - \mu)}) \frac{1}{(4\pi)^{d/2}} \sum_{l=0,1/2,1,\dots}^{\infty} a_l \frac{\delta^{\alpha-d/2+l}}{\alpha - \frac{d}{2} + l} \quad (3.30)$$

Here, we want to go back to heat kernel expansion. The first six terms of a_l coefficients are known for an arbitrarily shaped smooth cavity and an elliptic second order operator with proper boundary conditions on its boundary. For Schrödinger equation and our arbitrarily shaped cavity we will use only the first two terms.

We would like to explain why we take only the first two terms of heat kernel expansion. Here, we follow the article by Zayed[11]. There, the first four terms of the asymptotic expansion of the trace of the heat kernel for two and three dimensional Robin problem are explicitly given. We now quote the 3 dimensional case here, we

start with formulating the Robin problem.

$$-\Delta_n \phi = \lambda \phi \quad , \quad \left(\frac{\partial}{\partial n} + \gamma \right) \phi = 0 \quad (3.31)$$

Here, $\frac{\partial}{\partial n}$ is the inward pointing normal. Volume is defined as Ω and $\partial\Omega$ is the boundary. Asymptotic expansion of the trace of the heat kernel is

$$\begin{aligned} K(t) &= \frac{V}{(4\pi t)^{\frac{3}{2}}} + \frac{S}{16\pi t} + \frac{1}{12\pi^{\frac{3}{2}}t^{\frac{1}{2}}} \int_{\partial\Omega} H(\sigma) d\sigma \\ &+ \frac{7}{128\pi} \int_{\partial\Omega} [H^2(\sigma) - N^*(\sigma)] d\sigma + \dots \quad \text{lower orders as } t \rightarrow 0^+ \end{aligned} \quad (3.32)$$

where, V is the volume of the domain, S is the area of the boundary, H is the mean curvature and N^* is the Gaussian curvature of the boundary considered as an embedded surface in \mathbb{R}^3 . H and N^* for a smooth cavity which has well behaved boundary are given in terms of the principal radii of the curvature of the boundary, R_1 and R_2 as below.

$$H = \frac{1}{2} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \quad (3.33)$$

$$N^* = \frac{1}{R_1 R_2} \quad (3.34)$$

It is an interesting idea that, if the cavity is not surrounded by a smooth boundary, for example if it is a fractal boundary, the formulae of H and N^* may not be negligible as R_1 and R_2 are not well-defined. We encounter with an expression for the trace of the heat kernel in Lipschitz domains in Brown's article[10]. As stated in this article, for example where $|\Omega|$ is the volume and $\mathcal{H}^{d-1}(\partial\Omega)$ is the Hausdorff dimension of the boundary; the heat kernel for the Laplacian with Dirichlet boundary conditions on the boundary has an asymptotic expansion

$$tr(g)(t) = (4\pi t)^{-\frac{n}{2}} [|\Omega| - \frac{\sqrt{\pi t}}{2} \mathcal{H}^{d-1}(\partial\Omega) + o(t^{\frac{1}{2}})]$$

This is exactly in the same form with (3.25). However, we could not carry out this idea further since we needed an example of a domain with fractal boundary such that we know its boundary term in terms of the volume element and Hausdorff dimension.

In our case, we assume that our domain is such that the last two terms of (3.32) will remain small since typically R_1 and R_2 will grow as the volume $V \rightarrow \infty$. Indeed, $\int_{\partial\Omega} H(\sigma)d\sigma$ is the Euler number hence it is negligible. Therefore, also in our case, we will only need the first two terms a_0 and $a_{1/2}$.

$$a_0 = \left(\frac{2m}{\hbar^2}\right)^{(d/2)} V \quad (3.35)$$

$$a_{\frac{1}{2}} = \left(\frac{2m}{\hbar^2}\right)^{(d-1)/2} \frac{\sqrt{\pi}}{2} (\partial V) b \quad (3.36)$$

Here, V is the volume of the cavity, ∂V is the area of its boundary and b is a parameter depending on the boundary conditions being $b = -1$ for Dirichlet and $b = 1$ for Neumann boundary conditions.

We put these residues and the a_0 and $a_{1/2}$ coefficients back in the partition function expression.

$$\begin{aligned} q &= q_0 + (kT)^{\frac{d}{2}} Li_{\frac{d+2}{2}}(e^{-\beta(\mu_c-\mu)}) \left(\frac{2m}{\hbar^2}\right)^{\frac{d}{2}} \frac{V}{(4\pi)^{\frac{d}{2}}} + (kT)^{\frac{d-1}{2}} Li_{\frac{d+1}{2}}(e^{-\beta(\mu_c-\mu)}) \left(\frac{2m}{\hbar^2}\right)^{\frac{d-1}{2}} \frac{\sqrt{\pi}}{2} \frac{\partial V b}{(4\pi)^{\frac{d}{2}}} \\ &= q_0 + \left(\frac{2mkT}{\hbar^2 4\pi}\right)^{\frac{d}{2}} Li_{\frac{d+2}{2}}(e^{-\beta(\mu_c-\mu)}) V + \left(\frac{2mkT}{\hbar^2 4\pi}\right)^{\frac{d-1}{2}} Li_{\frac{d+1}{2}}(e^{-\beta(\mu_c-\mu)}) \frac{\sqrt{\pi}}{2} \frac{\partial V b}{(4\pi)^{\frac{1}{2}}} \end{aligned} \quad (3.37)$$

We use the known Planck constant and thermal wavelength expressions

$$\hbar = \frac{h}{2\pi}, \quad \lambda_T = \frac{h}{\sqrt{2\pi mkT}} \quad (3.38)$$

We put the above expressions in our partition function and it becomes

$$q = q_0 + \underbrace{\frac{V}{\lambda_T^{\frac{d}{2}}} Li_{\frac{d+2}{2}}(e^{-\beta(\mu_c-\mu)}) + \frac{\partial V b}{4\lambda_T^2} Li_{\frac{d+1}{2}}(e^{-\beta(\mu_c-\mu)})}_{\text{Typical expansion of the cavity}} \quad (3.39)$$

Here we see that the leading term goes with volume and the latter goes with area, L^{d-1} which demonstrates the typical geometrical expansion of the cavity. Here, L represents the typical dimension of the cavity.

A dimensionless expansion parameter, ξ is defined as below.

$$\xi^d = \frac{V}{\lambda_T^d} \quad (3.40)$$

Before we write the last form of the partition function we make another assumption which is related with the boundary term.

$$\kappa L^{d-1} = \partial V \quad (3.41)$$

where L is the diameter of the cavity. κ is again a dimensionless parameter and it has some information about shape of the boundary. These assumptions mean that the cavity grows equally in all directions and its boundary is sufficiently well-behaved. Now we can write the partition function in its last form.

$$q = q_0 + Li_{\frac{d+2}{2}}(e^{-\beta(\mu_c-\mu)})\xi^d + \frac{\kappa b}{4} Li_{\frac{d+1}{2}}(e^{-\beta(\mu_c-\mu)})\xi^{d-1} + \dots \quad (3.42)$$

When the system condensates and the ground state occupation gets large, μ gets close to $\mu_c = E_0$ and $Li_n(1)$ goes to $\zeta_R(n)$ for the appropriate dimensions. Here, the index R indicates that the zeta function is the Riemann zeta function. After we do the arrangements, we reach the expression of partition function

$$q = q_0 + \zeta_R\left(\frac{d+2}{2}\right)\xi^d + \frac{\kappa b}{4}\zeta_R\left(\frac{d+1}{2}\right)\xi^{d-1} \quad (3.43)$$

which contains the first order correction.

3.2. Number of Particles

Basically, below the critical temperature the total number of particles is

$$\begin{aligned}
 N &= \beta^{-1} \frac{\partial q}{\partial \mu} \Big|_{T,V} = \beta^{-1} \left[\frac{\partial q_0}{\partial \mu} - \frac{\partial}{\partial \mu} \sum'_N \ln(1 - e^{-\beta(E_N - \mu)}) \right] \\
 &= \beta^{-1} \left[\beta N_0 + \sum'_N \beta \frac{e^{-\beta(E_N - \mu)}}{1 - e^{-\beta(E_N - \mu)}} \right] = N_0 + \sum'_N \frac{e^{-\beta(E_N - \mu)}}{1 - e^{-\beta(E_N - \mu)}}
 \end{aligned} \tag{3.44}$$

where

$$N_0 = \frac{d_0}{e^{\beta(\mu_c - \mu)} - 1} = d_0 f_{BE} \tag{3.45}$$

being d_0 is the degeneracy and f_{BE} is the occupation function of the ground state.

Expansion of N will be calculated from the derivative of the other representation of the partition function that was written in terms of Li functions. Below, we note the derivative of the Li functions and the ξ parameter that will be used repeatedly.

$$Li_n(x) = \frac{1}{x} Li_{n-1}(x) \tag{3.46}$$

$$\frac{\partial \xi^d}{\partial \beta} \Big|_V = \beta^{-1} \left(-\frac{d}{2}\right) \xi^d \tag{3.47}$$

Now, we write the total number of particles.

$$\begin{aligned}
 N &= \beta^{-1} \frac{\partial q}{\partial \mu} \Big|_{T,V} \\
 &= \beta^{-1} \frac{\partial}{\partial \mu} (q_0 + Li_{\frac{d+2}{2}}(e^{-\beta(\mu_c - \mu)}) \xi^d + \frac{\kappa b}{4} Li_{\frac{d+1}{2}}(e^{-\beta(\mu_c - \mu)}) \xi^{d-1}) \Big|_{T,V} \\
 &= N_0 + Li_{\frac{d}{2}}(e^{-\beta(\mu_c - \mu)}) \xi^d + \frac{\kappa b}{4} Li_{\frac{d-1}{2}}(e^{-\beta(\mu_c - \mu)}) \xi^{d-1}
 \end{aligned} \tag{3.48}$$

Below the critical temperature the ground state is macroscopically occupied as $\mu \rightarrow \mu_c$ and the number of particles is in general

$$N_0 = \frac{d_0}{e^{\beta(E_0 - \mu)} - 1} \quad (3.49)$$

Toms and Kirsten keep this N_0 above the critical temperature and consider the ground state is microscopically occupied. However, this expression does not define N at regions where μ gets very close or equal to μ_c . Instead it specifies how μ gets close to μ_c as T is changing. At temperatures T above T_C , $\frac{N_0}{V}$ goes like $\frac{1}{L^2}$ and reaches macroscopic finite values including $\frac{1}{L}$ corrections when $T < T_C$. We will state the temperature dependence of N_0 more accurate. Keeping in mind that N is fixed, to figure out the temperature dependence of N_0 and the derivative of N_0 , we take the N_0 expression at condensate. Therefore, again for the adequate dimensions, all Li functions go directly to the zeta functions as μ goes to μ_c , below T_C .

$$N = N_0(T) + \zeta\left(\frac{d}{2}\right)\xi^d + \frac{\kappa b}{4}\zeta\left(\frac{d-1}{2}\right)\xi^{d-1} \quad (3.50)$$

which gives $N_0(T)$. We may also find $\frac{\partial N}{\partial T}$ by using

$$\frac{\partial N}{\partial \beta} = 0 = \frac{\partial N_0(T)}{\partial \beta} + \zeta\left(\frac{d}{2}\right)\left(-\frac{d}{2}\right)\beta^{-1}\xi^d + \frac{\kappa b}{4}\zeta\left(\frac{d-1}{2}\right)\left(-\frac{d-1}{2}\right)\beta^{-1}\xi^{d-1} \quad (3.51)$$

as:

$$\Rightarrow \frac{\partial N_0(T)}{\partial \beta} = \zeta\left(\frac{d}{2}\right)\frac{d}{2}\beta^{-1}\xi^d + \frac{\kappa b}{4}\zeta\left(\frac{d-1}{2}\right)\frac{d-1}{2}\beta^{-1}\xi^{d-1} \quad (3.52)$$

3.3. Discussion of The Critical Temperature in Terms of The Bulk Result

In this section, we will basically take out the critical temperature from the total number of particles expression. Since for each case the behaviour of the polylogarithmic function differs, we will make the critical temperature discussions for four cases as

$d = 2, 3$ and $d > 3$ separately. The total number of particles will be written with a fraction factor as

$$N_0 = fN \quad (3.53)$$

where N is the total number of particles, N_0 is the ground state occupation and f is the fraction of the particles in the ground state. When $N_0 \gg 1$, $T \simeq T_C$ and $\mu \simeq \mu_c$ condensate starts.

We start with $d > 3$. At the very beginning of the condensate, there is no macroscopic number of particles at the ground state. In this case, since $d > 3$, the polylogarithmic functions behave well, so the total number of particles can be directly written as

$$N \simeq \zeta_R\left(\frac{d}{2}\right)\xi_c^d + \frac{\kappa b}{4}\zeta_R\left(\frac{d-1}{2}\right)\xi_c^{d-1} + \dots, \quad N_0 \approx 0 \quad (3.54)$$

Now, moving to $f \ll 1$, where the condensate begins and the ground state occupation is approximately zero; we will try to solve the critical temperature with boundary effect in terms of the bulk critical temperature. We take only the first term of approximation above, write ξ parameter of the bulk, ξ_0^d , and solve the bulk critical temperature, T_0 .

$$\xi_0^d = \frac{V}{\lambda_{T_0}} = \frac{V(2m\pi kT_0)^{\frac{d}{2}}}{h^d} = \frac{N}{\zeta_R\left(\frac{d}{2}\right)} \quad (3.55)$$

$$\Rightarrow T_0^{\frac{d}{2}} = \frac{N}{\zeta_R\left(\frac{d}{2}\right)V} \frac{h^d}{(2m\pi k)^{\frac{d}{2}}} \quad (3.56)$$

$$\Rightarrow T_0 = \left(\frac{N}{\zeta_R\left(\frac{d}{2}\right)V} \right)^{\frac{2}{d}} \frac{h^2}{(2m\pi k)} \quad (3.57)$$

After that, we put back this bulk result in the total number of particles expression.

$$\begin{aligned}
N &= \zeta_R\left(\frac{d}{2}\right)\xi_c^d\left(1 + \frac{\kappa b}{4}\frac{\zeta_R\left(\frac{d-1}{2}\right)}{\zeta_R\left(\frac{d}{2}\right)\xi_c}\right) = \zeta_R\left(\frac{d}{2}\right)\xi_c^d\left(1 + \frac{\kappa b}{4}\frac{\zeta_R\left(\frac{d-1}{2}\right)\zeta_R^{\frac{1}{d}}\left(\frac{d}{2}\right)}{\zeta_R\left(\frac{d}{2}\right)N^{\frac{1}{d}}}\right) \\
&= \zeta_R\left(\frac{d}{2}\right)\xi_c^d\left(1 + \frac{\kappa b}{4}\frac{\zeta_R\left(\frac{d-1}{2}\right)}{\zeta_R^{\frac{d-1}{d}}\left(\frac{d}{2}\right)N^{\frac{1}{d}}}\right) \\
&= \zeta_R\left(\frac{d}{2}\right)\frac{V(\sqrt{2m\pi k})^d T_C^{\frac{d}{2}}}{h^d}\left(1 + \frac{\kappa b}{4}\frac{\zeta_R\left(\frac{d-1}{2}\right)}{\zeta_R^{\frac{d-1}{d}}\left(\frac{d}{2}\right)N^{\frac{1}{d}}}\right) \tag{3.58}
\end{aligned}$$

Finally, we extract T_C from the above expression.

$$\begin{aligned}
\left[T_C^{-\frac{d}{2}} = \zeta_R\left(\frac{d}{2}\right)\frac{V(\sqrt{2m\pi k})^d}{Nh^d}\left(1 + \frac{\kappa b}{4}\frac{\zeta_R\left(\frac{d-1}{2}\right)}{\zeta_R^{\frac{d-1}{d}}\left(\frac{d}{2}\right)N^{\frac{1}{d}}}\right)\right]^{-\frac{2}{d}} \tag{3.59} \\
\Rightarrow T_C = \zeta_R^{-\frac{2}{d}}\left(\frac{d}{2}\right)\frac{V^{-\frac{2}{d}}(\sqrt{2m\pi k})^{-2}}{N^{-\frac{2}{d}}h^{-2}}\left(1 + \frac{\kappa b}{4}\frac{\zeta_R\left(\frac{d-1}{2}\right)}{\zeta_R^{\frac{d-1}{d}}\left(\frac{d}{2}\right)N^{\frac{1}{d}}}\right)^{-\frac{2}{d}} \\
= \frac{\left(\frac{N}{V}\right)^{\frac{2}{d}}h^2}{\underbrace{\zeta_R^{\frac{2}{d}}\left(\frac{d}{2}\right)(2m\pi k)}_{T_0}}\left(1 + \frac{\kappa b}{4}\frac{\zeta_R\left(\frac{d-1}{2}\right)}{\zeta_R^{\frac{d-1}{d}}\left(\frac{d}{2}\right)N^{\frac{1}{d}}}\right)^{-\frac{2}{d}} \tag{3.60}
\end{aligned}$$

Lastly, we will write T_C in terms of T_0 by using the approximation $(1+x)^n = 1+nx$, where $n = -\frac{2}{d}$ in this case.

$$T_C = T_0\left(1 - \frac{\kappa b}{2d}\frac{\zeta_R\left(\frac{d-1}{2}\right)}{\left(\zeta_R\left(\frac{d}{2}\right)\right)^{\frac{d-1}{d}}N^{\frac{1}{d}}} + \dots\right) \tag{3.61}$$

As it seems, the correction of boundary effects to the critical temperature vanishes as $N \rightarrow \infty$. Additionally, T_C value increases or decreases depending on b being plus or minus 1.

We will also look up the $d = 3$ case. We already know

$$Li_n(x) = \sum_{l=1}^{\infty} \frac{x^l}{l^n} \quad \text{and} \quad \ln(1-x) = -\sum_{l=1}^{\infty} \frac{x^l}{l}, \quad |x| < 1 \quad (3.62)$$

Here, since $E_N - \mu_c$ goes to zero, the Li function is not directly reduced to $\zeta(1)$. In $d = 3$ case, the Li function of the boundary term turns into ordinary logarithm.

$$-\ln(1-x) = Li_1(x) \quad (3.63)$$

$$\Rightarrow Li_1(e^{-\beta(\mu_c - \mu)}) = -\ln(1 - e^{-\beta(\mu_c - \mu)}) = -\ln(1 - 1 + \beta(\mu_c - \mu)) \quad (3.64)$$

We know the ground state occupation number is $N_0 = \frac{d_0}{e^{\beta(\mu_c - \mu)} - 1}$. We take \ln of both sides then we have

$$\ln\left(e^{\beta(\mu_c - \mu)} = \frac{d_0 + N_0}{N_0} \right) \quad (3.65)$$

$$\Rightarrow \beta(\mu_c - \mu) = \ln\left(\frac{d_0}{N_0} + 1\right) \simeq \frac{1}{N_0} \quad (3.66)$$

$$\Rightarrow Li_1(e^{-\beta(\mu_c - \mu)}) = -\ln\left(\frac{1}{N_0}\right) = -\ln 1 + \ln N_0 = \ln N_0 = \ln(fN) \quad (3.67)$$

Now, putting these information back in the equation, we reach the last structure of total number of particles expression.

$$N - N_0 = N - fN \simeq \zeta_R\left(\frac{3}{2}\right)\xi^3 + \frac{\kappa b}{4}\ln(fN)\xi^2 \quad (3.68)$$

We make the arrangements and obtain Toms and Kirsten's expression.

$$\begin{aligned} N(1-f) &= \zeta_R\left(\frac{3}{2}\right)\frac{L^3}{\lambda_T^3} + \frac{\kappa b}{4}\zeta_R(1)\frac{L^2}{\lambda_T^2} \\ &= \zeta_R\left(\frac{3}{2}\right)\frac{L^3}{h^3}(2\pi m k T)^{\frac{3}{2}} + \frac{\kappa b}{4}\zeta_R(1)\frac{L^2}{h^2}(2\pi m k T) \end{aligned} \quad (3.69)$$

Again, we use only the first term (f is moved back at the right hand side of the equation) to write the bulk critical temperature.

$$N \simeq \zeta_R\left(\frac{3}{2}\right)\xi_0^3 = \zeta_R\left(\frac{3}{2}\right)\frac{V}{h^3}(2\pi mkT_0)^{\frac{3}{2}} \quad (3.70)$$

$$\Rightarrow T_0 = \left(\frac{N}{\zeta_R\left(\frac{3}{2}\right)V}\right)^{\frac{2}{3}} \frac{h^2}{2\pi mk} \quad (3.71)$$

We continue with putting T_0 back in N to see the boundary contribution to the critical temperature.

$$\begin{aligned} N &= \zeta_R\left(\frac{3}{2}\right)\xi_0^3 + \frac{\kappa b}{4}\ln(fN)\xi_0^2 + fN + \dots \\ &= \zeta_R\left(\frac{3}{2}\right)\xi_0^3 \left(1 + \frac{\kappa b}{4}\ln(fN)\frac{1}{\zeta_R\left(\frac{3}{2}\right)\xi_0} + \frac{fN}{\zeta_R\left(\frac{3}{2}\right)\xi_0^3}\right) \end{aligned} \quad (3.72)$$

Here, we insert the $\xi_0^3 = \frac{N}{\zeta_R\left(\frac{3}{2}\right)}$ formula that we know from the earlier calculations.

$$N = \zeta_R\left(\frac{3}{2}\right)\frac{V(2\pi mkT)^{\frac{3}{2}}}{h^3} \left(1 + \frac{\kappa b}{4}\ln(fN)\frac{(\zeta_R\left(\frac{3}{2}\right))^{\frac{1}{3}}}{\zeta_R\left(\frac{3}{2}\right)N^{\frac{1}{3}}} + \frac{fN\zeta_R\left(\frac{3}{2}\right)}{\zeta_R\left(\frac{3}{2}\right)N}\right) \quad (3.73)$$

We take out T , which can be described as T_C , from this equation:

$$T_C = \underbrace{\frac{N^{\frac{2}{3}}h^3}{(\zeta_R\left(\frac{3}{2}\right))^{\frac{2}{3}}V^{\frac{2}{3}}(2\pi mk)}}_{T_0} \left[1 + \frac{\kappa b}{4N^{\frac{1}{3}}}\ln(fN)(\zeta_R\left(\frac{3}{2}\right))^{-\frac{2}{3}} + \frac{fN}{N}\right]^{\frac{2}{3}} \quad (3.74)$$

Here, again we will use the approximation $(1+x)^n = 1+nx$, where $n = -\frac{2}{3}$ in our case:

$$\begin{aligned} T_C &= T_0 \left(1 - \frac{2}{3}\frac{\kappa b}{4N^{\frac{1}{3}}}\ln(fN)(\zeta_R\left(\frac{3}{2}\right))^{-\frac{2}{3}} - \frac{2}{3}f\right) \\ &= T_0 \left(1 - \frac{2}{3}\left(\frac{\kappa b}{4}\frac{\ln(fN)}{(\zeta_R\left(\frac{3}{2}\right))^{\frac{2}{3}}N^{\frac{1}{3}}} + f\right)\right) \end{aligned} \quad (3.75)$$

After we define an α parameter as

$$\alpha = \frac{\kappa b}{4} \frac{\ln(fN)}{(\zeta_R(\frac{3}{2}))^{\frac{2}{3}} N^{\frac{1}{3}}} \quad (3.76)$$

we reach the summarized expression for T as in Toms and Kirsten's paper.

$$T_C = T_0 \left(1 - \frac{2}{3}(\alpha + f) \right) \quad (3.77)$$

Even though we know there is no condensation at two dimension, let us continue with the $d = 2$ case to see what the explicit critical temperature looks like. We know that (as given in equation (3.90))

$$Li_{\frac{1}{2}}(e^{-\beta(\mu_c - \mu)}) \simeq \sqrt{\frac{\pi}{\beta(\mu_c - \mu)}} \quad (3.78)$$

for $\mu \simeq \mu_c$ limit. If we write the fraction on the number of particles accordingly

$$\begin{aligned} N(1 - f) &\simeq Li_1(e^{-\beta(\mu_c - \mu)})\xi^2 + \frac{\kappa b}{4} Li_{\frac{1}{2}}(e^{-\beta(\mu_c - \mu)})\xi + \dots \\ &\simeq \ln(fN)\xi^2 + \frac{\kappa b}{4} \sqrt{\frac{\pi}{1/N_0}} \xi \quad , \quad (N_0 = fN) \\ &\simeq \ln(fN)\xi^2 + \frac{\kappa b}{4} \sqrt{\pi} \xi \sqrt{fN} \end{aligned} \quad (3.79)$$

This is an inconsistent equation for $N \rightarrow \infty$ limit if f is small but finite so that $fn \gg 1$. Therefore, BEC is impossible for $d = 1$ and $d = 2$ cases as a phase transition.

3.4. Recalculation of $\frac{\partial \beta(\mu_c - \mu)}{\partial \beta}$

To see the finite size effects on each thermodynamical quantity that we will work out, we will recalculate $\frac{\partial \beta(\mu_c - \mu)}{\partial \beta}$ expression by keeping the boundary terms which go like ξ^{d-1} .

We will now enforce the total number of particles N to be fixed, therefore derivatives of N with respect to β at constant volume is zero.

$$\left. \frac{\partial N}{\partial \beta} \right|_{\mu} + \left. \frac{\partial N}{\partial \mu} \right|_{\beta} \frac{\partial \mu}{\partial \beta} = 0 \quad (3.80)$$

This can be also written as

$$\frac{\partial N}{\partial(e^{-\beta(\mu_c-\mu)})} \frac{\partial(e^{-\beta(\mu_c-\mu)})}{\partial \beta} \Big|_{\mu} + \frac{\partial N}{\partial \xi} \frac{\partial \xi}{\partial \beta} + \frac{\partial N}{\partial(e^{-\beta(\mu_c-\mu)})} \frac{\partial(e^{-\beta(\mu_c-\mu)})}{\partial \mu} \Big|_{\beta} \frac{\partial \mu}{\partial \beta} = 0 \quad (3.81)$$

We take out the $\frac{\partial \mu}{\partial \beta}$ term from the equation above and we will calculate $\left. \frac{\partial N}{\partial \beta} \right|_{\mu}$ and $\left. \frac{\partial N}{\partial \mu} \right|_{\beta}$ derivatives:

$$\left. \frac{\partial N}{\partial \beta} \right|_{\mu} = \frac{\partial N_0}{\partial \beta} + \frac{\partial}{\partial \beta} (Li_{\frac{d}{2}}(e^{-\beta(\mu_c-\mu)})\xi^d) + \frac{\partial}{\partial \beta} \left(\frac{\kappa b}{4} Li_{\frac{d-1}{2}}(e^{-\beta(\mu_c-\mu)})\xi^{d-1} \right) \quad (3.82)$$

$$\left. \frac{\partial N}{\partial \mu} \right|_{\beta} = \frac{\partial N_0}{\partial \mu} + \frac{\partial}{\partial \mu} (Li_{\frac{d}{2}}(e^{-\beta(\mu_c-\mu)})\xi^d) + \frac{\partial}{\partial \mu} \left(\frac{\kappa b}{4} Li_{\frac{d-1}{2}}(e^{-\beta(\mu_c-\mu)})\xi^{d-1} \right) \quad (3.83)$$

Here, since N_0 is microscopic, its derivatives with respect to both temperature and chemical potential are zero above T_C . We can write the rest clearly as:

$$\begin{aligned} \left. \frac{\partial N}{\partial \beta} \right|_{\mu} = & 0 - Li_{\frac{d-2}{2}}(e^{-\beta(\mu_c-\mu)})(\mu_c - \mu)\xi^d - Li_{\frac{d}{2}}(e^{-\beta(\mu_c-\mu)})\frac{d}{2}\beta^{-1}\xi^d \\ & - \frac{\kappa b}{4} Li_{\frac{d-3}{2}}(e^{-\beta(\mu_c-\mu)})(\mu_c - \mu)\xi^{d-1} - \frac{\kappa b}{4} Li_{\frac{d-1}{2}}(e^{-\beta(\mu_c-\mu)})\frac{d-1}{2}\beta^{-1}\xi^{d-1} \end{aligned} \quad (3.84)$$

$$\left. \frac{\partial N}{\partial \mu} \right|_{\beta} = 0 + Li_{\frac{d-2}{2}}(e^{-\beta(\mu_c-\mu)})\beta\xi^d + \frac{\kappa b}{4} Li_{\frac{d-3}{2}}(e^{-\beta(\mu_c-\mu)})\beta\xi^{d-1} \quad (3.85)$$

Dividing $\frac{\partial N}{\partial \beta} \Big|_{\mu}$ to $\frac{\partial N}{\partial \mu} \Big|_{\beta}$, we get

$$\begin{aligned}
\frac{\partial \mu}{\partial \beta} &= - \frac{\frac{\partial N}{\partial \beta} \Big|_{\mu}}{\frac{\partial N}{\partial \mu} \Big|_{\beta}} \\
&= - \left[- Li_{\frac{d-2}{2}}(e^{-\beta(\mu_c - \mu)})(\mu_c - \mu)\xi^d - Li_{\frac{d}{2}}(e^{-\beta(\mu_c - \mu)})\frac{d}{2}\beta^{-1}\xi^d \right. \\
&\quad \left. - \frac{\kappa b}{4} Li_{\frac{d-3}{2}}(e^{-\beta(\mu_c - \mu)})(\mu_c - \mu)\xi^{d-1} - \frac{\kappa b}{4} Li_{\frac{d-1}{2}}(e^{-\beta(\mu_c - \mu)})\left(\frac{d-1}{2}\right)\beta^{-1}\xi^{d-1} \right] \\
&\quad \cdot \left[Li_{\frac{d-2}{2}}(e^{-\beta(\mu_c - \mu)})\beta\xi^d + \frac{\kappa b}{4} Li_{\frac{d-3}{2}}(e^{-\beta(\mu_c - \mu)})\beta\xi^{d-1} \right]^{-1} \tag{3.86}
\end{aligned}$$

To reach the exact form of the expression which is written by Toms and Kirsten, we will multiply $\frac{\partial \mu}{\partial \beta}$ with $-\beta$ and then add $(\mu_c - \mu)$ to it. We will reach the desired expression after taking both the numerator and denominator in proper terms parenthesis which are the leading terms going like volume. For simplicity, we will not bother writing the exponential arguments of polylogarithmic functions.

$$\frac{\partial \beta(\mu_c - \mu)}{\partial \beta} = -\beta \frac{\partial \mu}{\partial \beta} + (\mu_c - \mu) = \frac{-\beta^{-1} \frac{d}{2} Li_{\frac{d}{2}} \left(1 + \frac{\frac{\kappa b}{4} \frac{d-1}{2} Li_{\frac{d-1}{2}} \xi^{-1}}{\frac{d}{2} Li_{\frac{d}{2}}} \right)}{Li_{\frac{d-2}{2}} \left(1 + \frac{\frac{\kappa b}{4} Li_{\frac{d-3}{2}} \xi^{-1}}{Li_{\frac{d-2}{2}}} \right)} \tag{3.87}$$

Now, let us establish the approximation that we will use to see the boundary effects. Since the terms with κb are order of $V^{-\frac{1}{d}}$ we can use the approximation

$$\frac{1}{1 + \epsilon} \simeq 1 - \epsilon, \text{ for small } \epsilon \tag{3.88}$$

However, the terms with κ parameter having lower dimension of volume is not enough to make this approximation. The other important condition to use this approximation is that the term $\frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}}$ should remain finite at the limit $T \rightarrow T_C$. We will use three expressions which are stated proceeding from Robinson's result in Pathria's book[7] and describing the behaviour of Li functions at this limit.

First expression is the result for m as a positive integer:

$$Li_m(e^{-\alpha}) = \frac{(-1)^{m-1}}{(m-1)!} \left[\sum_{i=1}^{m-1} \frac{1}{i} - \ln \alpha \right] \alpha^{m-1} + \sum_{i=0, i \neq m-1}^{\infty} \frac{(-1)^i}{i!} \zeta(m-i) \alpha^i, \quad (3.89)$$

secondly, for all $m < 1$ and non-integer $m > 1$:

$$Li_m(e^{-\alpha}) = \frac{\Gamma(1-m)}{\alpha^{1-m}} + \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \zeta(m-i) \alpha^i, \quad (3.90)$$

and lastly for $m = 1$:

$$Li_1(e^{-\alpha}) = \int_0^{\infty} \frac{dx}{e^{\alpha} e^x - 1} = \ln(1 - e^{-\alpha} e^{-x}) \Big|_0^{\infty} = -\ln(1 - e^{-\alpha}) \quad (3.91)$$

where $\alpha = -\mu\beta$.

We can show that for $d = 3, 4$ and 5 cases, $\frac{\partial}{\partial \beta} [\beta(\mu_c - \mu)]$ derivative disappears as $\mu \rightarrow \mu_c$. Then, let us make a dimension analysis whether we can make our expansion or not.

Since for $d = 1$ and $d = 2$ there is no condensation, there is no need to check the consistency. Starting with $d = 3$ case,

$$\begin{aligned} \frac{\partial}{\partial \beta} [\beta(\mu_c - \mu)] &= -\frac{3}{2} \beta^{-1} \frac{Li_{\frac{3}{2}}}{Li_{\frac{1}{2}}} \frac{1 + \frac{\kappa b}{4} \frac{Li_1}{Li_{\frac{3}{2}}} \frac{2}{3} \xi^{-1}}{1 + \frac{\kappa b}{4} \frac{Li_0}{Li_{\frac{1}{2}}} \xi^{-1}} \\ &= -\frac{3}{2} \beta^{-1} \frac{\frac{\Gamma(-\frac{1}{2})}{\alpha^{-\frac{1}{2}}} + \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \zeta(\frac{3}{2} - i) \alpha^i}{\frac{\Gamma(\frac{1}{2})}{\alpha^{\frac{1}{2}}} + \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \zeta(\frac{1}{2} - i) \alpha^i} \frac{1 + \frac{\kappa b}{4} \frac{-\ln(1-e^{-\alpha})}{\frac{\Gamma(-\frac{1}{2})}{\alpha^{-\frac{1}{2}}} + \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \zeta(\frac{3}{2} - i) \alpha^i} \frac{2}{3} \xi^{-1}}{1 + \frac{\kappa b}{4} \frac{\frac{\Gamma(1)}{\alpha} + \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \zeta(-i) \alpha^i}{\frac{\Gamma(\frac{1}{2})}{\alpha^{\frac{1}{2}}} + \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \zeta(\frac{1}{2} - i) \alpha^i} \xi^{-1}} \\ \lim_{\alpha \rightarrow 0} \left\{ -\frac{3}{2} \beta^{-1} \frac{\Gamma(-\frac{1}{2}) \alpha + \alpha^{\frac{1}{2}} \zeta(\frac{3}{2}) - \zeta(\frac{1}{2}) \alpha^{\frac{3}{2}}}{\Gamma(\frac{1}{2}) + \zeta(\frac{1}{2}) \alpha^{\frac{1}{2}} - \zeta(-\frac{1}{2}) \alpha^{\frac{3}{2}}} \frac{1 + \frac{\kappa b}{4} \frac{-\ln(1-e^{-\alpha}) \alpha^{-\frac{1}{2}}}{\Gamma(-\frac{1}{2}) + \zeta(\frac{3}{2}) \alpha^{-\frac{1}{2}} - \zeta(\frac{1}{2}) \alpha^{\frac{1}{2}}} \frac{2}{3} \xi^{-1}}{1 + \frac{\kappa b}{4} \frac{\Gamma(1) + \zeta(0) \alpha - \zeta(-1) \alpha^2}{(\Gamma(\frac{1}{2}) + \alpha^{\frac{1}{2}} \zeta(\frac{1}{2}) - \zeta(-\frac{1}{2}) \alpha^{\frac{3}{2}}) \alpha^{\frac{1}{2}}} \xi^{-1}} \right\} &= 0 \end{aligned} \quad (3.92)$$

$d = 4$ case:

$$\begin{aligned} \frac{\partial}{\partial \beta} [\beta(\mu_c - \mu)] &= -2\beta^{-1} \frac{Li_2}{Li_1} \frac{1 + \frac{\kappa b}{4} \frac{Li_{\frac{3}{2}}}{Li_{\frac{1}{2}}} \frac{3}{4} \xi^{-1}}{1 + \frac{\kappa b}{4} \frac{Li_{\frac{1}{2}}}{Li_1} \xi^{-1}} \\ &= -2\beta^{-1} \frac{-(1 - \ln \alpha)\alpha + \zeta(2)}{-\ln(1 - e^{-\alpha})} \frac{1 + \frac{\kappa b}{4} \frac{\Gamma(-\frac{1}{2})\alpha^{\frac{1}{2}} + \zeta(\frac{3}{2}) - \zeta(\frac{1}{2})\alpha}{-(1 - \ln \alpha)\alpha + \zeta(2)} \frac{3}{4} \xi^{-1}}{1 + \frac{\kappa b}{4} \frac{\frac{\Gamma(\frac{1}{2})}{\alpha^{\frac{1}{2}} + \zeta(\frac{1}{2}) - \zeta(-\frac{1}{2})\alpha}}{-\ln(1 - e^{-\alpha})} \xi^{-1}} \end{aligned} \quad (3.93)$$

$$\lim_{\alpha \rightarrow 0} \left\{ -2\beta^{-1} \frac{-(1 - \ln \alpha)\alpha + \zeta(2)}{-\ln(1 - e^{-\alpha})} \frac{1 + \frac{\kappa b}{4} \frac{\Gamma(-\frac{1}{2})\alpha^{\frac{1}{2}} + \zeta(\frac{3}{2}) - \zeta(\frac{1}{2})\alpha}{-(1 - \ln \alpha)\alpha + \zeta(2)} \frac{3}{4} \xi^{-1}}{1 + \frac{\frac{\Gamma(\frac{1}{2})}{\alpha^{\frac{1}{2}} + \zeta(\frac{1}{2}) - \zeta(-\frac{1}{2})\alpha}}{-\ln(1 - e^{-\alpha})} \xi^{-1}} \right\} = 0 \quad (3.94)$$

$d = 5$ case:

$$\frac{\partial}{\partial \beta} [\beta(\mu_c - \mu)] = -\frac{5}{2}\beta^{-1} \frac{Li_{\frac{5}{2}}}{Li_{\frac{3}{2}}} \frac{1 + \frac{\kappa b}{4} \frac{Li_{\frac{4}{5}}}{Li_{\frac{2}{5}}} \frac{4}{5} \xi^{-1}}{1 + \frac{\kappa b}{4} \frac{Li_1}{Li_{\frac{3}{2}}} \xi^{-1}} \quad (3.95)$$

$$\begin{aligned} &= -\frac{5}{2}\beta^{-1} \frac{\Gamma(-\frac{3}{2})\alpha + \zeta(\frac{5}{2})\alpha^{-\frac{1}{2}} - \zeta(\frac{3}{2})\alpha^{\frac{1}{2}}}{\Gamma(-\frac{1}{2}) + \zeta(\frac{3}{2})\alpha^{-\frac{1}{2}} - \zeta(\frac{1}{2})\alpha^{\frac{1}{2}}} \frac{1 + \frac{\kappa b}{4} \frac{-(1 - \ln \alpha)\alpha + \zeta(2)}{\Gamma(-\frac{3}{2})\alpha^{\frac{3}{2}} + \zeta(\frac{5}{2}) - \zeta(\frac{3}{2})\alpha} \frac{4}{5} \xi^{-1}}{1 + \frac{\kappa b}{4} \frac{-\ln(1 - e^{-\alpha})}{\Gamma(-\frac{1}{2})\alpha^{\frac{1}{2}} + \zeta(\frac{3}{2}) - \zeta(\frac{1}{2})\alpha} \xi^{-1}} \end{aligned} \quad (3.96)$$

$$\lim_{\alpha \rightarrow 0} \left\{ -\frac{5}{2}\beta^{-1} \frac{\Gamma(-\frac{3}{2})\alpha + \zeta(\frac{5}{2})\alpha^{-\frac{1}{2}} - \zeta(\frac{3}{2})\alpha^{\frac{1}{2}}}{\Gamma(-\frac{1}{2}) + \zeta(\frac{3}{2})\alpha^{-\frac{1}{2}} - \zeta(\frac{1}{2})\alpha^{\frac{1}{2}}} \frac{1 + \frac{\kappa b}{4} \frac{-(1 - \ln \alpha)\alpha + \zeta(2)}{\Gamma(-\frac{3}{2})\alpha^{\frac{3}{2}} + \zeta(\frac{5}{2}) - \zeta(\frac{3}{2})\alpha} \frac{4}{5} \xi^{-1}}{1 + \frac{\kappa b}{4} \frac{-\ln(1 - e^{-\alpha})}{\Gamma(-\frac{1}{2})\alpha^{\frac{1}{2}} + \zeta(\frac{3}{2}) - \zeta(\frac{1}{2})\alpha} \xi^{-1}} \right\} = 0 \quad (3.97)$$

Therefore, we can use our approximation only for the $d \geq 6$ dimensional cases.

Now, let us state the expansion that we will use for the sufficiently higher dimensions later on:

$$\begin{aligned}
\frac{\partial}{\partial\beta}[\beta(\mu_c - \mu)] &= \left[\frac{-\frac{d}{2}\beta^{-1}Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \right] \left[\frac{1 + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \frac{d-1}{d} \xi^{-1}}{1 + \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1}} \right] \\
&\simeq \left[\frac{-\frac{d}{2}\beta^{-1}Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \right] \left(1 + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \frac{d-1}{d} \xi^{-1} \right) \left(1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} \right) \\
&\simeq \left[\frac{-\frac{d}{2}\beta^{-1}Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \right] \left[1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \frac{d-1}{d} \xi^{-1} \right] \tag{3.98}
\end{aligned}$$

$$= -\frac{d}{2}\beta^{-1} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} + \frac{\kappa b}{4} \frac{d}{2} \beta^{-1} Li_{\frac{d}{2}} \frac{Li_{\frac{d-3}{2}}}{(Li_{\frac{d-2}{2}})^2} \xi^{-1} - \frac{\kappa b}{4} \beta^{-1} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}} \frac{d-1}{2} \xi^{-1} \tag{3.99}$$

We note that we do not keep the terms of order of $O(\xi^{-2})$.

3.5. Internal Energy

Since we already express the partition function q in terms of polylogarithmic functions, we can calculate the other related thermodynamical expressions in the same way. We start with internal energy of the system.

Internal energy can be found as the derivative of the partition function:

$$U = -\frac{\partial q}{\partial\beta}\Big|_{\mu} + \mu N = -\frac{\partial q}{\partial\beta}\Big|_{\mu} + \frac{\mu}{\beta} \frac{\partial q}{\partial\mu}\Big|_{\beta,V} \tag{3.100}$$

We stated the partition function as

$$q = q_0 + Li_{\frac{d+2}{2}}(e^{-\beta(\mu_c - \mu)})\xi^d + \frac{\kappa b}{4} Li_{\frac{d+1}{2}}(e^{-\beta(\mu_c - \mu)})\xi^{d-1}. \tag{3.101}$$

We will take these derivatives separately where $\frac{\partial[\beta(\mu_c - \mu)]}{\partial\beta}\Big|_{\mu} = \mu_c - \mu$ and $\frac{\partial[-\beta(\mu_c - \mu)]}{\partial\mu}\Big|_{\beta,V} = \beta$. We note that we did not use the expansion that we have found above since the quan-

titles that we keep constant are different:

$$\begin{aligned}
-\frac{\partial q}{\partial \beta} \Big|_{\mu} &= -\frac{\partial q_0}{\partial \beta} - Li_{\frac{d}{2}} \frac{\partial[-\beta(\mu_c - \mu)]}{\partial \beta} \Big|_{\mu} \xi^d - Li_{\frac{d+2}{2}} \left(-\frac{d}{2}\right) \beta^{-1} \xi^d \\
&\quad - \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \frac{\partial[-\beta(\mu_c - \mu)]}{\partial \beta} \Big|_{\mu} \xi^{d-1} - \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \left(-\frac{d-1}{2}\right) \beta^{-1} \xi^{d-1} \\
&= -\frac{\partial q_0}{\partial \beta} + Li_{\frac{d}{2}} (\mu_c - \mu) \xi^d + Li_{\frac{d+2}{2}} \frac{d}{2} \beta^{-1} \xi^d \\
&\quad + \frac{\kappa b}{4} Li_{\frac{d-1}{2}} (\mu_c - \mu) \xi^{d-1} + \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \frac{d-1}{2} \beta^{-1} \xi^{d-1} \tag{3.102}
\end{aligned}$$

$$\begin{aligned}
\frac{\mu}{\beta} \frac{\partial q}{\partial \mu} \Big|_{\beta, V} &= \frac{\mu}{\beta} \frac{\partial q_0}{\partial \mu} + \frac{\mu}{\beta} Li_{\frac{d}{2}} \frac{\partial[-\beta(\mu_c - \mu)]}{\partial \mu} \Big|_{\beta, V} \xi^d + \frac{\mu}{\beta} \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \frac{\partial[-\beta(\mu_c - \mu)]}{\partial \mu} \Big|_{\beta, V} \xi^{d-1} \\
&= \frac{\mu}{\beta} \frac{\partial q_0}{\partial \mu} + Li_{\frac{d}{2}} \xi^d \mu + \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{d-1} \mu \tag{3.103}
\end{aligned}$$

We take the chemical potential at the critical point, μ_c , equals to the ground state energy E_0 :

$$U = U_0 + \frac{d}{2} Li_{\frac{d+2}{2}} \beta^{-1} \xi^d + \frac{\kappa b}{4} \frac{d-1}{2} \beta^{-1} Li_{\frac{d+1}{2}} \xi^{d-1} + E_0 Li_{\frac{d}{2}} \xi^d + E_0 \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{d-1} \tag{3.104}$$

Here, d_0 is the degeneracy and E_0 is energy of the ground state. As we noted earlier, q_0 is the ground state partition function. Based on these, we can write the ground state contribution to the energy, U_0 as:

$$q_0 = -d_0 \ln(1 - ze^{-\beta E_0}) \quad , \quad U_0 = -\frac{\partial q_0}{\partial \beta} + \frac{\mu}{\beta} \frac{\partial q_0}{\partial \mu} = \frac{d_0 E_0}{e^{\beta(E_0 - \mu)} - 1} \tag{3.105}$$

this internal energy result is the same with the result that Toms and Kirsten wrote in their article.

3.6. Calculation of the Heat Capacity Above and Below Critical Temperature

The heat capacity with constant volume, C_V , will be calculated by taking the derivative of internal energy with respect to temperature. It will be calculated in two ways considering the behaviour of the system below and above the critical temperature, to check if there is a discontinuity around the critical temperature or not. Typically, we expect no discontinuity for the dimensions $d \leq 6$. We will check whether this is consistent or not after we write the discontinuity expression for higher dimensions.

3.6.1. Calculation of C_V^+

Let us start with C_V above the critical temperature. We basically take the temperature derivative of the internal energy expression.

$$\begin{aligned}
C_V^+ &= \frac{\partial U^+}{\partial T} \Big|_V = \frac{\partial U^+}{\partial \beta} \Big|_V (-k\beta^2) \\
&= \left[-\frac{d}{2} \beta^{-2} Li_{\frac{d+2}{2}}(e^{-\beta(\mu_c-\mu)}) \xi^d + \frac{d}{2} \beta^{-1} Li_{\frac{d}{2}}(e^{-\beta(\mu_c-\mu)}) \left(-\frac{\partial \beta(\mu_c-\mu)}{\partial \beta} \right) \xi^d \right. \\
&\quad + \frac{d}{2} \beta^{-1} Li_{\frac{d+2}{2}}(e^{-\beta(\mu_c-\mu)}) \beta^{-1} \left(-\frac{d}{2} \right) \xi^d - \frac{\kappa b d - 1}{4} \frac{d-1}{2} \beta^{-2} Li_{\frac{d+1}{2}}(e^{-\beta(\mu_c-\mu)}) \xi^{d-1} \\
&\quad + \frac{\kappa b d - 1}{4} \frac{d-1}{2} \beta^{-1} Li_{\frac{d-1}{2}}(e^{-\beta(\mu_c-\mu)}) \left(-\frac{\partial \beta(\mu_c-\mu)}{\partial \beta} \right) \xi^{d-1} \\
&\quad \left. + \frac{\kappa b d - 1}{4} \frac{d-1}{2} \beta^{-1} Li_{\frac{d+1}{2}}(e^{-\beta(\mu_c-\mu)}) \beta^{-1} \left(-\frac{d-1}{2} \right) \xi^{d-1} \right] (-k\beta^2) \tag{3.106}
\end{aligned}$$

Here, we did not write the terms with E_0 and the term coming from the derivative of U_0 since the ground state energy will be taken as zero. Note that

$$E_0 \sim \frac{h^2}{2mV^{\frac{2}{d}}} \tag{3.107}$$

thus of a very small order in general.

For simplicity, we will not write the exponential arguments of the Li functions.

We will replace all the $-\frac{\partial\beta(\mu_c-\mu)}{\partial\beta}$ derivatives with the expansion we have found earlier.

$$\begin{aligned}
C_V^+ = & \left[-\frac{d}{2}\beta^{-2}Li_{\frac{d+2}{2}}\xi^d + \frac{d}{2}\beta^{-1}Li_{\frac{d}{2}}\left(\frac{d}{2}\beta^{-1}\frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} - \frac{\kappa b d}{4}\frac{\beta^{-1}Li_{\frac{d}{2}}}{(Li_{\frac{d-2}{2}})^2}\xi^{-1} \right. \right. \\
& + \frac{\kappa b}{4}\beta^{-1}\frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}}\frac{d-1}{2}\xi^{-1}\xi^d + \frac{d}{2}\beta^{-1}Li_{\frac{d+2}{2}}\beta^{-1}\left(-\frac{d}{2}\right)\xi^d - \frac{\kappa b d-1}{4}\frac{\beta^{-2}Li_{\frac{d+1}{2}}}{2}\xi^{d-1} \\
& + \frac{\kappa b d-1}{4}\frac{\beta^{-1}Li_{\frac{d-1}{2}}}{2}\left(\frac{d}{2}\beta^{-1}\frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} - \frac{\kappa b d}{4}\frac{\beta^{-1}Li_{\frac{d}{2}}}{(Li_{\frac{d-2}{2}})^2}\xi^{-1} \right. \\
& \left. \left. + \frac{\kappa b}{4}\beta^{-1}\frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}}\frac{d-1}{2}\xi^{-1}\right)\xi^{d-1} - \frac{\kappa b d-1}{4}\frac{\beta^{-2}Li_{\frac{d+1}{2}}}{2}\frac{d-1}{2}\xi^{d-1} \right] (-k\beta^2) \quad (3.108)
\end{aligned}$$

After some arrangements, we can write C_V^+ explicitly as

$$\begin{aligned}
C_V^+ = & k\left(\frac{d}{2} + \frac{d^2}{4}\right)Li_{\frac{d+2}{2}}\xi^d + \frac{\kappa b}{4}\left(\frac{(d-1)}{2} + \frac{(d-1)^2}{4}\right)kLi_{\frac{d+1}{2}}\xi^{d-1} \\
& - k\frac{d^2}{4}\xi^d\frac{(Li_{\frac{d}{2}})^2}{Li_{\frac{d-2}{2}}} + k\frac{\kappa b d^2}{4}\frac{(Li_{\frac{d}{2}})^2Li_{\frac{d-3}{2}}}{(Li_{\frac{d-2}{2}})^2}\xi^{d-1} - k2\frac{d-1}{2}\frac{d}{2}\frac{\kappa b}{4}\frac{Li_{\frac{d}{2}}Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}}\xi^{d-1} \quad (3.109)
\end{aligned}$$

3.6.2. Calculation of C_V^-

In the calculation of the heat capacity below T_C , each term is the same with C_V^+ except there will be some terms vanishing. Since chemical potential will be a constant in the internal energy expression below T_C , the terms coming from the derivative of the chemical potential will vanish. Additionally, the polylogarithmics will again go to zeta functions.

$$\begin{aligned}
C_V^- = & \frac{\partial U^-}{\partial T}|_V = \frac{d}{2}k\zeta\left(\frac{d+2}{2}\right)\xi^d + k\frac{\kappa b (d-1)}{4}\frac{\zeta\left(\frac{d+1}{2}\right)}{2}\xi^{d-1} \\
& + \frac{d^2}{4}k\zeta\left(\frac{d+2}{2}\right)\xi^d + \frac{\kappa b (d-1)^2}{4}k\zeta\left(\frac{d+1}{2}\right)\xi^{d-1} \quad (3.110)
\end{aligned}$$

Here, we can check the bulk result, taking $d = 3$ and dropping the boundary terms:

$$\frac{C_V^-}{Nk} = \zeta\left(\frac{5}{2}\right)\xi^3\left(\frac{3}{2} + \frac{9}{4}\right) = \frac{15}{4}\zeta\left(\frac{5}{2}\right)\frac{v}{\lambda^3} \quad (3.111)$$

where $v = \frac{V}{N}$ and $\frac{v}{\lambda^3} = \frac{1}{\zeta(\frac{3}{2})}$; same expression with the result written by Pathria[7].

3.6.3. Discontinuity of C_V Around T_C

Now, looking at the discontinuity on C_V , we will subtract C_V^- from C_V^+ . Therefore, need to take the $\mu \rightarrow \mu_c$ limit at C_V^+ also.

$$\begin{aligned}
C_V^+ - C_V^- &= k \left(\frac{d}{2} + \frac{d^2}{4} \right) \zeta \left(\frac{d+2}{2} \right) \xi^d + \frac{\kappa b}{4} \left(\frac{d-1}{2} + \frac{(d-1)^2}{4} \right) k \zeta \left(\frac{d+1}{2} \right) \xi^{d-1} \\
&\quad - k \frac{d^2}{4} \xi^d \frac{(\zeta(\frac{d}{2}))^2}{\zeta(\frac{d-2}{2})} + k \frac{\kappa b}{4} \frac{d^2}{4} \frac{(\zeta(\frac{d}{2}))^2 \zeta(\frac{d-3}{2})}{(\zeta(\frac{d-2}{2}))^2} \xi^{d-1} - k \frac{\kappa b}{4} \frac{d}{2} \frac{\zeta(\frac{d}{2}) \zeta(\frac{d-1}{2})}{\zeta(\frac{d-2}{2})} \frac{d-1}{2} \xi^{d-1} \\
&\quad - \left(\frac{d}{2} k \zeta_R \left(\frac{d+2}{2} \right) \xi^d + k \frac{\kappa b}{4} \frac{(d-1)}{2} \zeta_R \left(\frac{d+1}{2} \right) \xi^{d-1} \right. \\
&\quad \left. + \frac{d^2}{4} k \zeta_R \left(\frac{d+2}{2} \right) \xi^d + \frac{\kappa b}{4} \frac{(d-1)^2}{4} k \zeta_R \left(\frac{d+1}{2} \right) \xi^{d-1} \right) \\
&= -k \frac{d^2}{4} \frac{(\zeta(\frac{d}{2}))^2}{\zeta(\frac{d-2}{2})} \xi^d + k \frac{d^2}{4} \frac{\kappa b}{4} \frac{(\zeta(\frac{d}{2}))^2 \zeta(\frac{d-3}{2})}{(\zeta(\frac{d-2}{2}))^2} \xi^{d-1} - k \frac{d(d-1)}{2} \frac{\kappa b}{4} \frac{\zeta(\frac{d}{2}) \zeta(\frac{d-1}{2})}{\zeta(\frac{d-2}{2})} \xi^{d-1} \quad (3.112)
\end{aligned}$$

As we can see, $C_V^+ - C_V^- \neq 0$ in general for the sufficiently higher dimensions, even at the bulk level. Since the discontinuity contribution to the bulk term comes from $\frac{\partial \beta(\mu_c - \mu)}{\partial \beta}$, we know it should vanish for $d = 3, 4$ and 5 .

3.6.4. Discontinuity of the Derivative of the Heat Capacity Around T_C

In this section, the derivative of the heat capacity with respect to temperature again above and below the critical temperature will be calculated.

We will start with the below T_C derivative since the chemical potential is zero below the critical temperature, the derivative of C_V^- will be easy. The only contribution

will come from the ξ 's derivatives.

$$\begin{aligned}\frac{\partial C^-}{\partial T} &= (-k\beta^2)\frac{\partial C^-}{\partial \beta} \\ &= \left(\frac{d^2}{4} + \frac{d^3}{8}\right)k^2\beta\zeta\left(\frac{d+2}{2}\right)\xi^d + k^2\frac{\kappa b}{4}\beta\left(\frac{(d-1)^2}{4} + \frac{(d-1)^3}{8}\right)\zeta\left(\frac{d+1}{2}\right)\xi^{d-1}\end{aligned}\quad (3.113)$$

$$\begin{aligned}\frac{1}{Nk}\frac{\partial C^-}{\partial T} &= \left(\frac{d^2}{4} + \frac{d^3}{8}\right)k\beta\frac{\zeta\left(\frac{d+2}{2}\right)}{N_0(T) + \zeta\left(\frac{d}{2}\right)\xi^d + \frac{\kappa b}{4}\zeta\left(\frac{d-1}{2}\right)\xi^{d-1}}\xi^d \\ &\quad + \frac{\kappa b}{4}\left(\frac{(d-1)^2}{4} + \frac{(d-1)^3}{8}\right)k\beta\frac{\zeta\left(\frac{d+1}{2}\right)}{N_0(T) + \zeta\left(\frac{d}{2}\right)\xi^d + \frac{\kappa b}{4}\zeta\left(\frac{d-1}{2}\right)\xi^{d-1}}\xi^{d-1}\end{aligned}\quad (3.114)$$

Here, $N = N_0(T) + Li_{\frac{d}{2}}(e^{-\beta(\mu_c - \mu)})\xi^d + \frac{\kappa b}{4}Li_{\frac{d-1}{2}}(e^{-\beta(\mu_c - \mu)})\xi^{d-1}$; if we drop N_0 as $T \rightarrow T_C$ from below we get:

$$\begin{aligned}\lim_{\mu \rightarrow \mu_c} \frac{1}{Nk}\frac{\partial C^-}{\partial T} &= \left(\frac{d^2}{4} + \frac{d^3}{8}\right)k\beta\frac{\zeta\left(\frac{d+2}{2}\right)}{\zeta\left(\frac{d}{2}\right)}\left(1 - \frac{\kappa b}{4}\frac{\zeta_R\left(\frac{d-1}{2}\right)}{\zeta_R\left(\frac{d}{2}\right)}\xi^{-1}\right) \\ &\quad + \frac{\kappa b}{4}\left(\frac{(d-1)^2}{4} + \frac{(d-1)^3}{8}\right)k\beta\frac{\zeta\left(\frac{d+1}{2}\right)}{\zeta\left(\frac{d}{2}\right)}\xi^{-1} \\ &= \left(\frac{d^2}{4} + \frac{d^3}{8}\right)k\beta\frac{\zeta\left(\frac{d+2}{2}\right)}{\zeta\left(\frac{d}{2}\right)} - \left(\frac{d^2}{4} + \frac{d^3}{8}\right)k\beta\frac{\kappa b}{4}\zeta\left(\frac{d+2}{2}\right)\frac{\zeta\left(\frac{d-1}{2}\right)}{\left(\zeta\left(\frac{d}{2}\right)\right)^2}\xi^{-1} \\ &\quad + \frac{\kappa b}{4}\left(\frac{(d-1)^2}{4} + \frac{(d-1)^3}{8}\right)k\beta\frac{\zeta\left(\frac{d+1}{2}\right)}{\zeta\left(\frac{d}{2}\right)}\xi^{-1}\end{aligned}\quad (3.115)$$

Again, if we take only the volume terms and insert $d = 3$ to check the consistency,

$$\frac{\partial C^-}{\partial T} = k^2\frac{V}{\lambda^3}\beta\zeta_R\left(\frac{5}{2}\right)\left(\frac{9}{4} + \frac{27}{8}\right) = \frac{45}{8}\frac{V}{\lambda^3}\frac{k}{T}\zeta_R\left(\frac{5}{2}\right)\quad (3.116)$$

our expression looks the same as written by Pathria[7].

Secondly, since the $\frac{\partial}{\partial \beta}[\beta(\mu_c - \mu)] \neq 0$, the derivative of C_V^+ will be a bit more complicated. Also, we should be careful with expanding this derivative whether we can or not depending on $\frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}}$ finite or not. Here, we used the expanded version of $\frac{\partial}{\partial \beta}[\beta(\mu_c - \mu)]$, in other words, we make our calculations for sufficiently higher dimen-

sions.

$$\begin{aligned}
\frac{\partial C_V^+}{\partial \beta} = & \frac{d^2}{4} k \frac{(Li_{\frac{d}{2}})^2}{Li_{\frac{d-2}{2}}} \beta^{-1} \xi^d - \frac{d^2}{4} k \frac{(Li_{\frac{d}{2}})^2}{Li_{\frac{d-2}{2}}} \beta^{-1} \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{d-1} \\
& + \frac{d}{2} k \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \beta^{-1} \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \frac{d-1}{2} \xi^{d-1} - \frac{d^2}{4} k Li_{\frac{d+2}{2}} \beta^{-1} \xi^d \\
& + \frac{\kappa b d d-1}{4 \cdot 2 \cdot 2} k Li_{\frac{d-1}{2}} \beta^{-1} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \xi^{d-1} - \frac{\kappa b (d-1)^2}{4 \cdot 4} k Li_{\frac{d+1}{2}} \beta^{-1} \xi^{d-1} \\
& + \left(-k \frac{d^3}{8} \frac{2(Li_{\frac{d}{2}})^2 \beta^{-1}}{Li_{\frac{d-2}{2}}} \xi^d \left[1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \frac{d-1}{d} \xi^{-1} \right] \right. \\
& + k \frac{d^3}{8} Li_{\frac{d-4}{2}} \beta^{-1} \frac{(Li_{\frac{d}{2}})^3}{(Li_{\frac{d-2}{2}})^3} \xi^d \left[1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \frac{d-1}{d} \xi^{-1} \right] \\
& + k \frac{d^3}{8} \beta^{-1} \frac{(Li_{\frac{d}{2}})^2}{Li_{\frac{d-2}{2}}} \xi^d \left. \left[1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \frac{d-1}{d} \xi^{-1} \right] \right. \\
& - k \frac{d^2}{4} \frac{(Li_{\frac{d}{2}})^2}{Li_{\frac{d-2}{2}}} \xi^d \left[-\frac{\kappa b d}{4 \cdot 2} Li_{\frac{d-5}{2}} \beta^{-1} \frac{Li_{\frac{d}{2}}}{(Li_{\frac{d-2}{2}})^2} \xi^{-1} + \frac{\kappa b d}{4 \cdot 2} Li_{\frac{d-3}{2}} \beta^{-1} Li_{\frac{d-4}{2}} \frac{Li_{\frac{d}{2}}}{(Li_{\frac{d-2}{2}})^3} \xi^{-1} \right. \\
& + \left. \frac{\kappa b d-1}{4 \cdot 2} \beta^{-1} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} - \frac{\kappa b d-1}{4 \cdot 2} \beta^{-1} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \right] \\
& - k \frac{\kappa b d-1}{4 \cdot 2} Li_{\frac{d-3}{2}} \frac{d^2}{4} \beta^{-1} \frac{(Li_{\frac{d}{2}})^2}{(Li_{\frac{d-2}{2}})^2} \xi^{d-1} - k \frac{\kappa b d-1}{4 \cdot 2} Li_{\frac{d-1}{2}} \frac{d^2}{4} \beta^{-1} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \xi^{d-1} \\
& + k \frac{\kappa b d-1}{4 \cdot 2} Li_{\frac{d-1}{2}} \frac{d^2}{4} \beta^{-1} Li_{\frac{d-4}{2}} \frac{(Li_{\frac{d}{2}})^2}{(Li_{\frac{d-2}{2}})^3} \xi^{d-1} + k \frac{\kappa b (d-1)^2}{4 \cdot 4} Li_{\frac{d-1}{2}} \frac{d}{2} \beta^{-1} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \xi^{d-1} \\
& + \frac{d^3}{8} k \frac{(Li_{\frac{d}{2}})^2}{Li_{\frac{d-2}{2}}} \xi^d \left[1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \frac{d-1}{d} \xi^{-1} \right] - \frac{d^3}{8} k Li_{\frac{d+2}{2}} \beta^{-1} \xi^d \\
& + \frac{\kappa b}{4} k \frac{(d-1)^2}{4} Li_{\frac{d-1}{2}} \frac{d}{2} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \beta^{-1} \xi^{d-1} - \frac{\kappa b (d-1)^3}{4 \cdot 8} Li_{\frac{d+1}{2}} \beta^{-1} \xi^{d-1} \quad (3.117)
\end{aligned}$$

If we write it more clearly dropping the terms of the order of κ^2 ; multiplying by $-k\beta^2$ and divide it with Nk properly, some terms cancel each other. After the simplifications

we get

$$\begin{aligned}
\frac{1}{Nk} \frac{\partial C_V^+}{\partial T} &= \left[-\frac{1}{k Li_{\frac{d}{2}} \xi^d} \left(1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \right) \right] \frac{\partial C_V^+}{\partial T} \\
&= -\frac{d^2}{4} k \beta \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} + \frac{d}{4} k \beta \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + \left(\frac{d^2}{4} + \frac{d^3}{8} \right) k \beta \frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} \\
&\quad + k \frac{\kappa b}{4} \left(\frac{(d-1)^2}{4} + \frac{(d-1)^3}{8} \right) \beta \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \\
&\quad - k \frac{d^3}{8} Li_{\frac{d-4}{2}} \beta \frac{(Li_{\frac{d}{2}})^2}{(Li_{\frac{d-2}{2}})^3} + k 3 \frac{d^3}{8} \frac{\kappa b}{4} \beta Li_{\frac{d-4}{2}} Li_{\frac{d-3}{2}} \frac{(Li_{\frac{d}{2}})^2}{(Li_{\frac{d-2}{2}})^4} \xi^{-1} \\
&\quad - k \frac{d^2}{2} (d-1) \frac{\kappa b}{4} \beta Li_{\frac{d-4}{2}} Li_{\frac{d-1}{2}} \frac{Li_{\frac{d}{2}}}{(Li_{\frac{d-2}{2}})^3} \xi^{-1} - k \frac{d^3}{8} \frac{\kappa b}{4} \beta Li_{\frac{d-5}{2}} \frac{(Li_{\frac{d}{2}})^2}{(Li_{\frac{d-2}{2}})^3} \xi^{-1} \\
&\quad - k \frac{\kappa b}{4} \left(\frac{d^2}{4} + \frac{d^3}{8} \right) \beta Li_{\frac{d+2}{2}} \frac{Li_{\frac{d-1}{2}}}{(Li_{\frac{d}{2}})^2} \xi^{-1} + k \frac{\kappa b}{4} \frac{d^3}{8} \beta Li_{\frac{d}{2}} \frac{Li_{\frac{d-1}{2}}}{(Li_{\frac{d-2}{2}})^3} \xi^{-1} \quad (3.118)
\end{aligned}$$

As we want to look at the discontinuity in the derivative of C_V around T_C , we will take the limit $\mu \rightarrow \mu_c$. In this limit, all polylogarithmic functions go to zeta functions: $Li_d \rightarrow \zeta(d)$.

$$\begin{aligned}
\lim_{\mu \rightarrow \mu_c} \frac{1}{Nk} \frac{\partial C_V^+}{\partial T} &= -\frac{d^2}{4} k \beta \frac{\zeta(\frac{d}{2})}{\zeta(\frac{d-2}{2})} + \frac{d}{4} k \beta \frac{\kappa b}{4} \frac{\zeta(\frac{d-1}{2})}{\zeta(\frac{d-2}{2})} \xi^{-1} + \left(\frac{d^2}{4} + \frac{d^3}{8} \right) k \beta \frac{\zeta(\frac{d+2}{2})}{\zeta(\frac{d}{2})} \\
&\quad + k \frac{\kappa b}{4} \left(\frac{(d-1)^2}{4} + \frac{(d-1)^3}{8} \right) \beta \frac{\zeta(\frac{d+1}{2})}{\zeta(\frac{d}{2})} \xi^{-1} - k \frac{d^3}{8} \zeta\left(\frac{d-4}{2}\right) \beta \frac{(\zeta(\frac{d}{2}))^2}{(\zeta(\frac{d-2}{2}))^3} \\
&\quad + k 3 \frac{d^3}{8} \frac{\kappa b}{4} \beta \zeta\left(\frac{d-4}{2}\right) \zeta\left(\frac{d-3}{2}\right) \frac{(\zeta(\frac{d}{2}))^2}{(\zeta(\frac{d-2}{2}))^4} \xi^{-1} \\
&\quad - k \frac{d^2}{2} (d-1) \frac{\kappa b}{4} \beta \zeta\left(\frac{d-4}{2}\right) \zeta\left(\frac{d-1}{2}\right) \frac{\zeta(\frac{d}{2})}{(\zeta(\frac{d-2}{2}))^3} \xi^{-1} \\
&\quad - k \frac{d^3}{8} \frac{\kappa b}{4} \beta \zeta\left(\frac{d-5}{2}\right) \frac{(\zeta(\frac{d}{2}))^2}{(\zeta(\frac{d-2}{2}))^3} \xi^{-1} - k \frac{\kappa b}{4} \left(\frac{d^2}{4} + \frac{d^3}{8} \right) \beta \zeta\left(\frac{d+2}{2}\right) \frac{\zeta(\frac{d-1}{2})}{(\zeta(\frac{d}{2}))^2} \xi^{-1} \\
&\quad + k \frac{\kappa b}{4} \frac{d^3}{8} \beta \zeta\left(\frac{d}{2}\right) \frac{\zeta(\frac{d-1}{2})}{(\zeta(\frac{d-2}{2}))^3} \xi^{-1} \quad (3.119)
\end{aligned}$$

Again, to compare our result with the expression given in Patrha's book (Problems 7.6), we drop the terms coming from the boundary:

$$\lim_{\mu \rightarrow \mu_c} \frac{1}{Nk} \frac{\partial C_V^+}{\partial T} = k\beta \left(-\frac{d^2}{4} \frac{\zeta(\frac{d}{2})}{\zeta(\frac{d-2}{2})} + \left(\frac{d^2}{4} + \frac{d^3}{8}\right) \frac{\zeta(\frac{d+2}{2})}{\zeta(\frac{d}{2})} - \frac{d^3}{8} \frac{\zeta(\frac{d-4}{2}) (\zeta(\frac{d}{2}))^2}{(\zeta(\frac{d-2}{2}))^3} \right) \quad (3.120)$$

and we put $d = 3$. The equation becomes

$$\frac{1}{Nk} \frac{\partial C^+}{\partial T} = \frac{1}{T} \left[-\frac{9}{4} \frac{\zeta(\frac{3}{2})}{\zeta(\frac{1}{2})} - \frac{27}{8} \zeta\left(\frac{-1}{2}\right) \frac{(\zeta(\frac{3}{2}))^2}{(\zeta(\frac{1}{2}))^3} + \frac{45}{8} \frac{\zeta(\frac{5}{2})}{\zeta(\frac{3}{2})} \right] \quad (3.121)$$

which is consistent.

Now, we subtract $\frac{1}{Nk} \frac{\partial C^-}{\partial T}$ from $\frac{1}{Nk} \frac{\partial C^+}{\partial T}$ and we get the explicit expression with the boundary contributions for the discontinuity of the derivative of the heat capacity around critical temperature as:

$$\begin{aligned} \frac{1}{Nk} \left[\frac{\partial C^+}{\partial T} - \frac{\partial C^-}{\partial T} \right] &= -\frac{d^2}{4} k\beta \frac{\zeta(\frac{d}{2})}{\zeta(\frac{d-2}{2})} + \frac{d}{4} k\beta \frac{\kappa b}{4} \frac{\zeta(\frac{d-1}{2})}{\zeta(\frac{d-2}{2})} \xi^{-1} - k \frac{d^3}{8} \zeta\left(\frac{d-4}{2}\right) \beta \frac{(\zeta(\frac{d}{2}))^2}{(\zeta(\frac{d-2}{2}))^3} \\ &+ 3k \frac{d^3}{8} \frac{\kappa b}{4} \beta \zeta\left(\frac{d-4}{2}\right) \zeta\left(\frac{d-3}{2}\right) \frac{(\zeta(\frac{d}{2}))^2}{(\zeta(\frac{d-2}{2}))^4} \xi^{-1} - k \frac{d^2}{2} (d-1) \frac{\kappa b}{4} \beta \zeta\left(\frac{d-4}{2}\right) \zeta\left(\frac{d-1}{2}\right) \frac{\zeta(\frac{d}{2})}{(\zeta(\frac{d-2}{2}))^3} \xi^{-1} \\ &- k \frac{d^3}{8} \frac{\kappa b}{4} \beta \zeta\left(\frac{d-5}{2}\right) \frac{(\zeta(\frac{d}{2}))^2}{(\zeta(\frac{d-2}{2}))^3} \xi^{-1} + k \frac{\kappa b}{4} \frac{d^3}{8} \beta \zeta\left(\frac{d}{2}\right) \frac{\zeta(\frac{d-1}{2})}{(\zeta(\frac{d-2}{2}))^3} \xi^{-1} \end{aligned} \quad (3.122)$$

3.7. Calculation of Compressibility Factor κ_T

Another thermodynamical factor that we would like to see under the boundary effect is compressibility. Isothermal compressibility factor is known as

$$\kappa_T = -\frac{1}{V} \frac{\partial V}{\partial P} \Big|_T = -\frac{1}{V} \left(-\frac{\frac{\partial V}{\partial T} \Big|_P}{\frac{\partial P}{\partial T} \Big|_V} \right) \quad (3.123)$$

Therefore, we need to calculate $\frac{\partial V}{\partial \beta}$ and $\frac{\partial P}{\partial \beta}$ first.

Starting with volume derivative, we will use an equation system of two equa-

tions that we will obtain from the derivatives of N and PV with respect to β . There will be no change in the derivative of the Li functions, however the derivative of the ξ functions will be changed since volume is not a constant from now on and its derivative needs to be taken with respect to temperature also. The ξ parameter can be written explicitly as below.

$$\xi^d = \frac{V}{\lambda_T^d} = V\alpha^d\beta^{-\frac{d}{2}} \quad (3.124)$$

$$\xi^{d-1} = \frac{V^{\frac{d-1}{d}}}{\lambda_T^{d-1}} = V^{\frac{d-1}{d}}\alpha^{d-1}\beta^{-\frac{d-1}{2}} \quad (3.125)$$

Here, we define $\alpha^d = (\frac{\sqrt{2\pi m}}{h})^d$ where h is the Planck constant. The ξ derivative is stated below to be used repeatedly later on :

$$\frac{\partial \xi^d}{\partial \beta} \Big|_P = -\frac{d}{2}\beta^{-\frac{d}{2}-1}V\alpha^d + \alpha^d\beta^{-\frac{d}{2}}\frac{\partial V}{\partial \beta} \Big|_P \quad (3.126)$$

$$\frac{\partial \xi^{d-1}}{\partial \beta} \Big|_P = -\frac{d-1}{2}\beta^{-\frac{d-1}{2}-1}V^{\frac{d-1}{d}}\alpha^{d-1} + \alpha^{d-1}\beta^{-\frac{d-1}{2}}\left(\frac{d-1}{d}\right)V^{-\frac{1}{d}}\frac{\partial V}{\partial \beta} \Big|_P \quad (3.127)$$

Now, we can start generating our equation system. Again, we will start with the fact that N is fixed:

$$\frac{\partial N}{\partial \beta} = 0 \quad ; \quad N = Li_{\frac{d}{2}}\xi^d + \frac{\kappa b}{4}Li_{\frac{d-1}{2}}\xi^{d-1} \quad (3.128)$$

$$\begin{aligned} 0 = & Li_{\frac{d-2}{2}}\frac{\partial(\mu/\beta)}{\partial \beta}\xi^d - Li_{\frac{d}{2}}\frac{d}{2}\beta^{-\frac{d}{2}-1}V\alpha^d + Li_{\frac{d}{2}}\alpha^d\beta^{-\frac{d}{2}}\frac{\partial V}{\partial \beta} + \frac{\kappa b}{4}Li_{\frac{d-3}{2}}\frac{\partial(\mu/\beta)}{\partial \beta}\xi^{d-1} \\ & - \frac{\kappa b}{4}Li_{\frac{d-1}{2}}V^{\frac{d-1}{d}}\alpha^{d-1}\frac{d-1}{2}\beta^{-\frac{d-1}{2}-1} + \frac{\kappa b}{4}Li_{\frac{d-1}{2}}V^{-\frac{1}{d}}\alpha^{d-1}\frac{d-1}{d}\beta^{-\frac{d-1}{2}}\frac{\partial V}{\partial \beta} \Big|_P \end{aligned} \quad (3.129)$$

Collecting the terms with $\frac{\partial V}{\partial \beta}$ at one side and $\frac{\partial(\mu\beta)}{\partial \beta}$ another, we get our first equation as:

$$\begin{aligned} & \left(-Li_{\frac{d}{2}}\alpha^d\beta^{-\frac{d}{2}} - \frac{\kappa b}{4}Li_{\frac{d-1}{2}}\alpha^{d-1}\beta^{-\frac{d-1}{2}}\frac{d-1}{d}V^{-\frac{1}{d}} \right) \frac{\partial V}{\partial \beta} \\ & + Li_{\frac{d}{2}}\frac{d}{2}\beta^{-1}\xi^d + \frac{\kappa b}{4}Li_{\frac{d-1}{2}}\frac{d-1}{2}\beta^{-1}\xi^{d-1} \\ & = \frac{\partial(\mu\beta)}{\partial \beta} \left(Li_{\frac{d-2}{2}}\xi^d + \frac{\kappa b}{4}Li_{\frac{d-3}{2}}\xi^{d-1} \right) \end{aligned} \quad (3.130)$$

Secondly, keeping the pressure constant, we will take the derivative of the equation of state with respect to temperature:

$$PV = \beta^{-1}q \quad , \quad \text{where } q = Li_{\frac{d+2}{2}}\xi^d + \frac{\kappa b}{4}Li_{\frac{d+1}{2}}\xi^{d-1} \quad (3.131)$$

$$\frac{\partial}{\partial \beta}[PV]|_P = \frac{\partial}{\partial \beta}[\beta^{-1}q]|_P \quad (3.132)$$

Only one term comes from the left hand side of the equation since the derivative of the pressure will be zero.

$$\begin{aligned} P \frac{\partial V}{\partial \beta} \Big|_P &= -\beta^{-2}q + \beta^{-1} \frac{\partial q}{\partial \beta} \\ &= -\beta^{-2}Li_{\frac{d+2}{2}}\xi^d - \beta^{-2}\frac{\kappa b}{4}Li_{\frac{d+1}{2}}\xi^{d-1} + \beta^{-1}Li_{\frac{d}{2}}\frac{\partial(\mu\beta)}{\partial \beta}\xi^d + \beta^{-1}Li_{\frac{d+2}{2}}\frac{\partial \xi^d}{\partial \beta} \\ & \quad + \beta^{-1}\frac{\kappa b}{4}Li_{\frac{d-1}{2}}\frac{\partial(\mu\beta)}{\partial \beta}\xi^{d-1} + \beta^{-1}\frac{\kappa b}{4}Li_{\frac{d+1}{2}}\frac{\partial \xi^{d-1}}{\partial \beta} \\ &= -\beta^{-2}Li_{\frac{d+2}{2}}\xi^d - \beta^{-2}\frac{\kappa b}{4}Li_{\frac{d+1}{2}}\xi^{d-1} + \beta^{-1}Li_{\frac{d}{2}}\frac{\partial(\mu\beta)}{\partial \beta}\xi^d + \beta^{-1}Li_{\frac{d+2}{2}}\left(-\frac{d}{2}\right)\beta^{-1}\xi^d + \\ & \quad + \beta^{-1}Li_{\frac{d+2}{2}}\alpha^d\beta^{-\frac{d}{2}}\frac{\partial V}{\partial \beta} + \beta^{-1}\frac{\kappa b}{4}Li_{\frac{d-1}{2}}\frac{\partial(\mu\beta)}{\partial \beta}\xi^{d-1} - \beta^{-1}\frac{\kappa b}{4}Li_{\frac{d+1}{2}}\frac{d-1}{2}\beta^{-1}\xi^{d-1} \\ & \quad + \beta^{-1}\frac{\kappa b}{4}Li_{\frac{d+1}{2}}\alpha^{d-1}\beta^{-\frac{d-1}{2}}\left(\frac{d-1}{d}\right)V^{-\frac{1}{d}}\frac{\partial V}{\partial \beta} \end{aligned} \quad (3.133)$$

Substituting $P = \frac{\beta^{-1}q}{V} = \beta^{-1}Li_{\frac{d+2}{2}}\alpha^d\beta^{-\frac{d}{2}} + \beta^{-1}\frac{\kappa b}{4}Li_{\frac{d+1}{2}}V^{-\frac{1}{d}}\alpha^{d-1}\beta^{-\frac{d-1}{2}}$ back in the left hand side and taking the expression in $\frac{\partial(\mu\beta)}{\partial \beta}$ and $\frac{\partial V}{\partial \beta}$ parenthesis, we get the second

equation:

$$\begin{aligned} & \left(\frac{1}{d} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}-1} \right) \frac{\partial V}{\partial \beta} + \frac{d+2}{2} \beta^{-2} Li_{\frac{d+2}{2}} \xi^d + \frac{d+1}{2} \beta^{-2} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1} \\ &= \frac{\partial(\mu\beta)}{\partial \beta} \left(\beta^{-1} Li_{\frac{d}{2}} \xi^d + \beta^{-1} \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{d-1} \right) \end{aligned} \quad (3.134)$$

At this moment, basically we have two different equations and two unknowns. Thus, we can solve this system of equations for $\frac{\partial V}{\partial \beta}$. If we take out the $\frac{\partial(\mu\beta)}{\partial \beta}$ terms in both equations and equate the rest, we get

$$\begin{aligned} & \frac{\partial V}{\partial \beta} \frac{[\frac{1}{d} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}-1}]}{\beta^{-1} Li_{\frac{d}{2}} \xi^d + \beta^{-1} \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{d-1}} + \frac{\frac{d+2}{2} \beta^{-2} Li_{\frac{d+2}{2}} \xi^d + \frac{d+1}{2} \beta^{-2} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1}}{\beta^{-1} Li_{\frac{d}{2}} \xi^d + \beta^{-1} \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{d-1}} \\ &= \frac{\partial V}{\partial \beta} \frac{[-Li_{\frac{d}{2}} \alpha^d \beta^{-\frac{d}{2}} - \frac{\kappa b}{4} Li_{\frac{d-1}{2}} (\frac{d-1}{d}) V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}}]}{Li_{\frac{d-2}{2}} \xi^d + \frac{\kappa b}{4} Li_{\frac{d-3}{2}} \xi^{d-1}} \\ &+ \frac{Li_{\frac{d}{2}} (\frac{d}{2}) \beta^{-1} \xi^d + \frac{\kappa b}{4} Li_{\frac{d-1}{2}} (\frac{d-1}{2}) \beta^{-1} \xi^{d-1}}{Li_{\frac{d-2}{2}} \xi^d + \frac{\kappa b}{4} Li_{\frac{d-3}{2}} \xi^{d-1}} \end{aligned} \quad (3.135)$$

Collecting the $\frac{\partial V}{\partial \beta}$ terms on one side:

$$\begin{aligned} & \frac{\partial V}{\partial \beta} \left[\frac{\frac{1}{d} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}-1}}{\beta^{-1} Li_{\frac{d}{2}} \xi^d + \beta^{-1} \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{d-1}} + \frac{Li_{\frac{d}{2}} \alpha^d \beta^{-\frac{d}{2}} + \frac{\kappa b}{4} Li_{\frac{d-1}{2}} (\frac{d-1}{d}) V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}}}{Li_{\frac{d-2}{2}} \xi^d + \frac{\kappa b}{4} Li_{\frac{d-3}{2}} \xi^{d-1}} \right] \\ &= \frac{Li_{\frac{d}{2}} (\frac{d}{2}) \beta^{-1} \xi^d + \frac{\kappa b}{4} Li_{\frac{d-1}{2}} (\frac{d-1}{2}) \beta^{-1} \xi^{d-1}}{Li_{\frac{d-2}{2}} \xi^d + \frac{\kappa b}{4} Li_{\frac{d-3}{2}} \xi^{d-1}} - \frac{\frac{d+2}{2} \beta^{-2} Li_{\frac{d+2}{2}} \xi^d + \frac{d+1}{2} \beta^{-2} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1}}{\beta^{-1} Li_{\frac{d}{2}} \xi^d + \beta^{-1} \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{d-1}} \\ &= \frac{Li_{\frac{d}{2}} (\frac{d}{2}) \beta^{-1} \xi^d}{Li_{\frac{d-2}{2}} \xi^d} \left[\frac{1 + \frac{\frac{\kappa b}{4} Li_{\frac{d-1}{2}} (\frac{d-1}{2}) \beta^{-1} \xi^{d-1}}{Li_{\frac{d}{2}} (\frac{d}{2}) \beta^{-1} \xi^d}}{1 + \frac{\frac{\kappa b}{4} Li_{\frac{d-3}{2}} \xi^{d-1}}{Li_{\frac{d-2}{2}} \xi^d}} \right] - \frac{\beta^{-2} Li_{\frac{d+2}{2}} (\frac{d+2}{2}) \xi^d}{\beta^{-1} Li_{\frac{d}{2}} \xi^d} \left[\frac{1 + \frac{\frac{d+1}{2} \beta^{-2} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1}}{\frac{d+2}{2} \beta^{-2} Li_{\frac{d+2}{2}} \xi^d}}{1 + \frac{\beta^{-1} \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{d-1}}{\beta^{-1} Li_{\frac{d}{2}} \xi^d}} \right] \\ &= \frac{Li_{\frac{d}{2}} (\frac{d}{2}) \beta^{-1}}{Li_{\frac{d-2}{2}}} \left[\frac{1 + \frac{\frac{d-1}{d} \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} \xi^{-1}}{Li_{\frac{d}{2}}}}{1 + \frac{\frac{\kappa b}{4} Li_{\frac{d-3}{2}} \xi^{-1}}{Li_{\frac{d-2}{2}}}} \right] - \frac{\beta^{-1} Li_{\frac{d+2}{2}} (\frac{d+2}{2})}{Li_{\frac{d}{2}}} \left[\frac{1 + \frac{\frac{d+1}{d+2} \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} \xi^{-1}}{Li_{\frac{d+2}{2}}}}{1 + \frac{\frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{-1}}{Li_{\frac{d}{2}}}} \right] \end{aligned} \quad (3.136)$$

Leaving the $\frac{\partial V}{\partial \beta}$ term alone on one side and continuing with the implication of the expansion method that we used earlier:

$$\begin{aligned}
\frac{\partial V}{\partial \beta} &= \left(\frac{Li_{\frac{d}{2}}(\frac{d}{2})\beta^{-1}}{Li_{\frac{d-2}{2}}} \left[\frac{1 + \frac{d-1}{d} \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}\xi^{-1}}{Li_{\frac{d}{2}}} \right] - \frac{\beta^{-1} Li_{\frac{d+2}{2}}(\frac{d+2})}{Li_{\frac{d}{2}}} \left[\frac{1 + \frac{d+1}{d+2} \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}}\xi^{-1}}{Li_{\frac{d+2}{2}}} \right] \right) \\
&\quad \left[\frac{\frac{1}{d} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}-1}}{\beta^{-1} Li_{\frac{d}{2}} \xi^d + \beta^{-1} \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \xi^{d-1}} + \frac{Li_{\frac{d}{2}} \alpha^d \beta^{-\frac{d}{2}} + \frac{\kappa b}{4} Li_{\frac{d-1}{2}}(\frac{d-1}) V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}}}{Li_{\frac{d-2}{2}} \xi^d + \frac{\kappa b}{4} Li_{\frac{d-3}{2}} \xi^{d-1}} \right]^{-1} \\
&= \left(\frac{Li_{\frac{d}{2}}(\frac{d}{2})\beta^{-1}}{Li_{\frac{d-2}{2}}} \left[1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}\xi^{-1}}{Li_{\frac{d-2}{2}}} + \frac{d-1}{d} \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}\xi^{-1}}{Li_{\frac{d}{2}}} \right] \right. \\
&\quad \left. - \frac{\beta^{-1} Li_{\frac{d+2}{2}}(\frac{d+2})}{Li_{\frac{d}{2}}} \left[1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}\xi^{-1}}{Li_{\frac{d}{2}}} + \frac{d+1}{d+2} \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}}\xi^{-1}}{Li_{\frac{d+2}{2}}} \right] \right) \\
&\quad \cdot \left[\frac{\frac{1}{d} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{-1}}{Li_{\frac{d}{2}} V} + \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}} V} \frac{1 + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}(\frac{d-1})\xi^{-1}}{Li_{\frac{d}{2}}} \right]^{-1} \tag{3.137}
\end{aligned}$$

We obtained an explicit expression for $\frac{\partial V}{\partial \beta}$. Now, since we need an extra $\frac{1}{V}$ factor to find κ_T , we will take the denominator in V parenthesis. Also, since we are not close to the critical temperature, the Li functions are well-behaved and we can use the $\frac{1}{1+\epsilon} \simeq 1 - \epsilon$ expansion without any concern about the dimension.

$$\begin{aligned}
\frac{1}{V} \frac{\partial V}{\partial \beta} &= \left[\frac{d}{2} \beta^{-1} - \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2} \beta^{-1} \right] \left[1 - \left(\frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} Li_{\frac{d}{2}} \xi^{-1}}{[Li_{\frac{d-2}{2}}]^2} \frac{d}{2} \beta^{-1} \right. \right. \\
&\quad \left. \left. + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} \xi^{-1}}{Li_{\frac{d-2}{2}}} \frac{d-1}{2} \beta^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} Li_{\frac{d+2}{2}} \xi^{-1}}{[Li_{\frac{d}{2}}]^2} \frac{d+2}{2} \beta^{-1} \right. \right. \\
&\quad \left. \left. - \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} \xi^{-1}}{Li_{\frac{d}{2}}} \frac{d+1}{2} \beta^{-1} \right) \left(\frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \frac{d}{2} \beta^{-1} - \frac{d+2}{2} \frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} \beta^{-1} \right)^{-1} \right] \\
&\quad \cdot \left(1 + \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} \xi^{-1}}{Li_{\frac{d-2}{2}}} - \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} \xi^{-1}}{Li_{\frac{d}{2}}} \frac{d-1}{d} - \frac{\kappa b}{4} \frac{1}{d} \frac{Li_{\frac{d+1}{2}}}{(Li_{\frac{d}{2}})^2} Li_{\frac{d-2}{2}} \xi^{-1} \right) \tag{3.138}
\end{aligned}$$

We make some simplifications to drop the terms of the order of κ^2 and we get:

$$\begin{aligned}
\frac{1}{V} \frac{\partial V}{\partial \beta} = & \left[\frac{d}{2} \beta^{-1} - \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2} \beta^{-1} \right] \left[1 - \left(\frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} Li_{\frac{d}{2}}}{[Li_{\frac{d-2}{2}}]^2} \xi^{-1} \frac{d}{2} \beta^{-1} \right. \right. \\
& + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} \frac{d-1}{2} \beta^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} Li_{\frac{d+2}{2}}}{[Li_{\frac{d}{2}}]^2} \xi^{-1} \frac{d+2}{2} \beta^{-1} \\
& \left. \left. - \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \frac{d+1}{2} \beta^{-1} \right) \left(\frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \frac{d}{2} \beta^{-1} - \frac{d+2}{2} \frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} \beta^{-1} \right)^{-1} \right. \\
& \left. + \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} - \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \frac{d-1}{d} - \frac{\kappa b}{4} \frac{1}{d} \frac{Li_{\frac{d+1}{2}}}{(Li_{\frac{d}{2}})^2} Li_{\frac{d-2}{2}} \xi^{-1} \right] \quad (3.139)
\end{aligned}$$

At this moment, we reached a check point. The formula of the thermal expansion coefficient is $\alpha_T = \frac{1}{V} \frac{\partial V}{\partial \beta}$. So, we will check if we have found α_T correctly or not by taking only the leading terms of $\frac{1}{V} \frac{\partial V}{\partial \beta}$ and take $d = 3$.

$$\alpha_T = \frac{1}{V} \frac{\partial V}{\partial \beta} = \frac{3}{2} \beta^{-1} - \frac{5}{2} \beta^{-1} \frac{Li_{\frac{5}{2}} Li_{\frac{1}{2}}}{[Li_{\frac{3}{2}}]^2} \quad (3.140)$$

As it can be seen clearly, when β is small, $exp(\mu\beta) \approx 1 + \mu\beta$, in other words at the high temperature region, the thermal expansion coefficient goes to $-\frac{1}{\beta}$ which is correct.

Now, returning back to the $\frac{1}{V} \frac{\partial V}{\partial T}$ calculation; we multiply $\frac{1}{V} \frac{\partial V}{\partial \beta}$ by $-k\beta^2$ and have the first expression that we need to obtain κ_T :

$$\begin{aligned}
\frac{1}{V} \frac{\partial V}{\partial T} \Big|_P = & \frac{1}{V} \frac{\partial V}{\partial \beta} (-k\beta^2) \\
= & -k \left[\frac{d}{2} \beta - \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2} \beta \right] \left[1 - \left(\frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} Li_{\frac{d}{2}}}{[Li_{\frac{d-2}{2}}]^2} \xi^{-1} \frac{d}{2} \beta^{-1} \right. \right. \\
& + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} \frac{d-1}{2} \beta^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} Li_{\frac{d+2}{2}}}{[Li_{\frac{d}{2}}]^2} \xi^{-1} \frac{d+2}{2} \beta^{-1} \\
& \left. \left. - \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \frac{d+1}{2} \beta^{-1} \right) \left(\frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \frac{d}{2} \beta^{-1} - \frac{d+2}{2} \frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} \beta^{-1} \right)^{-1} \right. \\
& \left. + \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} - \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \frac{d-1}{d} - \frac{\kappa b}{4} \frac{1}{d} \frac{Li_{\frac{d+1}{2}}}{(Li_{\frac{d}{2}})^2} Li_{\frac{d-2}{2}} \xi^{-1} \right] \quad (3.141)
\end{aligned}$$

Another derivative we need to calculate to obtain κ_T is $\frac{\partial P}{\partial T}|_V$:

$$\begin{aligned}
\frac{\partial P}{\partial T}|_V &= \frac{\partial P}{\partial \beta}|_V(-k\beta^2) \\
&= \frac{\partial}{\partial \beta} \left(Li_{\frac{d+2}{2}} \alpha^d \beta^{-\frac{d}{2}-1} + \frac{\kappa b}{4} Li_{\frac{d+1}{2}} V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}-1} \right) (-k\beta^2) \\
&= -k Li_{\frac{d}{2}} \frac{\partial(\mu\beta)}{\partial \beta}|_V \alpha^d \beta^{-\frac{d}{2}+1} - k Li_{\frac{d+2}{2}} \alpha^d \left(-\frac{d}{2} - 1 \right) \beta^{-\frac{d}{2}} \\
&\quad - k \frac{\kappa b}{4} Li_{\frac{d-1}{2}} \frac{\partial(\mu\beta)}{\partial \beta}|_V V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}+1} \\
&\quad + k \frac{\kappa b}{4} Li_{\frac{d+1}{2}} V^{-\frac{1}{d}} \alpha^{d-1} \frac{d+1}{2} \beta^{-\frac{d-1}{2}}
\end{aligned} \tag{3.142}$$

For simplicity, we took $\mu_c = 0$ ($E_0 = 0$). Again, we are not concerned about the behaviour of the Li functions. We can use the expanded expression that we had found for $\frac{\partial \beta(\mu_c - \mu)}{\partial \beta}$. We will drop μ_c and write it simpler as:

$$\frac{\partial(\mu\beta)}{\partial \beta}|_V = \left[\frac{\frac{d}{2} \beta^{-1} Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \right] \left[1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \frac{d-1}{d} \xi^{-1} \right] \tag{3.143}$$

After inserting this expression in the pressure derivative above and some simplifications, we get the second necessary equation as:

$$\begin{aligned}
\frac{\partial P}{\partial T}|_V &= -k \frac{d (Li_{\frac{d}{2}})^2}{2 Li_{\frac{d-2}{2}}} \left[1 - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \frac{d-1}{d} \xi^{-1} \right] \alpha^d \beta^{-\frac{d}{2}} \\
&\quad + k Li_{\frac{d+2}{2}} \alpha^d \frac{d+2}{2} \beta^{-\frac{d}{2}} - k \frac{\kappa b}{4} \frac{d}{2} Li_{\frac{d-1}{2}} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + k \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \frac{d+1}{2} \xi^{-1}
\end{aligned} \tag{3.144}$$

Combining the $\frac{1}{V}\frac{\partial V}{\partial T}|_P$ and $\frac{\partial P}{\partial T}|_V$ expressions that we obtained, we can write the isothermal compressibility factor:

$$\begin{aligned}
\kappa_T &= -\frac{1}{V}\left(-\frac{\partial V}{\partial T}\Big|_P\right) \tag{3.145} \\
&= -k\left[\frac{d}{2}\beta - \frac{Li_{\frac{d+2}{2}}Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2}\frac{d+2}{2}\beta\right]\left[1 - \left(\frac{\kappa b}{4}\frac{Li_{\frac{d-3}{2}}Li_{\frac{d}{2}}}{[Li_{\frac{d-2}{2}}]^2}\xi^{-1}\frac{d}{2}\beta^{-1}\right.\right. \\
&\quad + \frac{\kappa b}{4}\frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}}\xi^{-1}\frac{d-1}{2}\beta^{-1} + \frac{\kappa b}{4}\frac{Li_{\frac{d-1}{2}}Li_{\frac{d+2}{2}}}{[Li_{\frac{d}{2}}]^2}\xi^{-1}\frac{d+2}{2}\beta^{-1} \\
&\quad \left. - \frac{\kappa b}{4}\frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d}{2}}}\xi^{-1}\frac{d+1}{2}\beta^{-1}\right)\left(\frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}}\frac{d}{2}\beta^{-1} - \frac{d+2}{2}\frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}}\beta^{-1}\right)^{-1} \\
&\quad + \frac{\kappa b}{4}\frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}}\xi^{-1} - \frac{\kappa b}{4}\frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}}\xi^{-1}\frac{d-1}{d} - \frac{\kappa b}{4}\frac{1}{d}\frac{Li_{\frac{d+1}{2}}}{(Li_{\frac{d}{2}})^2}Li_{\frac{d-2}{2}}\xi^{-1}\left. \right] \\
&\quad \cdot \left[kLi_{\frac{d+2}{2}}\alpha^d\left(\frac{d+2}{2}\right)\beta^{-\frac{d}{2}} - k\frac{d}{2}\alpha^d\beta^{-\frac{d}{2}}\frac{(Li_{\frac{d}{2}})^2}{Li_{\frac{d-2}{2}}} \right]^{-1} \left[1 - \left(k\frac{d}{2}\frac{\kappa b}{4}\frac{Li_{\frac{d-3}{2}}(Li_{\frac{d}{2}})^2}{(Li_{\frac{d-2}{2}})^2}\xi^{-1}\alpha^d\beta^{-\frac{d}{2}} \right.\right. \\
&\quad + k\frac{d}{2}\frac{\kappa b}{4}\frac{Li_{\frac{d-1}}{2}Li_{\frac{d}{2}}}{Li_{\frac{d-2}}}\frac{d-1}{d}\xi^{-1}\alpha^d\beta^{-\frac{d}{2}} - k\frac{\kappa b}{4}\frac{d}{2}Li_{\frac{d-1}}{2}\frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}}}\xi^{-1} + k\frac{\kappa b}{4}Li_{\frac{d+1}}{2}\left(\frac{d+1}{2}\right)\xi^{-1} \left. \right) \\
&\quad \cdot \left. \left(kLi_{\frac{d+2}{2}}\alpha^d\left(\frac{d+2}{2}\right)\beta^{-\frac{d}{2}} - k\frac{d}{2}\alpha^d\beta^{-\frac{d}{2}}\frac{(Li_{\frac{d}{2}})^2}{Li_{\frac{d-2}}} \right)^{-1} \right]^{-1}
\end{aligned}$$

$$\begin{aligned}
&= -\frac{\frac{d}{2}\beta - \frac{Li_{\frac{d+2}{2}}Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2}\beta}{Li_{\frac{d+2}{2}}\alpha^d(\frac{d+2}{2})\beta^{-\frac{d}{2}} - \frac{d}{2}\alpha^d\beta^{-\frac{d}{2}}\frac{(Li_{\frac{d}{2}})^2}{Li_{\frac{d-2}{2}}}} \left[1 - \left(\frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}Li_{\frac{d}{2}}}{[Li_{\frac{d-2}{2}}]^2} \xi^{-1} \frac{d}{2} \beta^{-1} + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} \frac{d-1}{2} \beta^{-1} \right. \right. \\
&+ \left. \frac{\kappa b}{4} \frac{Li_{\frac{d-1}}{2}}[Li_{\frac{d}{2}}]^2} \xi^{-1} \frac{d+2}{2} \beta^{-1} - \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \frac{d+1}{2} \beta^{-1} \right) \left(\frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \frac{d}{2} \beta^{-1} - \frac{d+2}{2} \frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} \beta^{-1} \right)^{-1} \\
&+ \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} - \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \frac{d-1}{d} - \frac{\kappa b}{4} \frac{1}{d} \frac{Li_{\frac{d+1}{2}}}{(Li_{\frac{d}{2}})^2} Li_{\frac{d-2}{2}} \xi^{-1} + \left(k \frac{d}{2} \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}}Li_{\frac{d}{2}}}{(Li_{\frac{d-2}{2}})^2} \xi^{-1} \alpha^d \beta^{-\frac{d}{2}} \right. \\
&+ \left. k \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}} \frac{d-1}{2} \xi^{-1} \alpha^d \beta^{-\frac{d}{2}} - k \frac{\kappa b}{4} \frac{d}{2} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d-2}{2}}} \xi^{-1} + k \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d}{2}}} \left(\frac{d+1}{2} \right) \xi^{-1} \right) \\
&\cdot \left. \left(k \frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} \alpha^d \left(\frac{d+2}{2} \right) \beta^{-\frac{d}{2}} - k \frac{d}{2} \alpha^d \beta^{-\frac{d}{2}} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d-2}{2}}} \right)^{-1} \right] \tag{3.146}
\end{aligned}$$

To check the bulk result, we keep only the leading terms which go like volume and take $d = 3$. The result is

$$\kappa_T = -\frac{\frac{3}{2}\beta - \frac{5}{2} \frac{Li_{\frac{5}{2}}Li_{\frac{1}{2}}}{[Li_{\frac{3}{2}}]^2} \beta}{Li_{\frac{5}{2}}\alpha^3(\frac{5}{2})\beta^{-\frac{3}{2}} - \frac{3}{2} \frac{(Li_{\frac{3}{2}})^2}{Li_{\frac{1}{2}}} \alpha^3 \beta^{-\frac{3}{2}}} = \beta^{\frac{5}{2}} \frac{Li_{\frac{1}{2}}}{\alpha^3 [Li_{\frac{3}{2}}]^2} \tag{3.147}$$

consistent with the result given by Pathria[7].

3.8. Entropy Expression and Adiabatic Compressibility

Two other thermodynamic quantities that we would like to see under the boundary effect are entropy S and relevantly the adiabatic compressibility κ_S . The formula to find the adiabatic compressibility is known as $\kappa_S = -\frac{1}{V} \frac{\partial V}{\partial P} \Big|_S$.

Starting with the entropy, we will use the well-known expansion[7],

$$\frac{S}{Nk} = \frac{U - \mu N + PV}{NkT} \tag{3.148}$$

In this equality, we will place the elements we already know which are

$$\begin{aligned} U &= -\frac{\partial q}{\partial \beta} + \mu N \\ &= U_0 + \frac{d}{2}\beta^{-1}Li_{\frac{d+2}{2}}\xi^d + \frac{\kappa b}{4}\left(\frac{d-1}{2}\right)\beta^{-1}Li_{\frac{d+1}{2}}\xi^{d-1} \end{aligned} \quad (3.149)$$

$$U_0 = 0, \quad (3.150)$$

$$\mu\beta = \ln(z), \quad (3.151)$$

$$N = Li_{\frac{d}{2}}\xi^d + \frac{\kappa b}{4}Li_{\frac{d-1}{2}}\xi^{d-1} \quad (3.152)$$

and we get accordingly

$$\Rightarrow \frac{S}{Nk} = \beta^{-1} \frac{\frac{d}{2}Li_{\frac{d+2}{2}}\xi^d + \frac{\kappa b}{4}\frac{d-1}{2}Li_{\frac{d+1}{2}}\xi^{d-1} + Li_{\frac{d+2}{2}}\xi^d + \frac{\kappa b}{4}Li_{\frac{d+1}{2}}\xi^{d-1}}{kT Li_{\frac{d}{2}}\xi^d + kT \frac{\kappa b}{4}Li_{\frac{d-1}{2}}\xi^{d-1}} - \frac{\mu}{kT} \quad (3.153)$$

We expand this equation properly as we did many times, noting that again we are away from the critical temperature. We get the entropy expression as below.

$$\begin{aligned} \frac{S}{Nk} &= \frac{\frac{d+2}{2}Li_{\frac{d+2}{2}}\left(1 + \frac{\frac{\kappa b}{4}\left(\frac{d+1}{2}\right)Li_{\frac{d+1}{2}}\xi^{d-1}}{\frac{d+2}{2}Li_{\frac{d+2}{2}}\xi^d}\right)}{Li_{\frac{d}{2}}\left(1 + \frac{\frac{\kappa b}{4}Li_{\frac{d-1}{2}}\xi^{d-1}}{Li_{\frac{d}{2}}\xi^d}\right)} - \ln(z) \\ &= \frac{\frac{d+2}{2}Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}}\left(1 + \frac{d+1}{d+2}\frac{\frac{\kappa b}{4}Li_{\frac{d+1}{2}}\xi^{-1}}{Li_{\frac{d+2}{2}}}\right) - \frac{\frac{\kappa b}{4}Li_{\frac{d-1}{2}}\xi^{-1}}{Li_{\frac{d}{2}}} - \ln(z) \end{aligned} \quad (3.154)$$

To check the consistency, dropping the terms with κ and taking $d = 3$; the result we get is

$$\frac{S}{Nk} = \frac{\frac{5}{2}Li_{\frac{5}{2}}}{Li_{\frac{3}{2}}} - \ln(z) \quad (3.155)$$

and it is consistent with Pathria[7].

At this point, we have the entropy expression and we want to look at the adiabatic compressibility, κ_S . Two derivative expressions are needed to be calculated to reach

κ_S which are $\frac{1}{V} \frac{\partial V}{\partial T} \Big|_S$ and $\frac{\partial P}{\partial T} \Big|_S$. We need to keep entropy constant while taking the derivatives. Keeping the entropy constant, we look for other quantities that remains constant. Since we know already the number of particles, N , is constant, we will take out the ξ expression from the entropy equation and put it back in the N expression to see if ξ is also a constant.

$$\frac{S}{Nk} + \ln z = \frac{\frac{d+2}{2} Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} \left(1 + \left[\frac{d+1}{d+2} \frac{\frac{\kappa b}{4} Li_{\frac{d+1}{2}}}{Li_{\frac{d+2}{2}}} - \frac{\frac{\kappa b}{4} Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \right] \xi^{-1} \right) \quad (3.156)$$

$$\Rightarrow \quad \xi = \frac{\kappa b}{4} \left[\frac{\frac{d+1}{d+2} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d+2}{2}}} - \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}}}{\left(\frac{S}{Nk} + \ln z \right) \frac{2}{d+2} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d+2}{2}}} - 1} \right] \quad (3.157)$$

Putting ξ into the N expression:

$$\begin{aligned} N = & Li_{\frac{d}{2}} \left[\frac{\kappa b}{4} \frac{\frac{d+1}{d+2} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d+2}{2}}} - \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}}}{\left(\frac{S}{Nk} + \ln z \right) \frac{2}{d+2} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d+2}{2}}} - 1} \right]^d \\ & + Li_{\frac{d-1}{2}} \left[\frac{\kappa b}{4} \right]^d \left[\frac{\frac{d+1}{d+2} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d+2}{2}}} - \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}}}{\left(\frac{S}{Nk} + \ln z \right) \frac{2}{d+2} \frac{Li_{\frac{d}{2}}}{Li_{\frac{d+2}{2}}} - 1} \right]^{d-1} \end{aligned} \quad (3.158)$$

According to the equation above, since N is constant, $z = e^{-\beta\mu}$ should be a constant. This implies because of (3.157) that ξ is also a constant when S and N are constants. In this case, the derivative of the volume with respect to temperature will be found by the derivative of ξ because of that it becomes a constant if we keep the entropy constant. Volume dependence of ξ is explicitly known as we stated at the beginning.

$$\xi = \frac{V}{(\sqrt{2m\pi})^d} \beta^{-\frac{d}{2}} = \text{constant} \quad (3.159)$$

Taking the derivative of ξ with respect to T we get the $-\frac{1}{V}\frac{\partial V}{\partial T}\Big|_S$ expression that we desire:

$$\frac{\beta^{-\frac{d}{2}}}{(\sqrt{2m\pi})^d} \frac{\partial V}{\partial T} + \frac{V}{(\sqrt{2m\pi})^d} \frac{\partial}{\partial T} \beta^{-\frac{d}{2}} = 0 \quad (3.160)$$

$$\Rightarrow \frac{\partial V}{\partial T} = -k \frac{d}{2} \beta V \quad (3.161)$$

$$\Rightarrow -\frac{1}{V} \frac{\partial V}{\partial T} = k \frac{d}{2} \beta \quad (3.162)$$

There is one more expression we need to calculate keeping the entropy constant which is the derivative of the pressure with respect to temperature. It will be easy to calculate since both the argument of the polylogarithmic functions, z , and ξ are constants and there will be no contribution from their derivatives.

$$PV = \beta^{-1} q \quad (3.163)$$

$$\frac{\partial P}{\partial T} V + \frac{\partial V}{\partial T} P = (-k\beta^2) \left[-\beta^{-2} Li_{\frac{d+2}{2}} \xi^d - \beta^{-2} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1} \right] \quad (3.164)$$

Dividing by volume and inserting the terms which are known from before in the equation,

$$\frac{\partial P}{\partial T} + \frac{1}{V} \frac{\partial V}{\partial T} P = (-k\beta^2) \left[-\beta^{-2} Li_{\frac{d+2}{2}} \frac{\xi^d}{V} - \beta^{-2} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \frac{\xi^{d-1}}{V} \right] \quad (3.165)$$

$$\frac{\partial P}{\partial T} - k \frac{d}{2} \beta \beta^{-1} Li_{\frac{d+2}{2}} \frac{\xi^d}{V} - k \frac{d}{2} \beta \beta^{-1} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \frac{\xi^{d-1}}{V} = k Li_{\frac{d+2}{2}} \frac{\xi^d}{V} + k \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \frac{\xi^{d-1}}{V} \quad (3.166)$$

we get the $\frac{\partial P}{\partial T}\Big|_S$ expression as:

$$\frac{\partial P}{\partial T}\Big|_S = \left(Li_{\frac{d+2}{2}} \alpha^d \beta^{-\frac{d}{2}} + \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \alpha^{d-1} \beta^{-\frac{d-1}{2}} V^{-\frac{1}{d}} \right) \left(k \frac{2+d}{2} \right) \quad (3.167)$$

Now, combining all these equations, we can write the adiabatic compressibility expression as

$$\kappa_S = -\frac{1}{V} \frac{\partial V}{\partial P} \Big|_S = -\frac{1}{V} \frac{\frac{\partial V}{\partial T} \Big|_S}{\frac{\partial P}{\partial T} \Big|_S} = \frac{k \frac{d}{2} \beta}{(Li_{\frac{d+2}{2}} \alpha^d \beta^{-\frac{d}{2}} + \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \alpha^{d-1} \beta^{-\frac{d-1}{2}} V^{-\frac{1}{d}}) (k \frac{2+d}{2})} \quad (3.168)$$

Again, to obtain the bulk result, we take $d = 3$ and drop the terms except the leading terms of the κ_S , we get

$$\kappa_S = \frac{\frac{3}{2} \beta}{\frac{5}{2} \alpha^3 Li_{\frac{5}{2}} \beta^{-\frac{3}{2}}} = \frac{3}{5} \frac{\beta^{\frac{5}{2}}}{\alpha^3 Li_{\frac{5}{2}}} = \frac{3}{5} \frac{\beta^{\frac{5}{2}} \frac{N}{V}}{n \alpha^3 Li_{\frac{5}{2}}} = \frac{3}{5} \frac{\beta^{\frac{5}{2}} \alpha^3 Li_{\frac{3}{2}} \beta^{-\frac{3}{2}}}{n \alpha^3 Li_{\frac{5}{2}}} = \frac{3}{5} \frac{Li_{\frac{3}{2}}}{nkT Li_{\frac{5}{2}}} \quad (3.169)$$

which is consistent with the result written by Pathria[7].

3.9. Calculation of C_P

The heat capacity with constant pressure will also be investigated. Since the heat capacity with constant pressure is known as $C_P = \frac{\partial U}{\partial \beta} \Big|_P + P \frac{\partial V}{\partial \beta} \Big|_P$, we first need to rewrite the $\frac{\partial U}{\partial \beta}$ and $P \frac{\partial V}{\partial \beta}$ expressions at constant pressure. We will also check $\frac{C_P}{C_V}$ expression.

We start with the internal energy derivative at constant pressure:

$$U = \frac{\partial q}{\partial \beta} + \mu N \quad (3.170)$$

$$\begin{aligned} \frac{\partial U}{\partial \beta} \Big|_P &= \frac{d}{2} (-\beta^{-2}) Li_{\frac{d+2}{2}} \xi^d + \frac{d}{2} \beta^{-1} Li_{\frac{d}{2}} \frac{\partial(\mu\beta)}{\partial \beta} \Big|_P \xi^d + \frac{d}{2} \beta^{-1} Li_{\frac{d+2}{2}} (-\frac{d}{2}) \beta^{-1} \xi^d \\ &\quad + \frac{d}{2} \beta^{-1} Li_{\frac{d+2}{2}} \alpha^d \beta^{-\frac{d}{2}} \frac{\partial V}{\partial \beta} \Big|_P + \frac{\kappa b}{4} \frac{d-1}{2} (-\beta^{-2}) Li_{\frac{d+1}{2}} \xi^{d-1} \\ &\quad + \frac{\kappa b}{4} \frac{d-1}{2} \beta^{-1} Li_{\frac{d-1}{2}} \frac{\partial(\mu\beta)}{\partial \beta} \Big|_P \xi^{d-1} + \frac{\kappa b}{4} \frac{d-1}{2} \beta^{-1} Li_{\frac{d+1}{2}} (-\frac{d-1}{2}) \beta^{-1} \xi^{d-1} \\ &\quad + \frac{\kappa b}{4} \frac{d-1}{2} \beta^{-1} Li_{\frac{d+1}{2}} \alpha^{d-1} \beta^{-\frac{d-1}{2}} \frac{\partial}{\partial \beta} V^{\frac{d-1}{d}} \Big|_P \end{aligned} \quad (3.171)$$

Here, we need to remark that we calculated the expansion of $\frac{\partial}{\partial\beta}[\beta\mu]$ at constant volume before. However, now we need this derivative at constant pressure, so we will calculate it over again. We will take out $\frac{\partial}{\partial\beta}[\beta\mu]$ from the system of equations that we used to find $\frac{\partial V}{\partial\beta}$ earlier.

$$\begin{aligned} \frac{\partial}{\partial\beta}[\beta\mu]|_P &= \left[\frac{1}{d} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} V^{-\frac{1}{d}} \alpha^{d-1} \beta^{-\frac{d-1}{2}-1} \frac{\partial V}{\partial\beta} + \frac{d+2}{2} \beta^{-2} Li_{\frac{d+2}{2}} \xi^d + \frac{d+1}{2} \beta^{-2} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1} \right] \\ &\times \left[\beta^{-1} Li_{\frac{d}{2}} \xi^d \left(1 + \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \right) \right]^{-1} \end{aligned} \quad (3.172)$$

After making our expansion and some arrangements, we get the expression as below.

$$\begin{aligned} \frac{\partial}{\partial\beta}[\beta\mu]|_P &= \frac{d+2}{2} \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \beta^{-1} - \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{-1} \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^3} \frac{d+2}{2} \beta^{-1} \\ &+ \frac{d+2}{2} \beta^{-1} \frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} - \frac{d+2}{2} \beta^{-1} \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \xi^{-1} \end{aligned} \quad (3.173)$$

In addition to this expression, as used in the above calculation, we already have $\frac{\partial V}{\partial\beta}|_P$.

$$\begin{aligned} \frac{\partial V}{\partial\beta}|_P &= \frac{d}{2} \beta^{-1} V - \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2} \beta^{-1} V - \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} (d-1) \beta^{-1} V \xi^{-1} \\ &+ \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d}{2} \beta^{-1} V \xi^{-1} - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2} \beta^{-1} V \xi^{-1} \\ &+ \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} (Li_{\frac{d-2}{2}})^2 Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^4} \frac{d+2}{2d} \beta^{-1} V \xi^{-1} \end{aligned} \quad (3.174)$$

Now, we will replace these $\mu\beta$ and V derivatives in internal energy expression accordingly:

$$\begin{aligned}
\left. \frac{\partial U}{\partial \beta} \right|_P &= \frac{d}{2}(-\beta^{-2})Li_{\frac{d+2}{2}}\xi^d + \frac{d}{2}\beta^{-1}Li_{\frac{d}{2}}\left\{ \frac{d+2}{2} \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \beta^{-1} \right. \\
&\quad - \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{-1} \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^3} \frac{d+2}{2} \beta^{-1} \\
&\quad + \frac{d+2}{2} \beta^{-1} \frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} - \frac{d+2}{2} \beta^{-1} \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \xi^{-1} \left. \right\} \xi^d + \frac{d}{2} \beta^{-1} Li_{\frac{d+2}{2}} \left(-\frac{d}{2}\right) \beta^{-1} \xi^d \\
&\quad + \frac{d}{2} \beta^{-1} Li_{\frac{d+2}{2}} \alpha^d \beta^{-\frac{d}{2}} \left\{ \frac{d}{2} \beta^{-1} V - \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2} \beta^{-1} V - \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} (d-1) \beta^{-1} V \xi^{-1} \right. \\
&\quad + \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d}{2} \beta^{-1} V \xi^{-1} - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2} \beta^{-1} V \xi^{-1} \\
&\quad + \left. \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} (Li_{\frac{d-2}{2}})^2 Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^4} \frac{d+2}{2d} \beta^{-1} V \xi^{-1} \right\} + \frac{\kappa b}{4} \frac{d-1}{2} (-\beta^{-2}) Li_{\frac{d+1}{2}} \xi^{d-1} \\
&\quad + \frac{\kappa b}{4} \frac{d-1}{2} \beta^{-1} Li_{\frac{d-1}{2}} \left\{ \frac{d+2}{2} \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}}}{Li_{\frac{d}{2}}} \xi^{-1} \beta^{-1} - \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{-1} \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^3} \frac{d+2}{2} \beta^{-1} \right. \\
&\quad + \frac{d+2}{2} \beta^{-1} \frac{Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} - \frac{d+2}{2} \beta^{-1} \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \xi^{-1} \left. \right\} \xi^{d-1} \\
&\quad + \frac{\kappa b}{4} \frac{d-1}{2} \beta^{-1} Li_{\frac{d+1}{2}} \left(-\frac{d-1}{2}\right) \beta^{-1} \xi^{d-1} \\
&\quad + \frac{\kappa b}{4} \frac{d-1}{2} \beta^{-1} Li_{\frac{d+1}{2}} \alpha^{d-1} \beta^{-\frac{d-1}{2}} \frac{d-1}{d} V^{-\frac{1}{d}} \left\{ \frac{d}{2} \beta^{-1} V \right. \\
&\quad - \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2} \beta^{-1} V - \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} (d-1) \beta^{-1} V \xi^{-1} \\
&\quad + \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d}{2} \beta^{-1} V \xi^{-1} - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d+2}{2} \beta^{-1} V \xi^{-1} \\
&\quad + \left. \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} (Li_{\frac{d-2}{2}})^2 Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^4} \frac{d+2}{2d} \beta^{-1} V \xi^{-1} \right\} \tag{3.175}
\end{aligned}$$

After making some rearrangements and drop the terms of order of ξ^{d-2} , we get:

$$\begin{aligned}
\frac{\partial U}{\partial \beta} \Big|_P &= \frac{d^2}{4} \beta^{-2} Li_{\frac{d+2}{2}} \xi^d + \frac{d^2 + 2\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1} \beta^{-2} \\
&\quad - \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1} \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d^3 + d^2 + 3d + 2}{4d} \beta^{-2} \\
&\quad - \frac{2d^2 - d + 2}{4} \beta^{-2} \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}} Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} \xi^{d-1} - \frac{(Li_{\frac{d+2}{2}})^2 Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d + 2}{2} \frac{d}{2} \beta^{-2} \xi^d \\
&\quad + \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} Li_{\frac{d-2}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d^2}{4} \beta^{-2} \xi^{d-1} - \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} (Li_{\frac{d+2}{2}})^2}{(Li_{\frac{d}{2}})^2} \frac{d + 2}{2} \frac{d}{2} \beta^{-2} \xi^{d-1} \\
&\quad + \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} (Li_{\frac{d-2}{2}})^2 (Li_{\frac{d+2}{2}})^2}{(Li_{\frac{d}{2}})^4} \frac{d + 2}{4} \beta^{-2} \xi^{d-1} \tag{3.176}
\end{aligned}$$

The second term to be added to the internal energy derivative is $P \frac{\partial V}{\partial \beta} \Big|_P$ which was also calculated earlier:

$$\begin{aligned}
P \frac{\partial V}{\partial \beta} \Big|_P &= \beta^{-1} Li_{\frac{d+2}{2}} \xi^d \frac{d}{2} \beta^{-1} - \beta^{-1} Li_{\frac{d+2}{2}} \xi^d \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d + 2}{2} \beta^{-1} \\
&\quad - \beta^{-1} Li_{\frac{d+2}{2}} \xi^d \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} (d - 1) \beta^{-1} \xi^{-1} + \beta^{-1} Li_{\frac{d+2}{2}} \xi^d \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d}{2} \beta^{-1} \xi^{-1} \\
&\quad - \beta^{-1} Li_{\frac{d+2}{2}} \xi^d \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d + 2}{2} \beta^{-1} \xi^{-1} \\
&\quad + \beta^{-1} Li_{\frac{d+2}{2}} \xi^d \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} (Li_{\frac{d-2}{2}})^2 Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^4} \frac{d + 2}{2d} \beta^{-1} \xi^{-1} + \beta^{-1} \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1} \frac{d}{2} \beta^{-1}
\end{aligned}$$

Combining these two derivatives in C_P formula, we get:

$$C_P = \left(\frac{\partial U}{\partial \beta} \Big|_P + P \frac{\partial V}{\partial \beta} \Big|_P \right) (-k\beta^2) \tag{3.177}$$

$$\begin{aligned}
C_P = & -k \frac{d^2}{4} Li_{\frac{d+2}{2}} \xi^d - k \frac{d^2 + 2\kappa b}{4} \frac{Li_{\frac{d+1}{2}}}{4} \xi^{d-1} \\
& + k \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1} \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d^3 + d^2 + 3d + 2}{4d} \\
& + k \frac{2d^2 - d + 2\kappa b}{4} \frac{Li_{\frac{d-1}{2}} Li_{\frac{d+2}{2}}}{Li_{\frac{d}{2}}} \xi^{d-1} + k \frac{(Li_{\frac{d+2}{2}})^2 Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d + 2}{2} \frac{d}{2} \xi^d \\
& - k \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} Li_{\frac{d-2}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d^2}{4} \xi^{d-1} + k \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} (Li_{\frac{d+2}{2}})^2}{(Li_{\frac{d}{2}})^2} \frac{d + 2}{2} \frac{d}{2} \xi^{d-1} \\
& - k \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} (Li_{\frac{d-2}{2}})^2 (Li_{\frac{d+2}{2}})^2}{(Li_{\frac{d}{2}})^4} \frac{d + 2}{4} \xi^{d-1} \\
& - k Li_{\frac{d+2}{2}} \xi^d \frac{d}{2} + k Li_{\frac{d+2}{2}} \xi^d \frac{Li_{\frac{d+2}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d + 2}{2} \\
& + k Li_{\frac{d+2}{2}} \xi^d \frac{\kappa b}{4} \frac{Li_{\frac{d-1}{2}}}{Li_{\frac{d}{2}}} (d-1) \xi^{-1} - k Li_{\frac{d+2}{2}} \xi^d \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} Li_{\frac{d-2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d}{2} \xi^{-1} \\
& + k Li_{\frac{d+2}{2}} \xi^d \frac{\kappa b}{4} \frac{Li_{\frac{d-3}{2}} Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^2} \frac{d + 2}{2} \xi^{-1} \\
& - k Li_{\frac{d+2}{2}} \xi^d \frac{\kappa b}{4} \frac{Li_{\frac{d+1}{2}} (Li_{\frac{d-2}{2}})^2 Li_{\frac{d+2}{2}}}{(Li_{\frac{d}{2}})^4} \frac{d + 2}{2d} \xi^{-1} - k \frac{\kappa b}{4} Li_{\frac{d+1}{2}} \xi^{d-1} \frac{d}{2} \quad (3.178)
\end{aligned}$$

If we take the leading terms of C_P with $d = 3$:

$$C_P = -k \frac{15}{4} Li_{\frac{5}{3}} \xi^3 + k \frac{25}{4} \frac{(Li_{\frac{5}{2}})^2 Li_{\frac{1}{2}}}{(Li_{\frac{3}{2}})^2} \xi^3 \quad (3.179)$$

Now, to check the consistency with Pathria[7], we will divide C_P to C_V . We already have the leading terms of C_V with $d = 3$ as we below:

$$C_V = k \frac{15}{4} Li_{\frac{5}{2}} \xi^3 - k \frac{9}{4} \frac{(Li_{\frac{3}{2}})^2}{Li_{\frac{1}{2}}} \xi^3 \quad (3.180)$$

Finally, checking the ratio between C_P and C_V :

$$\begin{aligned}
\frac{C_P}{C_V} = & \frac{-k \frac{15}{4} Li_{\frac{5}{3}} \xi^3 + k \frac{25}{4} \frac{(Li_{\frac{5}{2}})^2 Li_{\frac{1}{2}}}{(Li_{\frac{3}{2}})^2} \xi^3}{k \frac{15}{4} Li_{\frac{5}{2}} \xi^3 - k \frac{9}{4} \frac{(Li_{\frac{3}{2}})^2}{Li_{\frac{1}{2}}} \xi^3} = \frac{5}{2} \frac{Li_{\frac{1}{2}} Li_{\frac{5}{2}}}{(Li_{\frac{3}{2}})^2} \quad (3.181)
\end{aligned}$$

This result is also consistent with Pathria[7] being equal to $\frac{\kappa_T}{\kappa_S}$.

4. GENERALIZATION TO THE p^s CASE

We did all our calculations for a second degree differential operator. What we would like to do is generalizing our calculations to s^{th} degree operators. That will make some changes on the coefficients. We will look at the change on partition function which is indicated in (2.7) of [9].

$$\epsilon_N = \frac{p^2}{2m} \quad \Rightarrow \quad p^s = \tilde{\epsilon} \quad (4.1)$$

Here p is the momentum operator. However, dimension of p^s is not energy. Therefore we introduce the spectrum directly as

$$\frac{\epsilon_N^{s/2}}{\epsilon_0^{s/2-1}} = \tilde{\epsilon} \quad (4.2)$$

to keep the dimension correct. This can be thought of as a system of quasiparticles at low energies.

4.1. Partition Function Calculation

The partition function can be written as

$$\begin{aligned} q &= q_0 + \sum_{n=1}^{\infty} \sum'_N \frac{1}{n} e^{-\beta n(\tilde{\epsilon}-\mu)} \\ &= q_0 + \sum_{n=1}^{\infty} \frac{1}{n} e^{(\beta n\mu)} \sum'_N e^{-\tilde{\epsilon}} \end{aligned} \quad (4.3)$$

Let us remember the Mellin Barnes integral :

$$e^{-v} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) v^{-\alpha} \quad (4.4)$$

In our case $v = \tilde{\epsilon}$. We organize the partition function as writing the $\tilde{\epsilon}$ in terms of dimensionally corrected regular energy, ϵ_N .

$$\begin{aligned} q &= q_0 + \sum_{n=1}^{\infty} \frac{1}{n} e^{(\beta n \mu)} \sum_N' \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha (\beta n)^{-\alpha} \Gamma(\alpha) (\tilde{\epsilon})^{-\alpha} \\ &= q_0 + \sum_{n=1}^{\infty} \frac{1}{n} e^{(\beta n \mu)} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha (\beta n)^{-\alpha} \Gamma(\alpha) \sum_N' \left[\epsilon_0 \left(\frac{\epsilon_N}{\epsilon_0} \right)^{\frac{s}{2}} \right]^{-\alpha} \end{aligned} \quad (4.5)$$

We take the last term above to continue with the zeta function expression associated with the Schrödinger equation.

$$\begin{aligned} \sum_N' \frac{\epsilon_N^{-\frac{s\alpha}{2}}}{\epsilon_0^{-\frac{s\alpha}{2} + \alpha}} &= \frac{1}{\epsilon_0^{-\frac{s\alpha}{2} + \alpha}} \sum_N' \epsilon_N^{-\frac{s\alpha}{2}} = \epsilon_0^{\frac{s\alpha}{2} - \alpha} \zeta\left(\frac{s\alpha}{2}\right) \\ &= \epsilon_0^{\frac{s\alpha}{2} - \alpha} \frac{1}{\Gamma\left(\frac{s\alpha}{2}\right)} \sum_N' \int_0^{\infty} dt t^{\frac{s\alpha}{2} - 1} e^{-t\epsilon_N} \end{aligned} \quad (4.6)$$

We will again use the polylogarithmic expression for the n summation.

$$\sum_{n=1}^{\infty} \frac{x^n}{n^\alpha} = Li_\alpha(x) \quad (4.7)$$

Here, we need to note that $\mu_c = E_0$ ground state energy taken as zero to simplify our calculations. This essentially means that we restrict ourselves to Neumann boundary conditions. Also, we will ignore the ground state occupation and drop the q_0 's while we are away from the critical temperature. After we make the arrangements in accordance with the expressions we have found above, the ground partition function becomes the expression:

$$q = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha Li_{\alpha+1}(e^{\beta\mu}) (\beta)^{-\alpha} \Gamma(\alpha) \frac{1}{\Gamma\left(\frac{s\alpha}{2}\right)} \epsilon_0^{\alpha\left(\frac{s}{2}-1\right)} \sum_N' \int_0^{\infty} dt t^{\frac{s\alpha}{2}-1} e^{-t\epsilon_N}. \quad (4.8)$$

Now, the heat kernel corresponding to the N summation will be the same as that we used in the earlier section.

$$K(t) = \sum'_N e^{-t\epsilon_N} \quad \text{for small } t \simeq \frac{1}{(4\pi)^{\frac{d}{2}}} t^{-\frac{d}{2}} \sum_{l=0,1/2,1,\dots}^{\infty} a_l t^l \quad (4.9)$$

Since we need to find the poles to calculate the integral by the residue method, we will use the same trick. We will divide the infinite integral into two parts as from zero to a small δ and from δ to infinity. The pole structure here is very complicated in general unless s is an even integer. Second part will be convergent at any region, so we will take only the first integral. Inserting the heat kernel in the q equation;

$$q = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha Li_{\alpha+1}(e^{\beta\mu})(\beta)^{-\alpha} \frac{\Gamma(\alpha)}{\Gamma(\frac{s\alpha}{2})} \frac{\epsilon_0^{\alpha(\frac{s}{2}-1)}}{(4\pi)^{\frac{d}{2}}} \sum_{l=0,1/2,1,\dots}^{\infty} a_l \int_0^{\delta} dt t^{\frac{s\alpha}{2}-1+l-\frac{d}{2}} \quad (4.10)$$

Taking the t integral:

$$\begin{aligned} q &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha Li_{\alpha+1}(e^{\beta\mu})(\beta)^{-\alpha} \Gamma(\alpha) \frac{1}{\Gamma(\frac{s\alpha}{2})} \epsilon_0^{\alpha(\frac{s}{2}-1)} \frac{1}{(4\pi)^{\frac{d}{2}}} \sum_{l=0,1/2,1,\dots}^{\infty} a_l \frac{t^{\frac{s\alpha}{2}+l-\frac{d}{2}}}{\frac{s\alpha}{2}+l-\frac{d}{2}} \Big|_0^{\delta} \\ &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha Li_{\alpha+1}(e^{\beta\mu})(\beta)^{-\alpha} \frac{\Gamma(\alpha)}{\Gamma(\frac{s\alpha}{2})} \frac{\epsilon_0^{\alpha(\frac{s}{2}-1)}}{(4\pi)^{\frac{d}{2}}} \sum_{l=0,1/2,1,\dots}^{\infty} \frac{a_l}{\frac{s\alpha}{2}+l-\frac{d}{2}} e^{[\frac{s\alpha}{2}+l-\frac{d}{2}]l n \delta} \end{aligned} \quad (4.11)$$

Similar with the earlier section, we will take the two coefficients which are a_0 and $a_{1/2}$. At this point, we will use the duplication formula for Γ function which is stated below to get rid of the poles coming from the $\Gamma(\alpha)$.

Multiplication theorem:

$$\prod_{n=0}^{k-1} \Gamma\left(z + \frac{n}{k}\right) = (2\pi)^{\frac{k-1}{2}} k^{\frac{1}{2}-kz} \Gamma(kz) \quad (4.12)$$

A special case of multiplication theorem at $k = 2$ is called duplication theorem which has the form below:

$$\Gamma(z)\Gamma(z + \frac{1}{2}) = 2^{1-2z}\sqrt{\pi}\Gamma(2z) \quad (4.13)$$

We insert this identity in our integral by taking $k = \frac{s}{2}$ and we get:

$$q = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha Li_{\alpha+1}(e^{\beta\mu})(\beta)^{-\alpha} \Gamma(\alpha) \frac{(2\pi)^{\frac{s-1}{2}} (\frac{s}{2})^{\frac{1}{2}-\frac{s}{2}\alpha} \epsilon_0^{\alpha(\frac{s}{2}-1)}}{\prod_{n=0}^{\frac{s}{2}-1} \Gamma(\alpha + \frac{2n}{s}) (4\pi)^{\frac{d}{2}}} \sum_{l=0,1/2,\dots}^{\infty} \frac{a_l}{\frac{s\alpha}{2} + l - \frac{d}{2}} \quad (4.14)$$

To get rid of the poles of the gamma function, we will take $s = 2k$ and use the advantage of the duplication formula. When we change the lower index of the product from 0 to 1, the first term of the product will cancel the upper $\Gamma(\alpha)$ and thus the extra undesired poles of Γ disappear.

$$q = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha Li_{\alpha+1}(e^{\beta\mu})(\beta)^{-\alpha} \frac{(2\pi)^{\frac{k-1}{2}} k^{\frac{1}{2}-k\alpha}}{\prod_{n=1}^{k-1} \Gamma(\alpha + \frac{n}{k})} \epsilon_0^{\alpha(k-1)} \frac{1}{(4\pi)^{\frac{d}{2}}} \sum_{l=0,1/2,1,\dots}^{\infty} \frac{a_l}{k\alpha + l - \frac{d}{2}} \quad (4.15)$$

Now, where $l = 0, 1/2, 1, \dots$ this expression has poles at $k\alpha + l = \frac{d}{2}$. We will again take only first two of a_l coefficients as calculating the residues of the zeta function, which implies that α will be taken as $\frac{d}{2k}$ and $\frac{d-1}{2k}$ respectively. The partition function and all other related thermodynamic relations and expressions will be changed by some non-trivial factors. Inserting the residues, the integral goes away and the q expression becomes

$$q = Li_{\frac{d+2k}{2k}}(e^{\beta\mu})(\beta)^{-\frac{d}{2k}} \frac{(2\pi)^{\frac{k-1}{2}} k^{\frac{1}{2}-\frac{d}{2}}}{\prod_{n=1}^{k-1} \Gamma(\frac{d}{2k} + \frac{n}{k})} \epsilon_0^{\frac{d}{2k}(k-1)} \frac{a_0}{(4\pi)^{\frac{d}{2}}} + Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu})(\beta)^{-\frac{d-1}{2k}} \frac{(2\pi)^{\frac{k-1}{2}} k^{\frac{1}{2}-\frac{d-1}{2}}}{\prod_{n=1}^{k-1} \Gamma(\frac{d-1}{2k} + \frac{n}{k})} \epsilon_0^{\frac{d-1}{2k}(k-1)} \frac{a_{1/2}}{(4\pi)^{\frac{d}{2}}} \quad (4.16)$$

The a_0 and $a_{\frac{1}{2}}$ coefficients will be the same as earlier version.

$$a_0 = \left(\frac{2m}{\hbar^2}\right)^{(d/2)} V \quad , \quad a_{\frac{1}{2}} = \left(\frac{2m}{\hbar^2}\right)^{(d-1)/2} \frac{\sqrt{\pi}}{2} (\partial V) b \quad (4.17)$$

Inserting these coefficients and making some arrangements we get the final form of partition function as below.

$$\begin{aligned} q &= Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) \beta^{-\frac{d}{2k} + \frac{d}{2}} \underbrace{\frac{(2\pi)^{\frac{k-1}{2}} k^{\frac{1}{2} - \frac{d}{2}}}{\prod_{n=1}^{k-1} \Gamma\left(\frac{d}{2k} + \frac{n}{k}\right)} \epsilon_0^{\frac{d}{2k}(k-1)} \xi^d}_{\text{The bulk factor, } a_{nk}} \\ &+ Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} \frac{\kappa b}{4} \underbrace{\frac{(2\pi)^{\frac{k-1}{2}} k^{\frac{1}{2} - \frac{d-1}{2}}}{\prod_{n=1}^{k-1} \Gamma\left(\frac{d-1}{2k} + \frac{n}{k}\right)} \epsilon_0^{\frac{d-1}{2k}(k-1)} \xi^{d-1}}_{\text{The boundary factor, } b_{nk}} \\ &= Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) \beta^{-\frac{d}{2k} + \frac{d}{2}} a_{nk} \xi^d + \frac{\kappa b}{4} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} b_{nk} \xi^{d-1} \end{aligned} \quad (4.18)$$

For simplicity, we will write the extra coefficients coming to the both bulk term and the boundary term shortly as a_{nk} and b_{nk} respectively.

4.2. Number of Particles

Next thing we do is calculate the total number of particles for our generalized case basically taking the derivative of the partition function as we did earlier.

$$N = \beta^{-1} \frac{\partial q}{\partial \mu} \Big|_{T,V} = \beta^{-\frac{d}{2k} + \frac{d}{2}} Li_{\frac{d}{2k}}(e^{\beta\mu}) a_{nk} \xi^d + \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) b_{nk} \xi^{d-1} \quad (4.19)$$

4.3. Critical Temperature Expression

We will write T_C also for the generalized $s = 2k$ case. Below, the 0 index indicates the bulk temperature:

$$N = \beta_0^{-\frac{d}{2k} + \frac{d}{2}} \zeta\left(\frac{d}{2k}\right) a_{nk} \xi_0^d \left(1 + \frac{\kappa b}{4} \beta_0^{-\frac{1}{2k} - \frac{1}{2}} \frac{\zeta\left(\frac{d-1}{2k}\right) b_{nk}}{\zeta\left(\frac{d}{2k}\right) a_{nk}} \xi_0^{-1} \right) \quad (4.20)$$

If we take the first term as bulk result, we will find T_0 in terms of N

$$N = (k_B T_0)^{\frac{d}{2k} - \frac{d}{2}} \zeta\left(\frac{d}{2k}\right) a_{nk} \frac{V(2m\pi k_B T_0)^{\frac{d}{2}}}{h^d} \quad (4.21)$$

$$\Rightarrow \xi_0 = \left[\frac{N}{\beta_0^{-\frac{d}{2k} + \frac{d}{2}} \zeta\left(\frac{d}{2k}\right) a_{nk}} \right]^{\frac{1}{d}} \quad (4.22)$$

$$\Rightarrow T_0 = \frac{1}{k_B} \left[\frac{N}{V(2m\pi)^{\frac{d}{2}} \zeta\left(\frac{d}{2k}\right) a_{nk}} \frac{h^d}{\beta_0^{-\frac{d}{2k} + \frac{d}{2}}} \right]^{\frac{2k}{d}} \quad (4.23)$$

Now we can write the critical temperature under the boundary effects in terms of the bulk critical temperature:

$$\begin{aligned} N &= \beta_C^{-\frac{d}{2k} + \frac{d}{2}} \zeta\left(\frac{d}{2k}\right) a_{nk} \xi_C^d + \frac{\kappa b}{4} \beta_C^{-\frac{d-1}{2k} + \frac{d-1}{2}} \zeta\left(\frac{d-1}{2k}\right) b_{nk} \xi_C^{d-1} \\ &= \beta_C^{-\frac{d}{2k} + \frac{d}{2}} \zeta\left(\frac{d}{2k}\right) a_{nk} \xi_C^d + \frac{\kappa b}{4} \beta_C^{-\frac{d-1}{2k} + \frac{d-1}{2}} \zeta\left(\frac{d-1}{2k}\right) b_{nk} \left[\frac{N}{\beta_C^{-\frac{d}{2k} + \frac{d}{2}} \zeta\left(\frac{d}{2k}\right) a_{nk}} \right]^{\frac{d-1}{d}} \\ &= \beta_C^{-\frac{d}{2k} + \frac{d}{2}} \zeta\left(\frac{d}{2k}\right) a_{nk} \xi_C^d + \frac{\kappa b}{4} \zeta\left(\frac{d-1}{2k}\right) b_{nk} \left[\frac{N}{\zeta\left(\frac{d}{2k}\right) a_{nk}} \right]^{\frac{d-1}{d}} \end{aligned} \quad (4.24)$$

We extract T_C from the expression above. We will use the $(1+x)^n = 1+nx$ expansion for small x , where $n = \frac{2k}{d}$ for this case:

$$\begin{aligned}
T_C &= \left[\frac{\frac{N}{V} h^d}{(k_B)^{\frac{d}{2k}} \zeta\left(\frac{d}{2k}\right) a_{nk} (2m\pi)^{\frac{d}{2}}} \right]^{\frac{2k}{d}} \left(1 - \frac{\kappa b}{4} \zeta\left(\frac{d-1}{2k}\right) b_{nk} \frac{N^{-\frac{1}{d}}}{\left(\zeta\left(\frac{d}{2k}\right) a_{nk}\right)^{\frac{d-1}{d}}} \right)^{\frac{2k}{d}} \\
&= \underbrace{\left[\frac{\frac{N}{V} h^d}{(k_B)^{\frac{d}{2k}} \zeta\left(\frac{d}{2k}\right) a_{nk} (2m\pi)^{\frac{d}{2}}} \right]^{\frac{2k}{d}}}_{T_0} \left(1 - \frac{2k}{d} \frac{\kappa b}{4} \zeta\left(\frac{d-1}{2k}\right) b_{nk} \frac{N^{-\frac{1}{d}}}{\left(\zeta\left(\frac{d}{2k}\right) a_{nk}\right)^{\frac{d-1}{d}}} \right) \quad (4.25)
\end{aligned}$$

4.4. Recalculation of $\frac{\partial\beta(\mu_c-\mu)}{\partial\beta}$

Before we continue with the internal energy and the heat capacity, the expression of $\frac{\partial(\mu\beta)}{\partial\beta}|_V$ will be calculated again for $s = 2k$ generalization. It must be noted that, our calculations are stated for the safe region of the polylogarithmic functions. In this case, the condition that we can make the expansion is that

$$\frac{Li_{\frac{d-1-2k}{2k}}}{Li_{\frac{d-2k}{2k}}} \quad \text{to be finite.} \quad (4.26)$$

This is true when we are away from the T_C . For sufficiently large dimensions the above condition will be satisfied even when we approach T_C .

Now we start the derivation of μ derivative:

$$\frac{\partial\mu}{\partial\beta} = - \frac{\partial N / \partial\beta|_{\mu}}{\partial N / \partial\mu|_{\beta}}, \quad \frac{\partial(\mu\beta)}{\partial\beta}|_V = \beta \frac{\partial\mu}{\partial\beta} + \mu \quad (4.27)$$

$$\begin{aligned}
\frac{\partial N}{\partial\beta}|_{\mu} &= \left(-\frac{d}{2k} + \frac{d}{2}\right) \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d}{2k}} a_{nk} \xi^d + \beta^{-\frac{d}{2k} + \frac{d}{2}} \mu Li_{\frac{d-2k}{2k}} a_{nk} \xi^d \\
&+ \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d}{2k}} a_{nk} \left(-\frac{d}{2}\right) \xi^d + \left(-\frac{d-1}{2k} + \frac{d-1}{2}\right) \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} Li_{\frac{d-1}{2k}} b_{nk} \xi^{d-1} \\
&+ \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} \mu Li_{\frac{d-1-2k}{2k}} b_{nk} \xi^{d-1} - \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} Li_{\frac{d-1}{2k}} b_{nk} \frac{d-1}{2} \xi^{d-1} \quad (4.28)
\end{aligned}$$

$$\frac{\partial N}{\partial \mu} \Big|_{\beta} = \beta^{-\frac{d}{2k} + \frac{d}{2} + 1} Li_{\frac{d-2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d + \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} + 1} Li_{\frac{d-1-2k}{2k}}(e^{\beta\mu}) b_{nk} \xi^{d-1} \quad (4.29)$$

We will divide these two, multiply the fraction with β and add μ . We will make the expansion which is $\frac{1}{1+\epsilon} \simeq 1 - \epsilon$ for small ϵ that we have used earlier.

$$\begin{aligned} \frac{\partial \mu}{\partial \beta} = & \left[\left(\frac{d}{2k} - \frac{d}{2} \right) \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d}{2k}}(e^{\beta\mu}) a_{nk} \xi^d - \beta^{-\frac{d}{2k} + \frac{d}{2}} \mu Li_{\frac{d-2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d \right. \\ & + \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d}{2k}}(e^{\beta\mu}) a_{nk} \left(\frac{d}{2} \right) \xi^d + \left(\frac{d-1}{2k} - \frac{d-1}{2} \right) \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) b_{nk} \xi^{d-1} \\ & \left. - \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} \mu Li_{\frac{d-1-2k}{2k}}(e^{\beta\mu}) b_{nk} \xi^{d-1} + \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) b_{nk} \left(\frac{d-1}{2} \right) \xi^{d-1} \right] \\ & \times \left[\beta^{-\frac{d}{2k} + \frac{d}{2} + 1} Li_{\frac{d-2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d + \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} + 1} Li_{\frac{d-1-2k}{2k}}(e^{\beta\mu}) b_{nk} \xi^{d-1} \right]^{-1} \quad (4.30) \end{aligned}$$

Multiplying by β and adding μ to the equation above, we have

$$\begin{aligned} \frac{\partial(\mu\beta)}{\partial \beta} = & \beta \frac{\partial \mu}{\partial \beta} + \mu \quad (4.31) \\ = & \left[\left(\frac{d}{2k} - \frac{d}{2} \right) \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d}{2k}} a_{nk} \xi^d - \beta^{-\frac{d}{2k} + \frac{d}{2}} \mu Li_{\frac{d-2k}{2k}} a_{nk} \xi^d \right. \\ & + \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d}{2k}} a_{nk} \frac{d}{2} \xi^d + \left(\frac{d-1}{2k} - \frac{d-1}{2} \right) \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} Li_{\frac{d-1}{2k}} b_{nk} \xi^{d-1} \\ & \left. - \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} \mu Li_{\frac{d-1-2k}{2k}} b_{nk} \xi^{d-1} + \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} Li_{\frac{d-1}{2k}} b_{nk} \frac{d-1}{2} \xi^{d-1} \right] \\ & \times \left[\beta^{-\frac{d}{2k} + \frac{d}{2}} Li_{\frac{d-2k}{2k}} a_{nk} \xi^d + \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} Li_{\frac{d-1-2k}{2k}} b_{nk} \xi^{d-1} \right]^{-1} + \mu \\ = & \left[\left(\frac{d}{2k} - \frac{d}{2} \right) \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d}{2k}}(e^{\beta\mu}) a_{nk} \xi^d + \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d}{2k}}(e^{\beta\mu}) a_{nk} \left(\frac{d}{2} \right) \xi^d \right. \\ & + \left(\frac{d-1}{2k} - \frac{d-1}{2} \right) \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) b_{nk} \xi^{d-1} \\ & \left. + \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) b_{nk} \left(\frac{d-1}{2} \right) \xi^{d-1} \right] \\ & \times \left[\beta^{-\frac{d}{2k} + \frac{d}{2}} Li_{\frac{d-2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d \right]^{-1} \left[1 + \frac{\kappa b}{4} \beta^{\frac{1}{2k} - \frac{1}{2}} \frac{Li_{\frac{d-1-2k}{2k}}(e^{\beta\mu}) b_{nk}}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu}) a_{nk}} \xi^{-1} \right]^{-1} \end{aligned}$$

$$\begin{aligned}
&= \left[\frac{d}{2k} \beta^{-1} \frac{Li_{\frac{d}{2k}}(e^{\beta\mu})}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu})} + \frac{d-1}{2k} \frac{\kappa b}{4} \beta^{\frac{1}{2k}-\frac{3}{2}} \frac{Li_{\frac{d-1}{2k}}(e^{\beta\mu})}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu})} \frac{b_{nk}}{a_{nk}} \xi^{-1} \right] \\
&\quad \times \left[1 - \frac{\kappa b}{4} \beta^{\frac{1}{2k}-\frac{1}{2}} \frac{Li_{\frac{d-1-2k}{2k}}(e^{\beta\mu})}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu})} \frac{b_{nk}}{a_{nk}} \xi^{-1} \right]. \tag{4.32}
\end{aligned}$$

Now, let us write down the ratio of b_{nk} to a_{nk} .

$$\frac{b_{nk}}{a_{nk}} = k^{\frac{1}{2}} \epsilon_0^{-\frac{1}{2}} \frac{\prod_{n=1}^{k-1} \Gamma(\frac{d}{2k} + \frac{n}{k})}{\prod_{n=1}^{k-1} \Gamma(\frac{d-1}{2k} - \frac{n}{k})} \tag{4.33}$$

Lastly, after some proper rearrangements we get the $\frac{\partial(\mu\beta)}{\partial\beta}$ expression.

$$\begin{aligned}
\frac{\partial(\mu\beta)}{\partial\beta} &= \frac{d}{2k} \beta^{-1} \frac{Li_{\frac{d}{2k}}(e^{\beta\mu})}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu})} + \frac{d-1}{2k} \frac{\kappa b}{4} \beta^{\frac{1}{2k}-\frac{3}{2}} \frac{Li_{\frac{d-1}{2k}}(e^{\beta\mu})}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu})} \frac{b_{nk}}{a_{nk}} \xi^{-1} \\
&\quad - \frac{d}{2k} \frac{\kappa b}{4} \beta^{\frac{1}{2k}-\frac{3}{2}} \frac{Li_{\frac{d}{2k}}(e^{\beta\mu}) Li_{\frac{d-1-2k}{2k}}(e^{\beta\mu})}{(Li_{\frac{d-2k}{2k}}(e^{\beta\mu}))^2} \frac{b_{nk}}{a_{nk}} \xi^{-1} \tag{4.34}
\end{aligned}$$

4.5. Internal Energy

After that, we can calculate the internal energy by using properly the above expression we have found for $\frac{\partial(\mu\beta)}{\partial\beta}$.

$$\begin{aligned}
U &= - \frac{\partial q}{\partial\beta} \Big|_{\mu} + \frac{\mu}{\beta} \frac{\partial q}{\partial\mu} \Big|_{\beta, V} \\
&= \left(- \frac{\partial}{\partial\beta} \Big|_{\mu} + \frac{\mu}{\beta} \frac{\partial}{\partial\mu} \Big|_{\beta, V} \right) \left[Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) \beta^{-\frac{d}{2k}+\frac{d}{2}} a_{nk} \xi^d + \frac{\kappa b}{4} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k}+\frac{d-1}{2}} b_{nk} \xi^{d-1} \right] \\
&= \frac{d}{2k} \beta^{-\frac{d}{2k}+\frac{d}{2}-1} Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d - \beta^{-\frac{d}{2k}+\frac{d}{2}} Li_{\frac{d}{2k}}(e^{\beta\mu}) \frac{\partial(\mu\beta)}{\partial\beta} \Big|_{\mu} a_{nk} \xi^d \\
&\quad + \frac{\kappa b}{4} \frac{d-1}{2k} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k}+\frac{d-1}{2}-1} b_{nk} \xi^{d-1} \\
&\quad - \frac{\kappa b}{4} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) \frac{\partial(\mu\beta)}{\partial\beta} \Big|_{\mu} \beta^{-\frac{d-1}{2k}+\frac{d-1}{2}} b_{nk} \xi^{d-1} \\
&\quad + \frac{\mu}{\beta} \left(\beta^{-\frac{d}{2k}+\frac{d}{2}+1} Li_{\frac{d}{2k}}(e^{\beta\mu}) a_{nk} \xi^d + \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k}+\frac{d-1}{2}+1} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) b_{nk} \xi^{d-1} \right)
\end{aligned}$$

$$\begin{aligned}
&= \frac{d}{2k} \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d - \beta^{-\frac{d}{2k} + \frac{d}{2}} Li_{\frac{d}{2k}}(e^{\beta\mu}) \mu a_{nk} \xi^d \\
&\quad + \frac{\kappa b}{4} \frac{d-1}{2k} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} b_{nk} \xi^{d-1} \\
&\quad - \frac{\kappa b}{4} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) \mu \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} b_{nk} \xi^{d-1} \\
&\quad + \mu \beta^{-\frac{d}{2k} + \frac{d}{2}} Li_{\frac{d}{2k}}(e^{\beta\mu}) a_{nk} \xi^d + \mu \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) b_{nk} \xi^{d-1} \\
&= \frac{d}{2k} \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d + \frac{\kappa b}{4} \frac{d-1}{2k} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} b_{nk} \xi^{d-1} \quad (4.35)
\end{aligned}$$

4.6. Calculation of the Heat Capacity

4.6.1. Calculation of C_V^+

We will use this internal energy expression to calculate C_V^+ . We note that we are above the critical temperature.

$$C_V^+ = \left. \frac{\partial U}{\partial T} \right|_{N,V} = \left. \frac{\partial U}{\partial \beta} \right|_{N,V} (-k_B \beta^2) \quad (4.36)$$

$$\begin{aligned}
\left. \frac{\partial U}{\partial \beta} \right|_{N,V} &= \frac{d}{2k} \left(-\frac{d}{2k} + \frac{d}{2} - 1 \right) \beta^{-\frac{d}{2k} + \frac{d}{2} - 2} Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d \\
&\quad + \frac{d}{2k} \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d}{2k}}(e^{\beta\mu}) \frac{\partial(\mu\beta)}{\partial \beta} \Big|_V a_{nk} \xi^d + \frac{d}{2k} \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) a_{nk} \beta^{-1} \left(-\frac{d}{2} \right) \xi^d \\
&\quad + \frac{\kappa b}{4} \left(-\frac{d-1}{2k} + \frac{d-1}{2} - 1 \right) \frac{d-1}{2k} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 2} b_{nk} \xi^{d-1} \\
&\quad + \frac{\kappa b}{4} \frac{d-1}{2k} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) \frac{\partial(\mu\beta)}{\partial \beta} \Big|_V \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} b_{nk} \xi^{d-1} \\
&\quad + \frac{\kappa b}{4} \frac{d-1}{2k} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} b_{nk} \beta^{-1} \left(-\frac{d-1}{2} \right) \xi^{d-1}
\end{aligned}$$

$$\begin{aligned}
&= \frac{d}{2k} \left(-\frac{d}{2k} - 1 \right) \beta^{-\frac{d}{2k} + \frac{d}{2} - 2} Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d + \frac{d}{2k} \frac{d}{2k} \beta^{-\frac{d}{2k} + \frac{d}{2} - 2} \frac{(Li_{\frac{d}{2k}}(e^{\beta\mu}))^2}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu})} a_{nk} \xi^d \\
&+ \frac{d}{2k} \frac{d-1}{2k} \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d}{2} - \frac{5}{2}} Li_{\frac{d}{2k}} \frac{Li_{\frac{d-1}{2k}}}{Li_{\frac{d-2k}{2k}}}(e^{\beta\mu}) b_{nk} \xi^{d-1} \\
&- \frac{d}{2k} \frac{d}{2k} \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d}{2} - \frac{5}{2}} \frac{(Li_{\frac{d}{2k}}(e^{\beta\mu}))^2 Li_{\frac{d-1-2k}{2k}}(e^{\beta\mu})}{(Li_{\frac{d-2k}{2k}}(e^{\beta\mu}))^2} b_{nk} \xi^{d-1} \\
&+ \frac{\kappa b}{4} \left(-\frac{d-1}{2k} - 1 \right) \frac{d-1}{2k} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 2} b_{nk} \xi^{d-1} \\
&+ \frac{\kappa b}{4} \frac{d-1}{2k} \frac{d}{2k} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 2} \frac{Li_{\frac{d}{2k}}(e^{\beta\mu})}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu})} b_{nk} \xi^{d-1} \tag{4.37}
\end{aligned}$$

Heat capacity at constant volume above the critical temperature will be written as:

$$\begin{aligned}
C_V^+ &= k_B \frac{d}{2k} \left(\frac{d}{2k} + 1 \right) \beta^{-\frac{d}{2k} + \frac{d}{2}} Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d - k_B \frac{d}{2k} \frac{d}{2k} \beta^{-\frac{d}{2k} + \frac{d}{2}} \frac{(Li_{\frac{d}{2k}}(e^{\beta\mu}))^2}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu})} a_{nk} \xi^d \\
&+ k_B \frac{d}{2k} \frac{d}{2k} \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d}{2} - \frac{1}{2}} \frac{(Li_{\frac{d}{2k}}(e^{\beta\mu}))^2 Li_{\frac{d-1-2k}{2k}}(e^{\beta\mu})}{(Li_{\frac{d-2k}{2k}}(e^{\beta\mu}))^2} b_{nk} \xi^{d-1} \\
&+ k_B \frac{\kappa b}{4} \left(\frac{d-1}{2k} + 1 \right) \frac{d-1}{2k} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} b_{nk} \xi^{d-1} \\
&- k_B \frac{\kappa b}{4} 2 \frac{d-1}{2k} \frac{d}{2k} Li_{\frac{d-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} \frac{Li_{\frac{d}{2k}}(e^{\beta\mu})}{Li_{\frac{d-2k}{2k}}(e^{\beta\mu})} b_{nk} \xi^{d-1} \tag{4.38}
\end{aligned}$$

4.6.2. Calculation of C_V^-

Now, we will calculate the heat capacity below the critical temperature. As before, we will drop the μ derivative terms since $\mu = 0$.

$$\begin{aligned}
C_V^- &= -k_B \beta^2 \cdot \left(\frac{d}{2k} \left(-\frac{d}{2k} + \frac{d}{2} - 1 \right) \beta^{-\frac{d}{2k} + \frac{d}{2} - 2} Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) a_{nk} \xi^d \right. \\
&+ \frac{d}{2k} \beta^{-\frac{d}{2k} + \frac{d}{2} - 1} Li_{\frac{d+2k}{2k}}(e^{\beta\mu}) a_{nk} \beta^{-1} \left(-\frac{d}{2} \right) \xi^d \\
&+ \frac{\kappa b}{4} \left(-\frac{d-1}{2k} + \frac{d-1}{2} - 1 \right) \frac{d-1}{2k} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 2} b_{nk} \xi^{d-1} \\
&\left. + \frac{\kappa b}{4} \frac{d-1}{2k} Li_{\frac{d+2k-1}{2k}}(e^{\beta\mu}) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2} - 1} b_{nk} \beta^{-1} \left(-\frac{d-1}{2} \right) \xi^{d-1} \right) \tag{4.39}
\end{aligned}$$

$$\begin{aligned}
&= k_B \frac{d}{2k} \left(\frac{d}{2k} + 1 \right) \beta^{-\frac{d}{2k} + \frac{d}{2}} \zeta \left(\frac{d+2k}{2k} \right) a_{nk} \xi^d \\
&\quad + k_B \frac{\kappa b}{4} \left(\frac{d-1}{2k} + 1 \right) \frac{d-1}{2k} \zeta \left(\frac{d+2k-1}{2k} \right) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} b_{nk} \xi^{d-1}
\end{aligned} \tag{4.40}$$

4.6.3. Discontinuity on C_V Around T_C

At last, we look at the discontinuity of the heat capacity around T_C .

$$\begin{aligned}
C_V^+ - C_V^- &= -k_B \frac{d}{2k} \frac{d}{2k} \beta^{-\frac{d}{2k} + \frac{d}{2}} \frac{(\zeta(\frac{d}{2k}))^2}{\zeta(\frac{d-2k}{2k})} a_{nk} \xi^d \\
&\quad + k_B \frac{d}{2k} \frac{d}{2k} \frac{\kappa b}{4} \beta^{-\frac{d-1}{2k} + \frac{d}{2} - \frac{1}{2}} \frac{(\zeta(\frac{d}{2k}))^2 \zeta(\frac{d-1-2k}{2k})}{(\zeta(\frac{d-2k}{2k}))^2} b_{nk} \xi^{d-1} \\
&\quad - k_B \frac{\kappa b}{4} 2 \frac{d-1}{2k} \frac{d}{2k} \zeta \left(\frac{d-1}{2k} \right) \beta^{-\frac{d-1}{2k} + \frac{d-1}{2}} \frac{\zeta(\frac{d}{2k})}{\zeta(\frac{d-2k}{2k})} b_{nk} \xi^{d-1}
\end{aligned} \tag{4.41}$$

5. CONCLUSIONS

In conclusion, the thermodynamic calculations that we make by using the Mellin-Barnes integral representation and heat kernel approximation gives interesting results. We have calculated the thermodynamic quantities such as the total number of particles, internal energy, heat capacity at constant volume and constant pressure, adiabatic and isothermal compressibility by using Toms and Kirsten's method and seen the boundary effects on these quantities. Also the consistency of the quantities in 3 dimensions at bulk level was checked. We have reached the interesting result that the heat capacity at constant volume is discontinuous at sufficiently high dimensions and this discontinuity basically comes from the temperature derivative of the chemical potential. This result inspired us to study further on the derivative of the chemical potential since the discontinuity on the heat capacity is not expected. In addition, we have generalized our results to an s^{th} order elliptic differential operator and saw that we can have an explicit form of partition function only for the even s values.

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