FINITE SIZE EFFECTS ON THE BOSE-EINSTEIN CONDENSATION

by

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ABSTRACT

FINITE SIZE EFFECTS ON THE BOSE-EINSTEIN CONDENSATION

In this thesis, the finite size effects for the Bose-Einstein condensation are investigated. The application of the Poisson summation method on the ideal Bose gas (both for relativistic and non-relativistic cases) is studied. The Bose gas is assumed to be enclosed in a cubical finite enclosure with periodic boundary conditions. The Bogoliubov theory for the weakly interacting Bose gas is reviewed and an expression for the ground state energy in terms of the heat kernel is obtained. We observed that a well known result of the ground state energy is obtainable via an alternative method. Then for the zero temperature case, the depletion of the condensate is treated with the heat kernel analysis combined with the Poisson summation method. The results show that for such configuration, finite size corrections turn out to be of order $1/L^2$. Finally, for the zero temperature case, the ground state energy is analysed by scaling the heat kernel. This yields finite size corrections of order $1/L$, a result which shows the necessity of a more elaborate treatment for more accurate results.

ÖZET

SONLU HACMİN BOSE-EINSTEIN YOĞUŞMASINDAKİ ETKİSİ

Bu tezde, Bose-Einstein yoğuşmasının sonlu hacimli bir sistemde gerçekleşmesi halinde sonlu hacmin yoğuşma üzerindeki etkilerinin neler olacağı konu alınmıştır. Poisson toplama yöntemi uygulanarak ideal Bose gazları (rölativistik ve rölativistik olmayan durumlarda) incelenmiştir. Söz konusu Bose gazı kübik şekilli sonlu bir hacim içerisinde ve periyodik sınır şartları altında olacak şekilde varsayılmıştır. Seyreltik gazlar için Bogoliubov teorisi tekrar edilmiş ve zemin hal enerjisi ifadesi ısı çekirdeği yöntemleri ile elde edilmiştir. Bilinen bir zemin enerjisi ifadesinin alternatif bir yöntem ile elde edilebileceği gösterilmiştir. Mutlak sıfır sıcaklığında, yoğuşuğun tükenimi Poisson toplama yöntemi ve ısı çekirdeği yöntemleri birlikte kullanılarak elde edilmiştir. Bunun sonucunda sonlu hacmin etkisini ifade eden terimlerin büyüklüklerinin $1/L^2$ seviyesinde olduğu gösterilmiştir. Son olarak da sıfır derece için zemin enerjisi ısı çekirdeğinin yeniden ölçeklendirilmesi ile tahmin edilmeye çalışılmış, sonucunda elde edilen büyüklüklerin ise $1/L$ seviyesinde olduğu gösterilmiştir.

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LIST OF SYMBOLS

$\hbar$	Reduced Planck constant
$\hat{H}$	Hamiltonian operator
k	Boltzmann constant
n	Particle number density
Tr	Trace
z	Fugacity
β	Temperature parameter
λ	Thermal wavelength
μ	Chemical potential
ρ	Single particle state
ρ_s	Scattering length
Ω_{gc}	Grand canonical potential

1. INTRODUCTION

Since its theoretical prediction nearly a century ago, Bose Einstein condensation has never ceased to be an attraction for physicists and has gradually grown in importance for understanding other major phenomena such as superfluidity, superconductivity, and so much more. Being the simplest amongst phenomena that display macroscopically observable quantum effects, Bose Einstein condensation is usually our best chance to have an understanding of the dynamics behind the other phenomena as well.

Study of the idealized Bose gas in the thermodynamic limit is the first step in understanding the dynamics behind the related phenomena; yet, more realistic cases require the volume to be finite or the gas molecules to be interacting, or both. The next simplest configuration to consider would be a non interacting system, not in the thermodynamic limit but a system constrained within a finite volume. This is a simple and unrealistic model, yet worth to be analysed: there is no *a priori* reason for the finite geometry effects to be absent for the configuration in question. More importantly, the results are even of more importance since the deviations from the bulk results will then be purely due to the finite size. For such a case, the conversion of the sum over states into an integral (plus its corrections), brings along additional approximations which may yield serious inaccuries in finite systems, especially macroscopically small systems.

A more accurate and elegant method for the same problem was proposed by Pathria for the specific case of cuboidal enclosures [1-6]. The motivation behind such a geometry constraint and the advantages of the choice of this method will become clear while proceeding with the method. By the Poisson summation technique, Pathria's work ingeniously interprets the phenomenon of Bose Einstein condensation as a 'gradual collapse of the lattice points of a thermogeometric space onto its origin as the temperature of the system is lowered' [2]. The idea of applying the Poisson summation method to these questions is inspired by a technique previously used by Krueger [9]

while investigating long range order in a partially finite geometry. Throughout the thesis, we will also be referring to the conventional approach for the Bose Einstein condensation, which can be found in many statistical physics coursebooks [1,7,8]. We will be mainly following the work of Pathria (both for nonrelativistic and relativistic cases) where he applied the Poisson summation method to the ideal Bose gas systems to get the finite size effects.

We will try to apply the same method to the weakly interacting Bose gas, with the help of another work [10] that uses the heat kernel techniques to study the weakly interacting bose gas on manifolds; this is an interesting problem since finite size effects have never been considered previously. The heat kernel approach allows one to get a first order glimpse of this correction. In this thesis, we will only study the corrections to ground state energy and the depletion at $T = 0^{\circ}K$. We hope to extend these methods to the finite temperature case.

2. FREE IDEAL BOSE GAS CASE

2.1. Introduction to the Poisson Summation Method

For the conventional study of the ideal bose gas in the thermodynamic limit as $T \to 0$, a separate treatment of the ground state from the excited states is required. This basic treatment contains an approximation: After the extraction of the condensate term ($\epsilon = 0$), sum over the discrete excited states is approximated by an integral ranging from $\epsilon = 0$ to $\epsilon = \infty$. The fact that the ground state is included within the integral despite being noted down separately does not matter; the contribution of the $\epsilon = 0$ term is insignificant within the integral.

Normally, trying to extend the calculations to finite systems brings along additional approximations that yield serious inaccuracies. Poisson summation technique proposes a more natural and consistent approach for calculating finite size effects in cuboidal geometries. It evaluates the sum as it is, without referring to approximations like the one mentioned above. At the exact stage where the necessity of approximating the sums by integrals arises, one can make use of the Poisson summation.

No constraints except periodic boundary conditions will be imposed. All of the following derivations will be valid for arbitrary N, though N is always large for practical reasons.

For a closed system of dimensions $L \times L \times L$ and of periodic boundary conditions, the single particle energy eigenvalues are:

$$\epsilon = \frac{h^2}{2mL^2}(n_1^2 + n_2^2 + n_3^2), \quad where\ n_i = \pm 1, \pm 2, ... \tag{2.1}$$

The total number of particles is the sum of the occupation number over all states:

$$N = \sum_{\varepsilon} \frac{1}{e^{\beta(\epsilon-\mu)} - 1} \tag{2.2}$$

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

$$N = \sum_{\varepsilon} \frac{1}{e^{(\alpha+\beta\varepsilon)} - 1} = \sum_{\varepsilon} \frac{1}{e^{(\alpha+\beta\varepsilon)}(1 - e^{-(\alpha+\beta\epsilon)})} \tag{2.3}$$

The geometric sum

$$\sum_{k=0}^{\infty} t^k = \frac{1}{1-t} = 1 + t + t^2 + t^3 + ... \ for \mid t \mid < 1 \tag{2.4}$$

seems to be applicable here, but we need to check whether $e^{-(\alpha+\beta\epsilon)} < 1$ is always satisfied or not. It is indeed satisfied, for it is compulsory to have $e^{(\alpha+\beta\epsilon)} \geq 1$ for a nonnegative particle number density. Changing the lower limit of the sum from $j = 0$ to $j = 1$, we get

$$N = \sum_{\varepsilon} e^{-(\alpha+\beta\epsilon)} \sum_{j=1}^{\infty} e^{-(\alpha+\beta\epsilon)(j-1)} = \sum_{\varepsilon} \sum_{j=1}^{\infty} e^{-j(\alpha+\beta\epsilon)} \tag{2.5}$$

Replacing the energy eigenvalues into the expression,

$$N = \sum_{\varepsilon} \sum_{j=1}^{\infty} e^{-j\alpha} e^{-j\frac{\beta h^2}{2mL^2}(n_1^2+n_2^2+n_3^2)} \tag{2.6}$$

while defining $w \equiv \frac{\beta h^2}{2mL^2} = \pi \left(\frac{\lambda}{L}\right)^2$ and $\lambda = \frac{h}{\sqrt{2\pi mkT}}$ with λ being the thermal wavelength, we can write

$$N = \sum_{j=1}^{\infty} e^{-j\alpha} \sum_{n_1,n_2,n_3} e^{-jw(n_1^2+n_2^2+n_3^2)} = \sum_{j=1}^{\infty} e^{-j\alpha} \left[\sum_{n_1} e^{-jwn_1^2} \sum_{n_2} e^{-jwn_2^2} \sum_{n_3} e^{-jwn_3^2} \right] \tag{2.7}$$

Conventionally one would approximate the sum over ϵ (or equally over n) with an integral, using an appropriate density of states. But instead we kept the sum as it is.

To evaluate it, we will now make use of the Poisson summation formula:

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{q=-\infty}^{\infty} F(q) \tag{2.8}$$

where

$$F(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{i2\pi kx} dx \tag{2.9}$$

is the Fourier transform of $f(n)$ which is an integrable function on the interval $[0, 2\pi]$. Replacing (2.9) into (2.8) we get,

$$\sum_{q=-\infty}^{\infty} F(k) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) e^{i2\pi kx} dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) \sum_{k=-\infty}^{\infty} e^{i2\pi kx} dx \tag{2.10}$$

Before moving on, we should emphasize a few points about the delta function: The delta function expression

$$\delta(x) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} e^{ikx} \tag{2.11}$$

takes the following form in (2.12) after the variable change $x \to 2\pi x'$:

$$\delta(2\pi x') = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} e^{2\pi ikx'} \tag{2.12}$$

At the same time, by means of the well known identity,

$$\delta(cx') = \frac{1}{\mid c \mid} \delta(x') \tag{2.13}$$

we note

$$\delta(2\pi x') = \frac{1}{2\pi} \delta(x') \tag{2.14}$$

of which we will make use to write:

$$\delta(x') = \sum_{k=-\infty}^{\infty} e^{ikx} = \sum_{n=-\infty}^{\infty} \delta(x' - n) \tag{2.15}$$

Basing ourselves on those properties of the delta function, we see that the Poisson summation formula appears almost naturally:

$$\int_{-\infty}^{\infty} f(x) \sum_{n=-\infty}^{\infty} \delta(x - n)dx = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x)\delta(x - n)dx = \sum_{n=-\infty}^{\infty} f(n) \tag{2.16}$$

2.2. Application of the Poisson Summation Method to the Non-relativistic Ideal Bose Gas (in a Finite Cubical Enclosure)

Looking back at the expression

$$N = \sum_{j=1}^{\infty} e^{-j\alpha} \sum_{n=-\infty}^{\infty} e^{-jwn^2} \tag{2.17}$$

we remark that the sum over n is a very suitable expression on which the Poisson summation can be applied to, having e^{-jwn^2} for $f(n)$.

At this point, we notice something: In reality we did not have anything special for the box geometry at the beginning. But it turns out that, it is this specific distribution of energy eigenvalues that encourages and permits us to apply the Poisson summation. For this reason, the application of the Poisson summation method is limited to cuboidal geometries and periodic boundary conditions. Applying the Poisson summation onto

the n-sum in (2.17), we get

$$\begin{aligned}
\sum_{n=-\infty}^{\infty} e^{-jwn^2} &= \sum_{q=-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-jwx^2} e^{2\pi iqx} dx \\
&= \sum_{q=-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-jw(x^2 - \frac{\pi iq}{jw})^2} dx \\
&= \sum_{q=-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-jw(x - \frac{\pi iq}{jw})^2} e^{-\frac{\pi^2 q^2}{jw}} dx \\
&= \sum_{q=-\infty}^{\infty} e^{-\frac{\pi^2 q^2}{jw}} \int_{-\infty}^{\infty} e^{-jw(x - \frac{\pi iq}{jw})^2} dx \\
&= \sqrt{\frac{\pi}{jw}} \sum_{q=-\infty}^{\infty} e^{-\frac{\pi^2 q^2}{jw}}
\end{aligned} \tag{2.18}$$

So (2.17) becomes:

$$= \sum_{j=1}^{\infty} e^{-j\alpha} \sum_{q_1=-\infty}^{\infty} \sqrt{\frac{\pi}{jw}} e^{-\frac{\pi^2 q_1^2}{jw}} \sum_{q_2=-\infty}^{\infty} \sqrt{\frac{\pi}{jw}} e^{-\frac{\pi^2 q_2^2}{jw}} \sum_{q_3=-\infty}^{\infty} \sqrt{\frac{\pi}{jw}} e^{-\frac{\pi^2 q_3^2}{jw}} \tag{2.19}$$

It is important to note that till here no information loss has occurred; every identity that has been used is exact.

It is a good idea to compare (2.19) to 'the conventional result' to figure out what we ended up with. But while going over the regular method, we might want to modify one step slightly: Instead of recognizing the Bose-Einstein functions and switching to the $g_\nu(z)$ notation, it will be more advantegous to leave them in their sum form. This will make it easier to compare their similarity to (2.19). So proceeding accordingly, at the end of the conventional approach, what we obtain for the ideal bose in the thermodynamic limit is

$$N_{bulk} = \sum_{j=1}^{\infty} e^{-j\alpha} L^3 \left[\frac{2\pi m}{(j\beta)h^2}\right]^{\frac{3}{2}} \tag{2.20}$$

Putting this N_{bulk} result aside and expanding the sum in (2.19), we find that

$$\begin{aligned} N &= \sum_{j=1}^{\infty} e^{-j\alpha} \left(\frac{\pi}{jw}\right)^{\frac{3}{2}} \prod_{i=1}^{3} \sum_{q_i} e^{-\frac{\pi^2(q_i^2)}{jw}} \\ &= \left(\frac{\pi}{w}\right)^{\frac{3}{2}} \sum_{\mathbf{q}} \sum_{j=1}^{\infty} \frac{e^{-j\alpha}}{j^{\frac{3}{2}}} e^{-\frac{\pi^2(q_1^2+q_2^2+q_3^2)}{jw}} \\ &= \frac{L^3}{\lambda^3} \sum_{\mathbf{q}} \sum_{j=1}^{\infty} \frac{e^{-j\alpha}}{j^{\frac{3}{2}}} e^{-\frac{\pi^2(q_1^2+q_2^2+q_3^2)}{jw}} \end{aligned} \tag{2.21}$$

where $\mathbf{q}$ is defined to be a vector of the magnitude $\sqrt{q_1^2+q_2^2+q_3^2}$ in the q-space. Separating the $\mathbf{q}=0$ from the rest, it turns out that

$$N = \frac{L^3}{\lambda^3} \sum_{j=1}^{\infty} \frac{e^{-j\alpha}}{j^{\frac{3}{2}}} + \frac{L^3}{\lambda^3} \sum_{j=1}^{\infty} {\sum_{\mathbf{q}}}' \frac{e^{-j\alpha}}{j^{\frac{3}{2}}} e^{-\frac{\pi^2(q_1^2+q_2^2+q_3^2)}{jw}} \tag{2.22}$$

where the primed sum stands for the sum excluding the $\mathbf{q}=0$ term. The first term in (2.22) is exactly the same expression as the N_{bulk} in (2.20), which is obtained by approximating the integral. We can identify the first part of (2.22) to correspond to the 'bulk term' in the condensation of the ideal bose gas. Then naturally, the following question would arise: What is the meaning of the following terms for which $\mathbf{q} \neq 0$? Obviously, they had been eliminated in the calculations for the thermodynamic limit. The physical meaning of those terms becomes obvious when one investigates their behaviour in the thermodynamic limit:

$$\frac{L^3}{\lambda^3} \sum_{j=1}^{\infty} {\sum_{\mathbf{q}}}' \frac{e^{-j\alpha}}{j^{\frac{3}{2}}} e^{\frac{-\pi L^2(q_1^2+q_2^2+q_3^2)}{j\lambda^2}} \tag{2.23}$$

is expected to become negligible compared to the bulk term as $L \to \infty$. Knowing that (2.22) is an exact expression while (2.20) is not, and observing the behaviour of (2.23), we come to the following conclusion: The second part of (2.22) contains both the condensate and the finite size effects. It brings along some sort of correction to the bulk result that considers the states to be continuous; corrections due to the -in reality- discreteness of the single particle states. And the discreteness of the states originate from the finite dimensionality of the enclosure; so any correction due to the discreteness

of the states is automatically a correction due to the finiteness of the system.

Once again, we can make a comparison between the Poisson summation technique and the conventional method: In the latter one, the only correction to the bulk result was the 'manual' addition of the ground state expression (or from another perspective, the separation of the ground state from the rest.) This way one could compensate for the fact as $T \to 0°K$, the $\epsilon = 0$ state was insignificant within the integral, whereas it had finite contribution in the N term in reality. The point that we should not miss here is the following: The insertion of the ground state into the total expression of N, while practically giving the correct results, is far from being the whole correction coming from the discrete nature of the energy states. On the other hand, the correction term that appears in the Poisson summation method is a global correction to the discreteness of states, with its infinite number of terms. In contrast to remarking a discrepancy and manually separating the ground state, here that separation is natural. To sum this idea up, we say that 'the part other than the bulk term' in (2.22) is 'the part that counts for the finite size effects of the system'.

Putting the bulk term aside, the finite size terms will be of interest to us from now on. The term containing the finite effects is:

$$\frac{L^3}{\lambda^3} \sum_{j=1}^{\infty} {\sum_{\mathbf{q}}}' \frac{e^{-j\alpha}}{j^{\frac{3}{2}}} e^{-\frac{\pi^2(q_1^2+q_2^2+q_3^2)}{jw}} \tag{2.24}$$

To proceed further with the j-sum, we need to make use of another identity related to the Poisson summation (For derivation, see [11].) It is:

$$\frac{1}{2}(f(a)+f(b)) + \sum_{n=a+1}^{b-1} f(n) = \lim_{L\to\infty} \sum_{|l|\leq L} \int_a^b f(t) e^{2\pi i l t} dt \tag{2.25}$$

Modifying the limits of the sum as $\sum_{n=a}^{b} f(n)$, and changing the variable from n to j we

acquire the identity

$$\sum_{j=a}^{b} f(j) = \frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{l=-\infty}^{\infty} \int_{a}^{b} f(t)e^{2\pi ilt}dt \tag{2.26}$$

which is applicable to our case.

To evaluate (2.24), (2.26) seems to be a convenient tool having

$$\frac{e^{-j\alpha}}{j^{\frac{3}{2}}} e^{\frac{-\pi^2(q_1^2+q_2^2+q_3^2)}{jw}} = f(j) \tag{2.27}$$

Yet the limits of the integration should be well selected, for the identity (2.26) also requires the information of $f(a)$ and $f(b)$. Thanks to the exponential, we are lucky enough to spot the limiting behaviours of (2.27) for the following cases:

$$\lim_{j\to 0} \frac{e^{-j\alpha}}{j^{\frac{3}{2}}} e^{\frac{-\pi^2(q_1^2+q_2^2+q_3^2)}{jw}} = 0 \tag{2.28}$$

and

$$\lim_{j\to \infty} \frac{e^{-j\alpha}}{j^{\frac{3}{2}}} e^{\frac{-\pi^2(q_1^2+q_2^2+q_3^2)}{jw}} = 0 \tag{2.29}$$

So with such choice of limits, $f(a)$ and $f(b)$ terms will be eliminated in (2.26). The next concern is that the summation in (2.24) starts from $j = 1$, not from $j = 0$ as required by (2.26) after setting a to be 0. But in (2.28) we saw that $j = 0$ term has no contribution, hence can be added to the summation, modifying the range of (2.24) to be from $j = 0$ to ∞. After this small trick, the identity (2.26) becomes perfectly applicable to (2.24). We should note that all these tricks have become possible only after the Poisson summation was applied, mainly because $-1/j$ was introduced as the power of the exponential after the Fourier transformation. This converts a slowly convergent sum into a rapidly convergent one.

Now we define

$$\gamma(\mathbf{q}) = \frac{\pi^2(q_1^2 + q_2^2 + q_3^2)}{w} = \frac{\pi q^2 L^2}{\lambda^2} \tag{2.30}$$

which clearly has a nonnegative value.

Using the identity (2.26), we can write:

$$\sum_{j=0}^{\infty} j^{-3/2} e^{-j\alpha} e^{-\gamma(\mathbf{q})j} = 0 + 0 + \sum_{l=-\infty}^{\infty} \int_0^{\infty} \frac{e^{-x\alpha}}{x^{3/2}} e^{-\gamma/x} e^{2\pi i l x} dx \tag{2.31}$$

This integral on the right hand side of (2.31) turns out to be an modified Bessel function of second kind with the form [12]:

$$K_\nu(z) = \frac{z^\nu}{2^{\nu+1}} \int_0^{\infty} e^{-t - \frac{z^2}{4t}} t^{-\nu-1} dt \tag{2.32}$$

Now that we have the following integral,

$$\int_0^{\infty} \frac{e^{-x(\alpha - 2\pi i l)} e^{-\gamma/x}}{x^{3/2}} dx \tag{2.33}$$

performing the variable change $x' = x(\alpha - 2\pi i l)$ gives us:

$$\int_0^{\infty} \frac{e^{-x(\alpha-2\pi i l)} e^{-\gamma/x}}{x^{3/2}} dx = (\alpha - 2\pi i l)^{1/2} \int_0^{\infty} \frac{e^{-x'} e^{-\frac{\gamma(\alpha-2\pi i l)}{x'}}}{(x')^{3/2}} dx' = (\alpha - 2\pi i l)^{1/2} \frac{K_{1/2}(z)\, 2^{\nu+1}}{z^\nu} \tag{2.34}$$

having $z = 2\gamma^2(\alpha - 2\pi i l)^{1/2}$ and with

$$K_{1/2}(z) = \sqrt{\frac{\pi}{2}} \frac{e^{-z}}{\sqrt{z}} \tag{2.35}$$

So the sum in (2.24) consecutively gets the form:

$$\begin{aligned}\sum_{j=1}^{\infty}\sum_{\mathbf{q}}{}' \frac{e^{-j\alpha}}{j^{\frac{3}{2}}} e^{\frac{-\pi^2(q_1^2+q_2^2+q_3^2)}{jw}} &= \sum_{q}{}' \sum_{j=0}^{\infty} j^{-3/2} e^{-j\alpha} e^{-\gamma(\mathbf{q})j} \\ &= \sum_{q}{}' \sum_{l=-\infty}^{\infty} \sqrt{\frac{\pi}{\gamma}} e^{-2\sqrt{\gamma}(\alpha-2\pi i l)^{1/2}} \\ &= \sum_{q}{}' \sqrt{\frac{\pi}{\gamma}} \sum_{l=-\infty}^{\infty} e^{-2\sqrt{\gamma\alpha}(1-\frac{2\pi i l}{\alpha})^{1/2}} \end{aligned} \tag{2.36}$$

And we get:

$$N = \frac{L^3}{\lambda^3}\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j^{\frac{3}{2}}} + \sum_{q}{}' \sum_{l=-\infty}^{\infty} \sqrt{\frac{\pi}{\gamma}} e^{-2\sqrt{\gamma}(\alpha-2\pi i l)^{1/2}} \tag{2.37}$$

At this stage, we will be doing an approximation for a first time. The l-sum in (2.36) is dominated by the $l = 0$ term for any value of α. A detailed derivation of this argument is made in Appendix A: All other terms having nonzero l are at most of order $e^{-L/\lambda}$, as can be seen from (A.48).

Omitting the $l \neq 0$ terms in (2.36), we get an approximate expression for N:

$$N \approx \frac{L^3}{\lambda^3}\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j^{\frac{3}{2}}} + \frac{L^3}{\lambda^3}\sum_{\mathbf{q}}{}' \sqrt{\frac{\pi}{\gamma}} e^{-2\sqrt{\gamma(\mathbf{q})}\alpha^{1/2}} = \frac{L^3}{\lambda^3} g_{3/2}(e^{-\alpha}) + \frac{L^3}{\lambda^3}\sum_{\mathbf{q}}{}' \frac{\lambda}{Lq} e^{-2\sqrt{\pi}\frac{Lq}{\lambda}\alpha^{1/2}} \tag{2.38}$$

While observing the above expression carefully, the exponential in (2.38) might call to one's attention. From (A.57) and (A.62), we know that the correlation length is defined to be

$$\xi = \frac{\lambda}{2\pi^{1/2}\alpha^{1/2}} \tag{2.39}$$

and often run into in the form of $e^{-R/\xi}$ within various expressions. Recognizing that,

$$e^{-2\sqrt{\pi}\frac{Lq}{\lambda}\alpha^{1/2}} = e^{-R/\xi} \tag{2.40}$$

with $R \equiv Lq$, we reorganize the expression within the q'-sum in (2.38) as

$$\frac{\lambda}{Lq} e^{-2\sqrt{\pi}\frac{Lq}{\lambda}\alpha^{1/2}} = \lambda \frac{e^{-R/\xi}}{R} \tag{2.41}$$

Defining

$$M(\mathbf{q}) \equiv R/2\xi = Lq/2\xi = (L\sqrt{q_1^2 + q_2^2 + q_3^2})/2\xi \tag{2.42}$$

(2.41) becomes

$$\lambda \frac{e^{-R/\xi}}{R} = \frac{\lambda}{2\xi} \frac{e^{-2M(\mathbf{q})}}{M(\mathbf{q})} = \sqrt{\pi}\sqrt{\alpha} \frac{e^{-2M(\mathbf{q})}}{M(\mathbf{q})} \tag{2.43}$$

We then define a new parameter y that is the dimension (L) of the system in units of its correlation length:

$$y = \frac{L}{2\xi} = \pi^{1/2}\alpha^{1/2}\frac{L}{\lambda} \text{ and } S(y) = \sum_q{}' \frac{e^{-2M(\mathbf{q})}}{M(\mathbf{q})} \tag{2.44}$$

Thus, we can write

$$N \approx \frac{L^3}{\lambda^3} \left[g_{3/2}(e^{-\alpha}) + \pi^{1/2}\alpha^{1/2} S(y) \right] \tag{2.45}$$

Here, we take a step back and look at the meaning and the behaviour of the parameter y: we said that it is the dimension (L) of the system in units of its correlation length. Approaching to the critical temperature from above, the correlation length behaves as in (A.61)

$$\xi \sim \lambda \left(\frac{T_{cr}}{T - T_{cr}} \right)^{1/(d-2)} \tag{2.46}$$

and suddenly reaches to very large values. This causes y to decrease to very small

values from very large values within a small temperature range. Since our region of interest is the region around the transition point (while approaching to it from above) and obviously $y \to 0$ within this region, we can use this fact to check our method roughly and see whether the Poisson summation method yields to a meaningful result or not. Within the region mentioned above, it is legitimate to replace the q-sum in $S(y)$ with an integral over y. This gives,

$$N \approx \frac{L^3}{\lambda^3}\left[g_{3/2}(e^{-\alpha}) + \pi^{1/2}\alpha^{1/2}\left(\frac{\pi}{y^3}\right)\right] = \frac{L^3}{\lambda^3}g_{3/2}(e^{-\alpha}) + \frac{1}{\alpha} \tag{2.47}$$

Although there is a considerable error coming from the replacement of the sum by an integral, even this rough result has what the Poisson summation had aimed for: It includes the condensate behaviour by itself. After seeing this step, one should not be confused by thinking that the Poisson summation also did what it was trying to avoid: 'approximating a sum by an integral'. In (2.47), it has been done to get an idea about the final result and till that step we have never referred to an approximation of that sort. But in the conventional method it plays part in an initial and essential step where it effects all the rest of the calculations. To see why (2.47) already carries the condensate behaviour, we will investigate the large and small temperature limits respectively. First looking for the large α values which correspond to the high temperature limit, we see that the second term is negligible compared to the first one. We are left with the usual bulk result, which is the correct expression of N for the high temperatures. But apart from the regular bulk result, it is this second term that makes it possible to observe the condensate behaviour; at least qualitatively. The behaviour of α around the critical point is a subtle thing to study; but from

$$n_0 = \frac{1}{e^{\alpha} - 1} \tag{2.48}$$

it can be seen that to obtain a 'large' value of n_0, one must have $\alpha << 1$. As $\alpha << 1$, the last term of (2.47) becomes considerable and dominates the bulk term more and more as $\alpha \to 0$. So instead of being implemented into the N expression manually, the condensate term appeared by itself while proceeding with this method. While far

from being precise, the N expression in (2.47) made sure that the Poisson summation method yields to the natural appereance of the condensate term. It is now time to evaluate the $S(y)$ sum up to a higher degree of accuracy: A method for evaluating the sums of the form $S(y) = \sum_{q}{}' \frac{e^{-2M(\mathbf{q})}}{M(\mathbf{q})}$ is developped by Chaba and Pathria [6]. The method is valid for a much broader group of lattice sums and (of arbitrary dimensions). They are of importance not only for the Bose-Einstein condensation, but also for the study of many other concepts such as electronic structure of crystalline solids, rotating superfluid He, type-II superconductors [13,14]. Taking the Poisson summation formula, sums on both sides can be labeled with the same indice as it does not effect the result: For any non negative a, we can write:

$$\sum_{q=-\infty}^{\infty} e^{-aq^2} = \left(\frac{\pi}{a}\right)^{1/2} \sum_{q=-\infty}^{\infty} e^{-\pi^2 q^2/a} \tag{2.49}$$

Generalizing this to m dimensions,

$$\sum_{q_1,q_2,...,q_m} e^{-a(q_1^2+q^2+...+q_m^2)} = \left(\frac{\pi}{a}\right)^{m/2} \sum_{q_1,q_2,...,q_m} e^{-\frac{\pi(q_1^2+q^2+...+q_m^2)}{a}} \tag{2.50}$$

Noting $R_m^2 = q_1^2 + q_2^2 + ... + q_m^2$ and separating the $\mathbf{R}_m = 0$ term, we have:

$$\sum_{\mathbf{R}_m}{}' \left[e^{-aR^2} - \left(\frac{\pi}{a}\right)^{m/2} e^{-\pi^2 R^2/a}\right] = \left(\frac{\pi}{a}\right)^{m/2} - 1 \tag{2.51}$$

Integrating (2.51) with respect to a, we obtain:

$$\begin{aligned} &= \sum_{\mathbf{R}_m}{}' \left[\frac{1}{R^2} e^{-aR^2} + \frac{\pi^{m/2}}{a^{(m-2)/2}} \int_1^{\infty} e^{-\frac{\pi^2 R^2}{a} t} t^{\frac{m-4}{2}} dt\right] \\ &= \begin{cases} \frac{2}{m-2}\pi^{m/2} a^{(2-m)/2} + a + C_m \ \ (\text{for } m \neq 2) \\ -\pi ln a + a + C_2 \ \ (\text{for } m = 2) \end{cases} \end{aligned} \tag{2.52}$$

Expressing the integral above in terms of the incomplete gamma function, which can

be expressed as: $\Gamma(s,x) = \int_x^\infty e^{-t}t^{s-1}dt$

$$\int_1^\infty e^{-\frac{\pi^2R^2}{a}t}t^{\frac{m-4}{2}} = \left(\frac{a}{\pi^2R^2}\right)^{(m-2)/2}\Gamma\left(\frac{m}{2}-1,\frac{\pi^2R^2}{a}\right) \tag{2.53}$$

Since we worked with three dimensions all the way along, $m = 3$. So we now have [6]

$$\sum_{\mathbf{R}_3}{}' \left[\frac{1}{R^2}e^{-aR^2} + \frac{\pi^{1/2}}{R}\Gamma\left(\frac{1}{2},\frac{\pi^2R^2}{a}\right)\right] = 2\frac{\pi^{3/2}}{a^{1/2}} + a + C_3 \tag{2.54}$$

Having this result at hand,

$$S(y) = \sum_{\mathbf{q}}{}' \frac{e^{-2M(\mathbf{q})}}{M(\mathbf{q})} = \frac{1}{y}\sum_{\mathbf{q}}{}' \frac{e^{-2yq}}{q} \tag{2.55}$$

sum can now be evaluated as

$$\sum_{\mathbf{R}_3}{}' \frac{1}{R^2}e^{-aR^2} \tag{2.56}$$

with $R^2 = q$ and $a = 2y$. The $S(y)$ sum is just ready to be extracted from (2.54), yet we still need an expression for the constant C_3. For that, we recall the fact that the region of interest is $y \to 0$ and hence $a \to 0$; this resulting in a zero contribution from the term containing the incomplete gamma function:

$$C_3 = \lim_{a\to 0}\left(\sum_{\mathbf{R}_3}{}' \frac{1}{R^2}e^{(-aR^2)} - \frac{2\pi^{3/2}}{a^{1/2}}\right) \tag{2.57}$$

C_3 evaluated for an acceptable value of a (not necessarily too small) is given in [6] as $C_3 = -8.913633$. Even if not directly related to our work, this constant has further importance: The behaviour of (2.54) is known to be relevant to the Madelung sums for small a values. These sums show up in the study of electronic structure of crystalline solids and C_3 has a direct relation to the Madelung constant of a simple cubic lattice

[14]. We can rewrite (2.54) to be:

$$\sum_{\mathbf{R}_3}{}' \frac{1}{R^2} e^{-aR^2} = \frac{2\pi^{3/2}}{a^{1/2}} + a + C_3 - O\left(\frac{1}{R} e^{-\pi^2 R^2/a}\right) \tag{2.58}$$

The order of the error belongs to the incomplete gamma function, and we see that it can be bounded from above by a term of the order of $e^{-\pi^2 R^2/a}$:

$$\begin{aligned}
\Gamma\left(\frac{1}{2}, \frac{\pi^2 R^2}{a}\right) &= \int_{\frac{\pi^2 R^2}{a}}^{\infty} e^{-t} t^{\frac{1}{2}-1} dt \\
&= \int_{\frac{\pi^2 R^2}{a}}^{\infty} e^{-\frac{t}{2}} e^{-\frac{t}{2}} t^{-\frac{1}{2}} dt \\
&\leq e^{-\frac{\pi^2 R^2}{a}} \int_{\frac{\pi^2 R^2}{a}}^{\infty} e^{-\frac{t}{2}} t^{-\frac{1}{2}}
\end{aligned} \tag{2.59}$$

All these results eventually yield to the following expression for our case [1]:

$$\sum_{\mathbf{q}}{}' \left[\frac{y^2}{q^2(y^2 + \pi^2 q^2)} + \frac{\pi}{q} e^{-2yq}\right] = 2\pi y + \frac{\pi^2}{y^2} + C_3 \tag{2.60}$$

Replacing $S(y)$ in (2.45):

$$N \approx \frac{L^3}{\lambda^3}\left[g_{3/2}(e^{-\alpha}) + \pi^{1/2}\alpha^{1/2}\frac{1}{\pi y}\left(2\pi y + \frac{\pi^2}{y^2} + C_3 - \sum_{\mathbf{q}}{}' \frac{y^2}{q^2(y^2 + \pi^2 q^2)}\right)\right] \tag{2.61}$$

Rearranging (2.61):

$$\begin{aligned}
N \approx{}& \left(\frac{L}{\lambda}\right)^3 g_{3/2}(e^{-\alpha}) + \left(\frac{L}{\lambda}\right)^2 \frac{\pi}{y^2} + \left(\frac{L}{\lambda}\right)^2 \frac{C_3}{\pi} + \left(\frac{L}{\lambda}\right)^2 2y \\
&- \left(\frac{L}{\lambda}\right)^2 \frac{y^2}{\pi} \sum_{\mathbf{q}}{}' \frac{y^2}{q^2(y^2 + \pi^2 q^2)}
\end{aligned} \tag{2.62}$$

It is seen that the second term on the right hand side is

$$\left(\frac{L}{\lambda}\right)^2 \frac{\pi}{y^2} = \frac{1}{\alpha} \tag{2.63}$$

Recalling that the fugacity z (z=$e^{\mu\beta}$) is

$$z = \frac{N_0}{N_0 + 1} \simeq 1 - \frac{1}{N_0} \tag{2.64}$$

and for $\alpha << 1$, we have

$$\alpha = -\ln z \approx \frac{1}{N_0} \tag{2.65}$$

We have a striking fact here: Taking a look at (2.62), we see that the second term is N_0. This means that the particle number of the ground state (the condensate term) has showed up in the expression by itself, with no intervention at all.

To simplify (2.62) further, we can make use of one more approximation. The Bose-Einstein function for $\nu < 1$ is [15]:

$$g_\nu(e^{-\alpha}) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1} dx}{e^{\alpha+x} - 1} \tag{2.66}$$

and for $\alpha \to 0$,

$$g_\nu(e^{-\alpha}) \approx \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1} dx}{\alpha + x} \tag{2.67}$$

Replacing $x = \alpha \tan^2\theta$ and recalling that the beta function was

$$B(\mu, \nu) = 2 \int_0^\infty \cos^{2\mu-1}\theta \sin^{2\nu-1}\theta d\theta = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu+\nu)} \text{ for } \mu, \nu > 0 \tag{2.68}$$

we see that

$$g_\nu(e^{-\alpha}) \approx \frac{\Gamma(1-\nu)}{\alpha^{1-\nu}} \text{ for } (0 < \nu < 1) \tag{2.69}$$

But the function we need has $\nu = 3/2$. Using the recurrence relation:

$$\frac{\partial}{\partial\alpha} g_\nu(e^{-\alpha}) = -g_{\nu-1}(e^{-\alpha}) \tag{2.70}$$

$$\frac{\partial g_{3/2}(e^{-\alpha})}{\partial\alpha} = -g_{1/2}(e^{-\alpha}) = -\frac{\Gamma(1/2)}{\alpha^{1/2}} = -\frac{\pi^{1/2}}{\alpha^{1/2}} \tag{2.71}$$

We end up with:

$$g_{3/2}(e^{-\alpha}) = -\int \pi^{1/2}\alpha^{-1/2} d\alpha = -2\pi^{1/2}\alpha^{1/2} + constant \tag{2.72}$$

Knowing that for $\alpha \to 0$, $g_{3/2}(e^{-\alpha}) \to g_{3/2}(1) = \zeta(3/2)$, it's clear that the constant is $\zeta(3/2)$. Then,

$$g_{3/2}(e^{-\alpha}) \approx -2\pi^{1/2}\alpha^{1/2} + \zeta(3/2) \tag{2.73}$$

With this result replaced into (2.62), we get:

$$\begin{aligned} N \approx \left(\frac{L}{\lambda}\right)^3 \zeta(3/2) - \left(\frac{L}{\lambda}\right)^3 2\pi^{1/2}\alpha^{1/2} + N_o + \left(\frac{L}{\lambda}\right)^2 \frac{C_3}{\pi} + \left(\frac{L}{\lambda}\right)^2 2y \\ - \left(\frac{L}{\lambda}\right)^2 \frac{y^2}{\pi} \sum_{\mathbf{q}}{}' \frac{1}{q^2(y^2 + \pi^2 q^2)} \end{aligned} \tag{2.74}$$

Second and fourth terms on the right hand side cancel out and eventually we end up with:

$$N \approx \left(\frac{L}{\lambda}\right)^3 \zeta(3/2) + N_0 + \left(\frac{L}{\lambda}\right)^2 \left[\frac{C_3}{\pi} - \frac{y^2}{\pi} \sum_{\mathbf{q}}{}' \frac{1}{q^2(y^2 + \pi^2 q^2)}\right] \tag{2.75}$$

The number of particles in the ground state is:

$$N_0 \approx N - \left(\frac{L}{\lambda}\right)^3 \zeta(3/2) - \left(\frac{L}{\lambda}\right)^2 \left[\frac{C_3}{\pi} - \frac{y^2}{\pi} \sum_{\mathbf{q}}{}' \frac{1}{q^2(y^2+\pi^2 q^2)}\right] \tag{2.76}$$

Using the expression for the critical temperature (in the thermodynamic limit, obtained by the conventional treatment)

$$T_c = T\frac{\lambda^2}{L^2}\left[\frac{N}{\zeta(3/2)}\right]^{2/3} \tag{2.77}$$

we can express the second term above in terms of N and T_c. Finally, we can say:

$$N_0 \approx N\left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right] + \left(\frac{L}{\lambda}\right)^2 \left[-\frac{C_3}{\pi} + \frac{y^2}{\pi} \sum_{\mathbf{q}}{}' \frac{1}{q^2(y^2+\pi^2 q^2)}\right] \tag{2.78}$$

Immediately recognizing the first term as the number of particles in the ground state for the bulk limit, we can easily say that the second term corresponds to the finite size effects. Thus, the finite size correction to N_0 has been obtained and can be seen to be of order $(L/\lambda)^2$, whereas the the bulk term is of $(L/\lambda)^3$. In other words, the bulk term is of order N while the correction is of order $N^{2/3}$. So in the thermodynamic limit (as $L \to \infty$), the correction term (differing from the bulk term by an order of (λ/L)) becomes negligible compared to the bulk term and the N_o expression reduces to the regular bulk result. While the transition has been smoothed out by the finiteness of the system, it can be reenforced to become a sharp one again (hence, creating singularities in thermodynamic functions) by taking the limit $V \to \infty$.

2.3. Application of the Poisson Summation Method to the Relativistic Ideal Bose Gas with Pair Production (in a Finite Cubical Enclosure)

What we have investigated in Section 2.2, we will now extend it to the ideal relativistic case. The condensation of a relativistic Bose gas is of interest for many domains, especially for cosmology and high energy. A few examples are the physics

within the core of a neutron star or of the primordial photon gas at the early epoch of the universe, pion condensation and quark confinement [16]. At the beginning, studies about the ideal relativistic Bose gas in arbitrary dimensions were carried out [17-20], but another study [21] showed that calculations concerning bosons with mass greater than zero must take the 'particle-antiparticle pair production' into account. This way, the temperature dependence of the charge density ρ changed from the previous T^3 result to T^2, thus changing the relation between the density and the critical temperature. On the other hand, another study [22] showed that the dependence of the condensation on the dimensions of the system was exactly parallel to the non-relativistic Bose gas, when particle-antiparticle pair production was taken into account. If the treatment did not include the pair production, the results drastically deviated from the non-relativistic case. These results gave Singh and Pathria enough motivation to extend the work of Zasada and Pathria and apply the Poisson summation to the ideal relativistic case [16]. We will now briefly cover this work. We will proceed by applying exactly the same steps of Section 2.2, except that we will now be considering the relativistic ideal Bose gas.

Defining the difference in the number of particles and antiparticles to be Q:

$$Q = N_1 - N_2 \tag{2.79}$$

where N_1 is the particle and N_2 is the antiparticle number. It is the difference between these two that drives the characteristics of the system, since the rest corresponds to the particle-antiparticle pairs. Q is a conserved quantity and might be considered to be some sort of 'generalized charge' for the system. In such configuration(a system with pair production) Q will undertake the role that N has in a non-relativistic system. Throughout the calculations, we will consider $k = c = \hbar = 1$ for simplicity. For the equilibrium, we can write,

$$N_1 = \sum_{\epsilon} \frac{1}{e^{\beta(\epsilon-\mu)} - 1} \tag{2.80}$$

and

$$N_2 = \sum_{\epsilon} \frac{1}{e^{\beta(\epsilon+\mu)} - 1} \tag{2.81}$$

since $\mu_1 = -\mu_2 = \mu$. By assuming that $\mu > 0$, we automatically defined $N_1 > N_2$ and hence the generalized charge to be $Q > 0$.

There has been no change with the boundary conditions or dimensions of the system. Any related convention that we will use in this section has the same meaning as in the previous one unless stated otherwise. But instead, our energy eigenvalues will be

$$\epsilon_i = (k_i^2 + m^2)^{1/2} \tag{2.82}$$

where k_i are the eigenvalues of the wave vector $\mathbf{k}$:

$$k_i = \frac{2\pi n_i}{L} \ (n_i = 0, \pm 1, \pm 2, ...) \tag{2.83}$$

We will not prefer the α notation for this section and will use $(-\beta\mu)$ instead. The presence of μ is of extreme importance for this case, because it is the only parameter that differs between a particle and an antiparticle.

By using exactly the same steps as in Section 2.2 while using the above energy eigenvalues, we get:

$$N_1 = \sum_{j=1}^{\infty} e^{j\beta\mu} \sum_{n_1,n_2,n_3} exp\left[-j\beta m\left(1 + \frac{4\pi^2(n_1^2 + n_2^2 + n_3^2)}{m^2 L^2}\right)^{1/2}\right] \tag{2.84}$$

which is the relativistic equivalent of our expression (2.7).

Applying the Poisson summation (2.8) to (2.84) we obtain:

$$N_1 = \sum_{j=1}^{\infty} e^{j\beta\mu} \sum_{\mathbf{q}} \left[\frac{L^3 m^2}{2\pi^2\beta}\right] \frac{j}{j^2 + \beta^{-2}\gamma^2(\mathbf{q})} K_2(\beta m[j^2 + \beta^{-2}\gamma^2(\mathbf{q})]^{1/2}) \tag{2.85}$$

where

$$\gamma(\mathbf{q}) = (q_1^2 + q_2^2 + q_3^2)^{1/2} L \tag{2.86}$$

Separating the $(\mathbf{q} = 0)$ term, we get:

$$N_1 = \sum_{j=1}^{\infty} e^{j\beta\mu} \left[\frac{L^3 m^2}{2\pi^2\beta}\right] \frac{1}{j} K_2(j\beta m) + \sum_{j=1}^{\infty} e^{j\beta\mu} \sum_{\mathbf{q}}{}' \left[\frac{L^3 m^2}{2\pi^2\beta}\right] \frac{j K_2(\beta m[j^2 + \beta^{-2}\gamma^2(\mathbf{q})]^{1/2})}{j^2 + \beta^{-2}\gamma^2(\mathbf{q})} \tag{2.87}$$

The first term in (2.87) is totally consistent with the expressions obtained in [10] for the relativistic ideal gas via the subordination identity. We recognize it as the bulk term:

$$N_{bulk(1)} = \left[\frac{L^3 m^2}{2\pi^2\beta}\right] \sum_{j=1}^{\infty} j^{-1} e^{j\beta\mu} K_2(j\beta m) \tag{2.88}$$

Then we can write,

$$N_1 = N_{bulk(1)} + \left[\frac{L^3 m^2}{2\pi^2\beta}\right] \sum_{\mathbf{q}}{}' \sum_{j=1}^{\infty} \frac{j e^{j\beta\mu} K_2(\beta m[j^2 + \beta^{-2}\gamma^2(\mathbf{q})]^{1/2})}{j^2 + \beta^{-2}\gamma^2(\mathbf{q})} \tag{2.89}$$

Our interest is once again not with the first(bulk) term but with the second one. The condensate expression and the finite size effects for an ideal relativistic bose gas will be unraveled due to the second term of the expression of (2.89). Focusing our attention on the second term, we use the identity (2.25) to convert the j-sum to an

l-sum. Thus we obtain:

$$\sum_{j=1}^{\infty} \frac{j e^{j\beta\mu} K_2(\beta m[j^2+\beta^{-2}\gamma^2(\mathbf{q})]^{1/2})}{j^2+\beta^{-2}\gamma^2(\mathbf{q})} = \sum_{l=-\infty}^{\infty} \int_0^{\infty} \frac{x e^{x(\beta\mu+2\pi i l)}}{x^2+\beta^{-2}\gamma^2(\mathbf{q})} K_2(\beta m[x^2+\beta^{-2}\gamma^2(\mathbf{q})]^{1/2}) dx \quad (2.90)$$

The same argument of retaining only the $l = 0$ values is equally valid here. But before continuing with that step, it will make things easier to put the expressions of (2.90) into a clearer form. From (2.32) we know that:

$$K_2(\beta m[x^2+\beta^{-2}\gamma^2(\mathbf{q})]^{1/2}) = \frac{\beta^2 m^2[x^2+\beta^{-2}\gamma^2(\mathbf{q})]}{2} \int_0^{\infty} exp\left[-\frac{1}{2}\left(t+\frac{\beta^2 m^2[x^2+\beta^{-2}\gamma^2(\mathbf{q})]}{t}\right)\right]\frac{1}{t^3}dt \quad (2.91)$$

Putting (2.91) into (2.90) and defining $\mu' \equiv \mu + \frac{2\pi i l}{\beta}$, we get

$$\sum_{l=-\infty}^{\infty} \int_0^{\infty} \frac{x e^{x(\beta\mu+2\pi i l)}}{x^2+\beta^{-2}\gamma^2(\mathbf{q})} K_2(\beta m[x^2+\beta^{-2}\gamma^2(\mathbf{q})]^{1/2}) dx) =$$
$$\frac{\beta^2 m^2}{2} \sum_{l=-\infty}^{\infty} \int_0^{\infty} exp\left[-\frac{1}{2}\left(t+\frac{m^2\gamma^2(\mathbf{q})}{t}\right)\right]\frac{1}{t^3}dt \left[\int_0^{\infty} exp\left(\beta\mu' x - \frac{\beta^2 m^2 x^2}{2t}\right) x dx\right] \quad (2.92)$$

In order to execute the integration over x, we need to make use of the parabolic cylinder function [23]:

$$D_\nu(t) = \frac{1}{\Gamma(-\nu)} e^{-\frac{t^2}{4}} \int_0^{\infty} x^{-\nu-1} e^{-\frac{x^2}{2}-tx} dx \ for\ \nu < 0 \quad (2.93)$$

For the integral in (2.92), we see that the required parabolic cylinder function is D_{-2}.

The integral then can be rewritten as:

$$\int_0^\infty \exp\left(\beta\mu' x - \frac{\beta^2 m^2 x^2}{2t}\right) x dx = \frac{t}{\beta^2 m^2} \exp\left[\frac{\mu'^2 t}{4m^2}\right] D_{-2}\left(-\frac{\mu' t^{1/2}}{m}\right) \tag{2.94}$$

Replacing this result in (2.90), we can now rewrite (2.89):

$$N_1 = N_{bulk(1)} + \left[\frac{L^3 m^2}{4\pi^2\beta}\right] \sum_{\mathbf{q}}{}' \sum_{l=-\infty}^{\infty} \int_0^\infty \frac{1}{t^2} D_{-2}\left(-\frac{\mu' t^{1/2}}{m}\right) \exp\left[-\frac{t}{2} + \frac{\mu'^2 t}{4m^2} - \frac{m^2\gamma^2(\mathbf{q})}{2t}\right] dt \tag{2.95}$$

Till here, we have not considered anything about the antiparticles yet. But at this stage it becomes an obligation: The t-integral in (2.95) can not be calculated without including the antiparticles into the discussion.

Had we repeated the whole process for the antiparticle, everything would be exactly the same except the sign of the chemical potential:

$$N_2 = N_{bulk(2)} + \left[\frac{L^3 m^2}{4\pi^2\beta}\right] \sum_{\mathbf{q}}{}' \sum_{l=-\infty}^{\infty} \int_0^\infty \frac{1}{t^2} D_{-2}\left(\frac{\mu' t^{1/2}}{m}\right) \exp\left[-\frac{t}{2} + \frac{\mu'^2 t}{4m^2} - \frac{m^2\gamma^2(\mathbf{q})}{2t}\right] dt \tag{2.96}$$

with the bulk term for the antiparticle:

$$N_{bulk(2)} = \left[\frac{L^3 m^2}{2\pi^2\beta}\right] \sum_{j=1}^{\infty} j^{-1} e^{-j\beta\mu} K_2(j\beta m) \tag{2.97}$$

Then for $Q = N_1 - N_2$, we have:

$$= N_{bulk(1)} - N_{bulk(2)} + \left[\frac{L^3 m^2}{4\pi^2\beta}\right] \sum_{\mathbf{q}}{}' \sum_{l=-\infty}^{\infty} \int_0^\infty \frac{1}{t^2} \left[D_{-2}\left(\frac{\mu' t^{1/2}}{m}\right) - D_{-2}\left(-\frac{\mu' t^{1/2}}{m}\right)\right] \times \exp\left[-\frac{t}{2} + \frac{\mu'^2 t}{2m^2} - \frac{m^2\gamma^2(\mathbf{q})}{2t}\right] dt \tag{2.98}$$

From [12], we get the required expression for the difference of parabolic cylinder functions:

$$D_{-2}(t) - D_{-2}(-t) = -\sqrt{2\pi}te^{t^2/4} \tag{2.99}$$

(2.98) then becomes,

$$Q = N_{bulk(1)} - N_{bulk(2)} + \left[\frac{L^3 m}{(2\pi)^{3/2}\beta}\right] \sum_{\mathbf{q}}{}' \sum_{l=-\infty}^{\infty} \mu' \int_0^{\infty} \frac{1}{t^{3/2}} \exp\left[-\frac{t}{2} + \frac{\mu'^2 t}{2m^2} - \frac{m^2\gamma^2(\mathbf{q})}{2t}\right] dt \tag{2.100}$$

Writing the bulk term differences in detail,

$$N_{bulk(1)} - N_{bulk(2)} = \frac{L^3 m^2}{\beta\pi^2} \sum_{j=1}^{\infty} \frac{1}{j} \sinh(j\beta\mu) K_2(j\beta m) \tag{2.101}$$

and getting the result of the integral from the table of the Laplace transforms [24], eventually we find:

$$Q = \frac{L^3 m^2}{\beta\pi^2} \sum_{j=1}^{\infty} \frac{1}{j} \sinh(j\beta\mu) K_2(j\beta m) + \frac{L^3}{2\pi\beta} \sum_{\mathbf{q}}{}' \sum_{l=-\infty}^{\infty} \frac{\mu'}{\gamma(\mathbf{q})} \exp[-(m'^2 - \mu'^2)^{1/2}\gamma(\mathbf{q})] \tag{2.102}$$

(2.102) is the equivalent expression of (2.37) in non-relativistic case, with no approximations made up to this stage. A very important point here would be to get the dependence of the condensate behaviour on the temperature. Examining the 'charge' of the condensate,

$$Q_0 = N_{0(1)} - N_{0(2)} \tag{2.103}$$

$$= \frac{1}{e^{\beta(m-\mu)} - 1} - \frac{1}{e^{\beta(m+\mu)} - 1} \tag{2.104}$$

we see that the emergence of a condensate behaviour requires $\mu \to m$. Thus, this limit also defines the critical temperature T_{cr} for the bulk system. We will examine the

behaviour of the bulk expression in (2.102) for this limit. Defining some $\varrho(\beta,\mu)$ would help us to do it easier:

$$\varrho(\beta,\mu)=\sum_{j=1}^{\infty}\frac{1}{j\beta m}\sinh(j\beta\mu)K_2(j\beta m) \tag{2.105}$$

Then clearly $N_{bulk(1)}-N_{bulk(2)}$ becomes,

$$N_{bulk(1)}-N_{bulk(2)}=\frac{L^3m^3}{\pi^2}\varrho(\beta,\mu) \tag{2.106}$$

In the limit of $\mu\to m$, $\varrho(\beta,\mu)$ becomes:

$$\varrho(\beta_{cr},\mu)=\sum_{j=1}^{\infty}\frac{1}{j\beta_{cr}m}\sinh(j\beta_{cr}m)K_2(j\beta_{cr}m) \tag{2.107}$$

Because this limit also defined T_{cr} for the bulk, we can say:

$$\varrho(\beta_{cr},\mu)=\frac{\pi^2Q}{L^3m^3} \tag{2.108}$$

For the non relativistic limit ($m >> kT_{cr}$), (2.107) reduces to [16]

$$\varrho(\beta_{cr},\mu)\approx\left[\frac{\pi}{4\beta_{cr}^3m^3}\right]^{1/2}\zeta\left(\frac{3}{2}\right)=\frac{\pi^2Q}{m^3L^3} \tag{2.109}$$

from which we get

$$\beta_{cr}=\frac{m}{2\pi}\left[\zeta\left(\frac{3}{2}\right)L^3/Q\right]^{2/3} \tag{2.110}$$

Replacing the Riemann zeta function in, we get:

$$Q_0=Q\left[1-\left(\frac{\beta_{cr}}{\beta}\right)^{3/2}\right]=Q\left[1-\left(\frac{T}{T_{cr}}\right)^{3/2}\right] \tag{2.111}$$

which is the usual non relativistic bulk result. For the extreme relativistic limit ($m << kT_{cr}$), (2.107) reduces to

$$\varrho(\beta_{cr}, \mu) \approx \frac{\pi^2}{3\beta_{cr}^2 m^2} = \frac{\pi^2 Q}{m^3 L^3} \tag{2.112}$$

from which

$$\beta_{cr} = \left(\frac{mL^3}{3Q}\right)^{1/2} \tag{2.113}$$

$$Q_0 = Q\left[1 - \left(\frac{T}{T_{cr}}\right)^2\right] \tag{2.114}$$

From (2.102), omitting all the terms except those having $l = 0$ and defining

$$y = \frac{1}{2}(m^2 - \mu^2)^{1/2} L \tag{2.115}$$

(2.102) becomes

$$Q = \frac{L^3 m^3}{\pi^2}\varrho(\beta, \mu) + \frac{L^3 \mu (m^2 - \mu^2)^{1/2}}{4\pi\beta} S(y) \tag{2.116}$$

with

$$S(y) = \sum_{\mathbf{q}}{}' \frac{1}{R(\mathbf{q})} e^{-2R(\mathbf{q})} \tag{2.117}$$

and

$$R(\mathbf{q}) = (q_1^2 + q_2^2 + q_3^2)^{1/2} y \tag{2.118}$$

similar to what we did in the previous section. Making use of a result from [22]:

$$\varrho(\beta,\mu) = \varrho(\beta,m) - \frac{\pi}{2\beta m^2}(m^2-\mu^2)^{1/2} + O(m^2-\mu^2) \tag{2.119}$$

and (2.60), it can be written that:

$$Q = \frac{L^3 m^3}{\pi^2}\varrho(\beta,\mu) + \frac{mL^2}{2\beta y^2} + \frac{mL^2}{2\pi^2\beta}\left[C_3 - y^2 {\sum_{\mathbf{q}}}' \frac{1}{q^2(y^2+\pi^2 q^2)}\right] \tag{2.120}$$

where the second term on the right hand side of (2.120) corresponds to the condensate and the third one, to the finite size effects for a relativistic ideal bose gas system.

3. WEAKLY INTERACTING BOSE GAS CASE

3.1. Bogoliubov Theory and the Finite Size Effects on the Ground State Energy

For the treatment of the weakly interacting Bose gas, we need to refer to the Bogoliubov theory [25]. First of all, the number preserving Hamiltonian can be defined as:

$$\hat{H} = \hat{H}' - \mu\hat{N} \tag{3.1}$$

with $\hat{H}'$ being the many body Hamiltonian with hard core repulsive potential [10]. This is a simple yet extremely rough assumption, far from being the realistic case.

$$\hat{H}' = \int d\mathbf{x} \left[\psi^\dagger(\mathbf{x})\hat{h}\hat{\psi}(\mathbf{x}) + \frac{u_0}{2}\psi^\dagger(\mathbf{x})\psi^\dagger(x)\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x})\right] \ (u_0 > 0) \tag{3.2}$$

The operator $\hat{h} \equiv -\Delta$ is the Hamiltonian for the single free particle. Knowing this, one remarks that the first term of (3.2) is the free many-body Hamiltonian. The expression to be defined as the field operator will be an approximation, consisting of a constant coherent state value and a fluctuation:

$$\hat{\psi}(\mathbf{x}) = \hat{\psi}_0(\mathbf{x}) + \hat{\eta}(\mathbf{x}) \tag{3.3}$$

where $\hat{\psi}_0(\mathbf{x})$ is

$$\psi_0 := \hat{\psi}_0(\mathbf{x}) = \hat{a}_0 f_0(\mathbf{x}) \sim \sqrt{N_0} f_0 = \sqrt{\frac{N_0}{V}} = \sqrt{n_0} \tag{3.4}$$

and the fluctuation $\hat{\eta}(\mathbf{x})$:

$$\hat{\eta}(\mathbf{x}) = \sum_{\sigma \neq 0} \hat{a}_\sigma f_\sigma \tag{3.5}$$

Writing (3.4) has been made possible with what is called the c-number substitution, justification of which can be found in [26,10]. The most crucial fact about the c-number substitution for us is that the error committed by this substitution is of order $\ln(V)/V$. Hence, it is due to this order that another term order of $(1/V^{1/3})$ that we will run into in the following part of the work will be considerable.

The c-number substitution is mainly based on the commutation of ground state's creation and annihilation operators for very large N_o values. This is due to the fact that N_0 and $N_0 + 1$ contain approximately the same information for $N_0 >> 1$. Thus, it becomes convenient to say that $\hat{a_0}|\Psi\rangle \rightarrow \sqrt{N_o}|\Psi\rangle$ and $\hat{a_0}^\dagger|\Psi\rangle \rightarrow \sqrt{N_o}|\Psi\rangle$, where $\hat{a_0}$ and $\hat{a_0}^\dagger$ operators are both approximated by the number $\sqrt{N_0}$.

Using the Neumann boundary conditions, the ground state wave function is given by: $f_0 = \frac{1}{\sqrt{V}}$

Now we will be expanding the Hamiltonian, replacing (3.3) into (3.2), while considering that the fluctuations are small and hence ignorable for orders higher than 2.

$$H'_{eff} = \int d(\mathbf{x}) \big[(\psi_0 \hat{h} \eta(\hat{\mathbf{x}}) + \hat{\eta}^\dagger(\mathbf{x}) \hat{h} \hat{\eta}(\mathbf{x}) + \frac{u_o}{2} \big(\psi_0^4 + 2\psi_0^3 (\hat{\eta}^\dagger(\mathbf{x}) + \hat{\eta}(\mathbf{x})) + \psi_0^2 \hat{\eta}^2(\mathbf{x}) + 4\hat{\eta}^\dagger(\mathbf{x}) \hat{\eta}(\mathbf{x}) + \hat{\eta}^{\dagger 2}(\mathbf{x}) \big) \big] \tag{3.6}$$

It should be added at this point that the laplacian eigenfunction f_σ's are orthogonal. They can also be chosen to be real, as indicated in [27]:

$$\int d(\mathbf{x}) f_\sigma(\mathbf{x}) f_\rho(\mathbf{x}) = \delta_{\sigma\rho} \tag{3.7}$$

If one of the eigenvalues is specifically chosen to be the ground state ($\sigma = 0$) and the other to be an excited one ($\sigma \neq 0$), we have:

$$\int d(\mathbf{x}) f_\sigma(\mathbf{x}) f_0(\mathbf{x}) = \frac{1}{\sqrt{V}} \int d(\mathbf{x}) f_\sigma(\mathbf{x}) = 0 \tag{3.8}$$

Making use of (3.8) and replacing (3.5) into (3.6), we end up expanding the effective Hamiltonian in terms of the creation and annihilation operators:

$$\hat{H}'_{eff} = \frac{u_0 n_0^2 V}{2} + \sum_{\sigma \neq 0} \left[(\epsilon_\sigma + 2u_0 n_0) \hat{a_\sigma}^\dagger \hat{a_\sigma} + \frac{u_0 n_0}{2} (\hat{a_\sigma}^\dagger \hat{a_\sigma}^\dagger + \hat{a_\sigma} \hat{a_\sigma}) \right] \tag{3.9}$$

The number operators, each for a state $\hat{N_\sigma} = \hat{a_\sigma}^\dagger \hat{a_\sigma}$, when summed over all states, yield to the total number operator:

$$\hat{N} = \sum_\sigma \hat{a_\sigma}^\dagger \hat{a_\sigma} = N_o + \sum_{\sigma \neq 0} \hat{a_\sigma}^\dagger \hat{a_\sigma} \text{ with } N_0 = n_0 V \tag{3.10}$$

Returning back to (3.1) and replacing the $\hat{H}'_{eff}$ and $\hat{N}$ expressions in it, finally we get:

$$\hat{H} = \hat{H_{eff}}' - \mu \hat{N} = \frac{u_0 n_0^2 V}{2} - \mu n_0 V + \sum_{\sigma \neq 0} \left[(\epsilon_\sigma + 2u_0 n_0 - \mu) \hat{a_\sigma}^\dagger \hat{a_\sigma} + \frac{u_0 n_0}{2} (\hat{a_\sigma}^\dagger \hat{a_\sigma}^\dagger + \hat{a_\sigma} \hat{a_\sigma}) \right] \tag{3.11}$$

Now, the Hamiltonian at hand (3.11) is already quadratic, but clearly not diagonal. Applying the Bogoliubov transformation permits us to transform our current basis to a new basis of 'quasi particle states' where the Hamiltonian will then be diagonal. Our system varies in energy and number of particles, hence a grand canonical treatment is natural. The grand canonical potential is

$$\Omega_{gc}(z, V, T) = -kT \ln Z_{gc}(z, V, T) = -kT \ln \left[\sum_\sigma e^{-\beta(H - \mu N)} \right] \tag{3.12}$$

where $z = e^{-\mu\beta}$ is the fugacity and Z_{gc}, the grand partition function. The main concern of our study is to calculate the finite size effects, so our system has constant volume; we can drop the volume dependency of the parameters. For the grand canonical case, Ω_{gc} is the quantity that needs to be minimized. But also, the thermodynamical pressure can be defined to be maximized, as both will carry a parallel argument for this specific case. To explain this fact in more detail, we write down the definition of the thermodynamic

pressure:

$$P(\mu, T, V) = -\frac{\partial}{\partial V}\Omega_{gc} \tag{3.13}$$

Due to the fact that the dimensions of the system are much larger than the range of any interaction, to a first order in extensive variables we can say:

$$P = -\frac{\Omega_{gc}}{V} \tag{3.14}$$

With the volume being constant, P can safely be chosen to be the quantity to be maximized. Rewriting P explicitly:

$$P = \frac{kT}{V}\ln Z_{gc} = \frac{kT}{V}\ln(Tr' e^{-\beta(\hat{H'_{eff}} - \mu\hat{N})}) \tag{3.15}$$

As a first step of an iterative process, we only take the part with order zero in η:

$$\hat{H_{eff}}' - \mu\hat{N} \approx \frac{u_0 n_0^2 V}{2} - \mu n_0 V \tag{3.16}$$

Replacing this expression for $(\hat{H_{eff}}' - \mu\hat{N})$ in (3.11) and taking the derivative with respect to μ, we see that P is maximized by the value

$$\mu = u_0 n_0 \tag{3.17}$$

Replacing (3.17) back in (3.11):

$$\hat{H_{eff}}' - \mu\hat{N} = -\frac{u_0 n_0^2 V}{2} + \sum_{\sigma \neq 0}\left[(\epsilon_\sigma + u_0 n_0)\hat{a_\sigma}^\dagger \hat{a_\sigma} + \frac{u_0 n_0}{2}(\hat{a_\sigma}^\dagger \hat{a_\sigma}^\dagger + \hat{a_\sigma}\hat{a_\sigma})\right] \tag{3.18}$$

With the approximation of c-number substitution, the ground state energy for the lowest order approximation for a constant particle number density can be expressed as

the following [28]:

$$E_0 = \frac{1}{2} u_0 n_0^2 V \tag{3.19}$$

Thus, again to zeroth order we find

$$\mu = \frac{\partial E_0}{\partial N}|_{V,S} = u_0 n_0 \tag{3.20}$$

Recognizing this term in (3.18) and removing $\mu\hat{N}$ from both sides, we come up with the effective Hamiltonian:

$$\hat{H_{eff}}' = \sum_{\sigma \neq 0} \left[(\epsilon_\sigma + 2u_0 n_0) \hat{a_\sigma}^\dagger \hat{a_\sigma} + \frac{u_0 n_0}{2} (\hat{a_\sigma}^\dagger \hat{a_\sigma}^\dagger + \hat{a_\sigma} \hat{a_\sigma}) \right] \tag{3.21}$$

And we see that the correction coming from the diagonalization is of the order of $(u_0 n_0)$. The next step would be to diagonalize (3.21). The Bogoliubov transformation is defined as [29]

$$a_\sigma = (\sinh \xi_\sigma) b_\sigma^\dagger + (\cosh \xi_\sigma) b_\sigma \tag{3.22}$$

with

$$\lambda_\sigma := \epsilon_\sigma + u_0 n_0 = w_\sigma \cosh 2\xi_\sigma \tag{3.23}$$

$$u_0 n_0 = -w_\sigma \sinh 2\xi_\sigma \tag{3.24}$$

$$w_\sigma := \sqrt{(\epsilon_\sigma + u_0 n_0)^2 - (u_0 n_0)^2} \tag{3.25}$$

After arranging the terms, we get the diagonalized effective Hamiltonian

$$\hat{H_{eff}} = -\frac{1}{2}\sum_{\sigma=1}^{\infty}(\lambda_\sigma - w_\sigma) + \sum_{\sigma\neq 0} w_\sigma \hat{b_\sigma}^\dagger \hat{b_\sigma} \tag{3.26}$$

Obviously

$$(\lambda_\sigma - w_\sigma) = \frac{u_0 n_0^2}{\lambda_\sigma + w_\sigma} \tag{3.27}$$

The convergence properties of the first sum in (3.26) is of primary interest. From (3.27), it can be seen that investigating the order of $(\lambda_\sigma + w_\sigma)$ would be equivalently good for this purpose. To understand the order of $(\lambda_\sigma + w_\sigma)$, we first rearrange w_σ.

$$w_\sigma = \sqrt{\left[\epsilon_\sigma\left(1 + \frac{u_0 n_0}{\epsilon_\sigma}\right)\right]^2 - (u_0 n_0)^2} = \epsilon_\sigma\sqrt{1 + \frac{2u_0 n_0}{\epsilon_\sigma}} \tag{3.28}$$

The critical element determining the behaviour of the w_σ is ϵ_σ. There is an infinite number of σ states and ϵ_σ increases by each successive term. This means that $\frac{u_0 n_0}{\epsilon_\sigma}$ can be considered to be small for values of σ above some large σ_0. This makes the square root term in (3.28) binomially expandable: $\left(1 + \frac{2u_0 n_0}{\epsilon_0}\right)^{1/2} \approx 1 + \frac{u_0 n_0}{\epsilon_0} - \frac{1}{8}\frac{u_0^2 n_0^2}{\epsilon_0^2} + ...$
So the first term of (3.26) becomes:

$$-\frac{1}{2}\sum_{\sigma_0}^{\infty}(\lambda_\sigma - w_\sigma) \tag{3.29}$$

$$= -\frac{1}{2}\sum_{\sigma_0}^{\infty}\frac{(gn_0)^2}{\lambda_\sigma + w_\sigma} \tag{3.30}$$

$$= -\frac{1}{2}\sum_{\sigma_0}^{\infty}\frac{(gn_0)^2}{2\epsilon_\sigma\left[1 + O\left(\frac{1}{\epsilon_0}\right)\right]} \tag{3.31}$$

$$= -\frac{1}{2}\sum_{\sigma_0}^{\infty}\frac{(gn_0)^2}{2\epsilon_\sigma} + O\left(\frac{1}{\epsilon_0^2}\right) \tag{3.32}$$

Recognizing the ground state energy E_0 as the first term of (3.32), we eventually write the final form expression of the diagonalized effective Hamiltonian as:

$$\hat{H_{eff}} = E_0 + \sum_{\sigma\neq 0} w_\sigma \hat{b_\sigma}^\dagger \hat{b_\sigma} \tag{3.33}$$

We also need a rigorous approach about the behaviour of the $\sum_{\sigma=1}^{\infty}\frac{1}{\epsilon_\sigma}$ that is present in the first term of (3.32). It is more advantegeous to take a look at the general case of

$$\sum_{\sigma=1}^{\infty}\frac{1}{\epsilon_\sigma^k} \tag{3.34}$$

To investigate that, we need to refer to a work by Li and Yau [30] that gives a lower bound expression for the Laplacian eigenvalues:

$$\epsilon_\sigma \geqslant \frac{C(d)}{D_M^2}\sigma^{2/d} \tag{3.35}$$

where $C(d)$ is a positive constant solely dependent on the dimension d and D_M is the diameter of the box. Based on (3.35), we can get an upper bound for (3.34):

$$\sum_{\sigma=1}^{\infty}\frac{1}{\epsilon_\sigma^k} \leq \frac{D_M^{2k}}{C^k(d)}\sum_{\sigma=1}^{\infty}\frac{1}{\sigma^{2k/d}} \tag{3.36}$$

The sum on the right side of the inequality is a Riemann zeta function $\zeta(2k/d)$, consequently (3.32) converges only for $\frac{2k}{d} > 1$ and diverges otherwise. For $k = 1$, dimensions equal to or higher than 2 lead to a divergence, which is exactly the case at hand. This is a non-physical defect originating from the extremely rough approximating nature of the hard-sphere potential. The hard sphere potential is characterized by [31]:

$$V_0(\mathbf{r}_1 - \mathbf{r}_2) \approx V_0\delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{3.37}$$

This assumption overlooks the fact that $\tilde{V}$ is a matrix in reality, while it replaces the matrix elements V_0's with a constant value. The divergence confronted arises exactly for this reason [28]. To eliminate this, the Born approximation can make a guiding model: the relation between V_0 and the scattering length σ_s in the Born approximation is equally relevant for our case. In the lowest order, the two body s-wave scattering length is given by:

$$\sigma_s = \frac{mV_0}{4\pi\hbar^2} \tag{3.38}$$

Based on the physically measurable scattering length, we introduce a renormalized coupling constant: $u_0 = \frac{4\pi\sigma_s\hbar^2}{m}$. Going to the next order in Born approximation, σ_s is expanded up to quadratic terms in V_0 [32] and gets the form:

$$\sigma_s = \frac{m}{4\pi\hbar^2}\left(V_0 - \frac{V_0^2}{V}\sum_{\sigma=1}^{\infty}\frac{1}{\epsilon_\sigma}\right) \tag{3.39}$$

Solving for physically measurable quantities, we reexpress V_0

$$V_0 = u_o\left(1 + \frac{u_0}{V}\sum_{\sigma=1}^{\infty}\frac{1}{\epsilon_\sigma}\right) \tag{3.40}$$

Corresponding to the new iterated values of σ_s, we now have a tuned u_0 value. The tuning of the coupling constant u_0 will yield to a cancellation of the previous divergency and result in a renormalized ground state energy (The detailed derivation can be found in [28].) The renormalized expression for the ground state is then

$$E_0 = -\frac{1}{2}\sum_{\sigma=1}^{\infty}\left[(\epsilon_\sigma + u_0 n_0) - w_\sigma - \frac{(u_0 n_o)^2}{2\epsilon_\sigma}\right] \tag{3.41}$$

and from now on, when we refer to u_0, we'll be referring to the renormalized coupling constant.

3.2. Ground State Energy in terms of the Heat Kernel

In the literature, the result of the sum (3.41) is not given and only described to be found by a replacement of the sum with an integral in momentum space [28]. The final result has been given by Lee and Yang [33] as

$$E_0 = u_0 \frac{N^2}{2V}\left[1 + \frac{128}{15\sqrt{\pi}}(n\sigma_s^3)^{1/2}\right] \tag{3.42}$$

But it is possible to recover (3.42), the same result of Lee and Yang, from a different perspective and this will be our main aim for the next few pages. It is possible to describe our aim roughly, by saying that we will analyze the ground state energy in terms of the heat kernel, following the steps developped in [10]. (A quick summary of the heat kernels is recovered in Appendix B.) Back to the expression (3.29), we define $s = \epsilon_\sigma$ and $a = u_0 n_0$ and obtain

$$(\lambda_\sigma - w_\sigma) = s + a - \sqrt{(s+a)^2 - a^2} = s + a - \sqrt{s^2 + 2sa} \tag{3.43}$$

Because σ is a constant(our system has constant number density) and s is a varying quantity (σ spans over all states), we can shift the variable s of an amount of a:

$$s' \to s + a \tag{3.44}$$

and get

$$s + a - \sqrt{s^2 + 2sa} = s' - \sqrt{s'^2 - a^2} \tag{3.45}$$

From now on, we'll omit the prime on s, and s will correspond to the shifted version. A first step would be to make use of the simple identity:

$$\left(s - \sqrt{s^2 - a^2}\right)\left(s + \sqrt{s^2 - a^2}\right) = a^2 s - \sqrt{s^2 - a^2} = \frac{a^2}{s + \sqrt{s^2 - a^2}} \tag{3.46}$$

From [12] we note

$$\int_0^\infty \frac{x^{n+1}dx}{(ax^2+2bx+c)^{n+3/2}} = \frac{n!}{(2n+1)!!\sqrt{a}(\sqrt{ac}+b)^{n+1}} \quad \text{for } a>0,\ c\geq 0 \text{ and } b>-\sqrt{ac} \tag{3.47}$$

We remark that for $n=0$, $a=1$, $c=(s^2-a^2)$ and $b=s$, we recognize (3.47) to be the right hand side of (3.46) divided by a factor or a^2:

$$\frac{1}{s+\sqrt{s^2-a^2}} = \int_0^\infty \frac{xdx}{[x^2+2sx+s^2-a^2]^{3/2}} \tag{3.48}$$

Remarking that

$$\frac{1}{[x^2+2sx+s^2-a^2]^{3/2}} = \frac{1}{[(x+s)^2-a^2]^{3/2}} \tag{3.49}$$

is a Laplace transform [24], we get:

$$= \int_0^\infty dt e^{-(s+x)t} \frac{\sqrt{\pi}}{\Gamma(3/2)} \left(\frac{t}{2a}\right) I_1(at) \tag{3.50}$$

where $I_1(t)$ is the modified Bessel function of the first kind of order 1. Putting (3.50) back in (3.48), and shifting s once again to $s+a$, we have

$$A\int_0^\infty dt \int_0^\infty xdx e^{-(s+a+x)t} \left(\frac{t}{a}\right) I_1(at) = A\int_0^\infty dt \left(\frac{1}{at}\right) e^{-at}e^{-st} I_1(at) \tag{3.51}$$

where $A=\frac{\sqrt{\pi}}{2\Gamma(3/2)}$ is a constant and can be omitted as it has no role on the present mathematical treatment. Summing both sides over non zero states of σ:

$$\sum_{\sigma=1}\int_0^\infty dt \int_0^\infty xdx e^{-(s+a+x)t} \left(\frac{t}{a}\right) I_1(at) = \sum_{\sigma=1} e^{-st} \int_0^\infty dt \left(\frac{1}{at}\right) e^{-at} I_1(at) \tag{3.52}$$

Noticing that

$$\sum_{\sigma=1} e^{-st} = \sum_{\sigma=1} e^{-\epsilon_\sigma t} = \mathrm{Tr}' e^{\Delta t} \tag{3.53}$$

At this point we should stop and have a look at the equality of the expressions:

$$E_0 = -\frac{1}{2}\sum_{\sigma=1}^{\infty}(\lambda_\sigma - w_\sigma) = -\frac{a^2}{2}\int_0^\infty \frac{dt}{at} I_1(at) e^{-at} \mathrm{Tr}' e^{\Delta t} \tag{3.54}$$

Earlier, we had seen that E_0 was divergent. That gives us enough motivation to investigate the convergence properties of the rightmost term in (3.54), and that means studying the convergence properties of $\mathrm{Tr}' e^{\Delta t}$ and $I_1(t)$. The asymptotic expansions of a modified Bessel function of order p are [34]: For $t << 1$,

$$I_p(t) \sim \frac{t^p}{2^p \Gamma(p+1)}\left(1 + \frac{t^2}{2.(2p+2)} + \frac{t^4}{2.4.(2p+2)(2p+4)} + ...\right) \tag{3.55}$$

For $t >> 1$,

$$I_p(t) \sim \frac{e^t}{\sqrt{2\pi t}}\left(1 - \frac{1}{2t}\left(p^2 - \frac{1}{4}\right) + ...\right) \tag{3.56}$$

With (3.55) and (3.56), it is easy to obtain the asymptotic behaviour of the Bessel function. As $t \to \infty$, clearly

$$I_1(t) \to \frac{e^t}{\sqrt{2\pi t}} \to \frac{e^t}{\sqrt{t}} \tag{3.57}$$

and as $t \to 0^+$,

$$I_1(t) \to \frac{t}{2} \tag{3.58}$$

To study the convergence of the trace, we need to consult to some upper and lower bounds of $\mathrm{Tr}' e^{\Delta t}$. Those bounds can be evaluated from some existing bounds for the

eigenvalue of the Laplacian. A lower bound had already been mentioned in (3.35) as

$$\epsilon_\sigma \geqslant \frac{C(d)}{D_M^2}\sigma^{2/d} \tag{3.59}$$

There also exists an upper bound by Colbois and Maerten [35]:

$$\epsilon_\sigma \leqslant B(d)\left(\frac{\sigma}{V}\right)^{2/d} \tag{3.60}$$

where B(d) is again a dimension dependent positive constant. With the help of these two bounds, the trace $\mathrm{Tr}' e^{\Delta t} = \sum_{\sigma=1}^{\infty} e^{-t\epsilon_\sigma}$ is seen to be bounded between:

$$\sum_{\sigma=1}^{\infty} e^{-\frac{tB}{V^{2/d}}\sigma^{2/d}} \leqslant \sum_{\sigma=1}^{\infty} e^{-t\epsilon_\sigma} \leqslant \sum_{\sigma=1}^{\infty} e^{-\frac{tC}{D_M^2}\sigma^{2/d}} \tag{3.61}$$

Using the integral test, it's trivial to bound these sums by their integral expressions. For the lower bound we write

$$\int_1^{\infty} dx e^{-\frac{tB}{V^{2/d}}x^{2/d}} \leqslant \sum_{x=1}^{\infty} e^{-\frac{tB}{V^{2/d}}x^{2/d}} \tag{3.62}$$

And for the upper bound as well:

$$D_M^d \int_0^{\infty} dx e^{-tCx^{2/d}} \geqslant \sum_{\sigma=1}^{\infty} e^{-\frac{tC}{D_M^2}\sigma^{2/d}} \tag{3.63}$$

After evaluating the integrals we are left with the following trace bounds originating from the bounds on the Laplacian eigenvalues:

$$\left(\frac{V}{B^{d/2}}\right)\left(\frac{d}{2}\right)\Gamma\left(\frac{d}{2}, \frac{tB}{V^{2/d}}\right)\left(\frac{1}{t}\right)^{d/2} \leqslant \mathrm{Tr}' e^{\Delta t} \leqslant \left(\frac{D_M^d}{C^{d/2}}\right)\Gamma\left(\frac{d}{2}\right)\left(\frac{1}{t}\right)^{d/2} \tag{3.64}$$

Now that we have bounds for the trace, its asymptotic behaviour can be predicted. Considering $d = 3$ and overlooking the coefficients, the integrand in (3.54)

$$\frac{1}{at} I_1(at) e^{-at} \mathrm{Tr}' e^{\Delta t} \tag{3.65}$$

is seen to behave with

$$\frac{1}{at} \frac{e^{at}}{(at)^{1/2}} e^{-at} \frac{1}{t^{3/2}} \propto \frac{1}{t^3} \text{ for } t \to \infty \tag{3.66}$$

and

$$\frac{1}{at} \frac{at}{2} e^{-at} \frac{1}{t^{3/2}} \propto \frac{1}{t^{3/2}} \text{ for } t \to 0^+ \tag{3.67}$$

The $t \to \infty$ limit converges whereas the $t \to 0^+$ limit obviously diverges. At this point, it should also be noted that had we taken the integral over t, the outcome would be divergent in the limit $t \to 0^+$ due to the limiting behaviour as $t \to 0^+$. To overcome this situation, Akant *et al.* [10] came up with the idea of substracting an extra term in order to cancel out the divergence. Based on the fact that it is the behaviour of the trace that gives rise to the divergency, the term $\frac{1}{2}\mathrm{Tr}' e^{\Delta t}$ is suggested to be substracted from (3.65):

$$\frac{1}{at} I_1(at) e^{-at} \mathrm{Tr}' e^{\Delta t} - \frac{1}{2} \mathrm{Tr}' e^{-\Delta t} = \mathrm{Tr}' e^{\Delta t} \left(\frac{1}{at} I_1(at) e^{-at} - \frac{1}{2} \right) \tag{3.68}$$

Since our region of interest is t close to 0 (a is a finite quantity), the power in the exponential e^{-at} is small and hence the expression can be expanded. For very small t, (3.68) behaves as

$$\sim \frac{at}{2} \frac{1}{t^{3/2}} \tag{3.69}$$

which yields a convergent result after being integrated over t. Now that it seems we are able to overcome the problem of divergence, we should understand for the substracted

part by reevaluating it in terms of $\mathrm{Tr}' e^{\Delta t}$. Taking the integral over t (and noting that the sum and the integral are interchangable as the sum is convergent), we find that:

$$\int_0^\infty dt\, \mathrm{Tr}' e^{\Delta t} = \sum_{\sigma \neq 0} \int_0^\infty dt\, e^{-\epsilon_\sigma t} \tag{3.70}$$

$$= \sum_{\sigma \neq 0} \frac{1}{2\epsilon_\sigma} \tag{3.71}$$

Remembering the $-\frac{a^2}{2}$ term in front of the whole expression in (3.54) and replacing it as well, we reobtain the term in (3.41):

$$-\frac{1}{2} \sum_{\sigma \neq 0} \frac{a^2}{2\epsilon_\sigma} \tag{3.72}$$

Now, one has to pay attention: this was the effective Hamiltonian's ground state. The ground state of the overall Hamiltonian is obtained by adding the chemical potential back to the right hand side:

$$E_g = \frac{u_0 n_o^2 V}{2} - \frac{a^2 V}{2} \int_0^\infty dt \left(\frac{1}{at} I_1(at) e^{-at} - \frac{1}{2} \right) \frac{1}{V} \mathrm{Tr} e^{\Delta t} \tag{3.73}$$

And rescaling the integral

$$E_g = \frac{u_0 n_o^2 V}{2} - \frac{a^2 V}{2} \int_0^\infty dt \left(\frac{1}{t} I_1(t) e^{-t} - \frac{1}{2} \right) \frac{1}{V} \mathrm{Tr} e^{\Delta t/a} \tag{3.74}$$

The explicit expression of the integrand in (3.74) is needed and from [12] one gets:

$$\frac{\pi I_1(a)}{2a} = \int_0^1 \sqrt{1 - x^2} \cosh(ax) dx \tag{3.75}$$

$$\frac{I_1(t)}{t} = \frac{2}{\pi}\int_0^1 \sqrt{1-x^2}\cosh(tx)dx \tag{3.76}$$

So (3.74) becomes,

$$E_g = \frac{u_0 n_0^2 V}{2} - \frac{aV}{\pi}\int_0^\infty dt \int_0^1 dx\sqrt{1-x^2}\left(\cosh(tx)e^{-t}-1\right)\frac{1}{V}\mathrm{Tr}e^{\Delta t/a} \tag{3.77}$$

$$E_g = \frac{u_0 n_0^2 V}{2} + \frac{aV}{2\pi}\int_0^\infty dt \int_0^1 dx\sqrt{1-x^2}\left[(1-e^{-t(1-x)})+(1-e^{-t(1+x)})\right]\frac{1}{V}\mathrm{Tr}e^{\Delta t/a} \tag{3.78}$$

And if we define

$$F(t,x) = \sqrt{1-x^2}\left[(1-e^{-t(1-x)})+(1-e^{-t(1+x)})\right] \tag{3.79}$$

can be rewritten as

$$E_g = \frac{u_0 n_0^2 V}{2} + \frac{aV}{2\pi}\int_0^\infty dt \int_0^1 dx F(t,x)\frac{1}{V}\mathrm{Tr}e^{\Delta t/a} \tag{3.80}$$

Looking at (3.80), getting bounds for the E_g seems feasible if we know the bounds for the trace. And we already do; we have bounds (by Li and Yau) for $\mathrm{Tr}e^{\Delta t}$ at hand [30]:

$$\frac{V}{(4\pi t)^{d/2}} \leq \mathrm{Tr}e^{\Delta t} \leq \tilde{C}(d)g(t) \tag{3.81}$$

where $\tilde{C}$ is again a positive constant depending only on the dimension. The leftmost expression in (3.80), the lower bound $\frac{V}{(4\pi t)^{d/2}}$ is, by no surprise, the exact expression of $\mathrm{Tr}e^{\Delta t}$ for the flat case. But before applying the bounds in (3.81) for the trace in (3.80), one final check about the sign of the terms preceeding it is required. For the interval

$0 \leq x < 1$, it's clear that $F(t,x)$ is strictly positive as

$$(1 - e^{-t(1-x)}) > 0 \quad \text{and } (1 - e^{-t(1+x)}) > 0 \text{ within the same interval.} \tag{3.82}$$

By this, it is guaranteed that the bounds in (3.81) are perfectly applicable.

We will move on by considering flat space; that means that we need to replace the trace expression with the lower bound in (3.81). Till this moment the Hamiltonian for the free particle was taken to be $\hat{h} = -\Delta$. But now if one desires to introduce the physical values for the energy eigenvalues, the omitted factor of $\hbar^2/2m$ should be reintroduced. Taking all these into consideration, we write

$$E_g = \frac{u_0 n_0^2 V}{2} + \frac{aV}{2\pi} \int_0^\infty dt \int_0^1 dx F(t,x) \frac{a^{3/2} 2^{3/2} m^{3/2}}{\hbar^3 (4\pi t)^{3/2}} \tag{3.83}$$

$$E_g = \frac{u_0 n_0^2 V}{2} + \frac{aV}{2\pi} \int_0^\infty dt \int_0^1 dx \sqrt{1-x^2} \left[(1 - e^{-t(1-x)}) + (1 - e^{-t(1+x)}) \right] \frac{a^{3/2} 2^{3/2} m^{3/2}}{\hbar^3 (4\pi t)^{3/2}} \tag{3.84}$$

$$= \frac{u_0 n_0^2 V}{2} + \frac{a^{5/2} 2^{1/2} m^{3/2} V}{\hbar^3 (4\pi)^{3/2}} \int_0^1 dx \sqrt{1-x^2} \left[\int_0^\infty \frac{dt}{t^{3/2}} \left(1 - e^{-t(1+x)}\right) + \int_0^\infty \frac{dt}{t^{3/2}} \left(1 - e^{-t(1-x)}\right) \right] \tag{3.85}$$

The integrand has the form

$$\int \frac{1 - e^{-t\kappa}}{t^{3/2}} dt = 2\sqrt{\pi}\sqrt{\kappa}\, \mathrm{erf}(\sqrt{\kappa}\sqrt{t}) + \frac{2e^{-t\kappa}}{\sqrt{t}} - \frac{2}{\sqrt{t}} + \text{constant} \tag{3.86}$$

Knowing that $\mathrm{erf}(0) = 0$ and $\mathrm{erf}(\infty) = 1$, the solution is

$$\int_0^\infty \frac{dt}{t^{3/2}} \left(1 - e^{-t(1\pm x)}\right) = 2\sqrt{\pi(1 \pm x)^{1/2}} \tag{3.87}$$

Using the result of (3.87) for the integrals over t in (3.85) and remembering that $a = u_0 n_0$, we write,

$$E_g = \frac{u_0 n_0^2 V}{2}\left[1 + \frac{2^{5/2} a^{3/2} m^{3/2}\sqrt{\pi}}{n_0 \hbar^3 \pi (4\pi)^{3/2}} \int_0^1 dx \sqrt{1-x^2}((1+x)^{1/2} + (1-x)^{1/2})\right] \tag{3.88}$$

The integral in (3.88) can be found with the help of [14] to be as

$$\int_0^1 \left[(1+x)^{\mu-1}(1-x)^{\nu-1} + (1+x)^{\nu-1}(1-x)^{\mu-1}\right] dx = 2^{\mu+\nu-1} B(\mu,\nu) \qquad [Re\mu > 0, Re\nu > 0] \tag{3.89}$$

where $B(\mu,\nu)$ is the beta function of which one of the expressions is

$$B(\mu,\nu) = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu+\nu)} \tag{3.90}$$

For our case we have $\mu = 3/2$ and $\nu = 1$. The integral in (3.88) then has the value

$$2^{5/2} B\left(\frac{3}{2}, 2\right) = 2^{5/2}\frac{4}{15} \tag{3.91}$$

and (3.88) becomes,

$$E_g = \frac{u_0 n_0^2 V}{2}\left[1 + \frac{2^{5/2} a^{3/2} m^{3/2}\sqrt{\pi}}{n_0 \hbar^3 \pi (4\pi)^{3/2}} 2^{5/2}\frac{4}{15}\right] \tag{3.92}$$

From (3.38), we can write the coupling constant in terms of the scattering cross section and replace it with u_0 in (3.92)

$$u_0 = \frac{4\pi\sigma_s \hbar^2}{m} \tag{3.93}$$

$$E_g = \frac{2\pi\sigma_s \hbar^2 N^2}{mV}\left[1 + \frac{128}{15\sqrt{\pi}}(n_0\sigma_s^3)^{1/2}\right] \tag{3.94}$$

which can also be written as

$$E_g = \frac{u_0 N^2}{2V}\left[1 + \frac{128}{15\sqrt{\pi}}(n_0\sigma_s^3)^{1/2}\right] \tag{3.95}$$

which is the same result as derived by Lee and Yang, cited in (3.42). So with a totally different approach, it became possible to obtain the correct expression for the system's ground state energy.

3.3. Heat Kernel Analysis of the Depletion of the Condensate at T=0°K with Poisson Summation Method

To evaluate the depletion coefficient at zero temperature, we start with

$$n_e = \frac{1}{V}\sum_{\sigma\neq 0}\langle a_\sigma^\dagger a_\sigma\rangle \tag{3.96}$$

where n_e is the particle number density of the excited states. As previously mentioned, the Bogoluibov transformations are [29]:

$$a_\sigma = (\sinh\xi_\sigma)b_\sigma^\dagger + (\cosh\xi_\sigma)b_\sigma \tag{3.97}$$

$$a_\sigma^\dagger = (\sinh\xi_\sigma)b_\sigma + (\cosh\xi_\sigma)b_\sigma^\dagger \tag{3.98}$$

Replaced in (3.96), one gets

$$n_e = \frac{1}{V}\sum_{\sigma\neq 0}\left[\sinh^2\xi_\sigma\langle b_\sigma^\dagger b_\sigma\rangle + \cosh\xi_\sigma\langle b_\sigma^\dagger b_\sigma\rangle + \frac{1}{2}\sinh 2\xi_\sigma\langle b_\sigma^{\dagger 2} + b_\sigma^2\rangle\right] \tag{3.99}$$

Ignoring the second order terms, (3.99) becomes

$$n_e = \frac{1}{V}\sum_{\sigma\neq 0}\left[\cosh 2\xi_\sigma\left(\frac{1}{2} + \langle b_\sigma^\dagger b_\sigma\rangle\right) - \frac{1}{2}\right] \tag{3.100}$$

$$= \frac{1}{V}\sum_{\sigma\neq 0}\left[\cosh 2\xi_\sigma \coth\frac{\beta w_\sigma}{2} - \frac{1}{2}\right] \tag{3.101}$$

$$= \frac{1}{2V}\sum_{\sigma\neq 0}\left[\frac{\lambda_\sigma}{w_\sigma}\coth\frac{\beta w_\sigma}{2} - 1\right] \tag{3.102}$$

For $T \to 0$,

$$n_0 = \frac{1}{2V}\sum_{\sigma\neq 0}\left[\frac{\lambda_\sigma}{w_\sigma} - 1\right] \tag{3.103}$$

$$= \frac{1}{2V}\sum_{\sigma\neq 0}\left[\frac{\lambda_\sigma}{\sqrt{\lambda_\sigma^2 - (u_0 n_0)^2}} - 1\right] \tag{3.104}$$

Once again, we spot the form of the Laplace transform [24]:

$$\frac{1}{\sqrt{\lambda_\sigma^2 - (u_0 n_0)^2}} = \int_0^\infty dt e^{-\lambda_\sigma t} I_0(u_0 n_0 t) \tag{3.105}$$

Then,

$$\frac{\lambda_\sigma}{\sqrt{\lambda_\sigma^2 - (u_0 n_0)^2}} = -\int_0^\infty dt \left[\frac{d}{dt}e^{-\lambda_\sigma t}\right] I_0(u_0 n_0 t) \tag{3.106}$$

Noting that $\frac{dI_0(t)}{dt} = I_1(t)$ and using integration by parts,

$$= 1 + u_0 n_0 \int_0^\infty dt e^{-\lambda_\sigma t} I_1(u_0 n_0 t) \tag{3.107}$$

Putting (3.106) into (3.104),

$$n_e = \frac{1}{2V}\sum_{\sigma\neq 0}\left[1 + u_0 n_0 \int_0^\infty dt e^{-\lambda_\sigma t} I_1(u_0 n_0 t) - 1\right] \tag{3.108}$$

$$= \frac{u_0 n_0}{2V}\int_0^\infty dt \sum_{\sigma\neq 0} e^{-\lambda_\sigma t} I_1(u_0 n_0 t) \tag{3.109}$$

$$= \frac{u_0 n_0}{2V}\int_0^\infty dt \left[\sum_{\sigma\neq 0} e^{-\epsilon_\sigma t}\right] e^{-u_0 n_0 t} I_1(u_0 n_0 t) \tag{3.110}$$

$$= \frac{u_0 n_0}{2}\int_0^\infty dt \left[\frac{1}{V}\mathrm{Tr}' e^{\Delta t}\right] e^{-u_0 n_0 t} I_1(u_0 n_0 t) \tag{3.111}$$

which is a perfectly convenient expression to be bounded with the bounds for the trace. But instead, we will continue with in a different direction where we will be applying the Poisson summation technique for the trace expression in (3.111), keeping the leading order in $(u_0 n_0)$ as well as $1/L$'s to find the finite size effects in the depletion coefficient.

Now starting with,

$$I_1(at) = \frac{2}{\pi}(at)\int_{-1}^{1} e^{atx}\sqrt{1-x^2}dx \tag{3.112}$$

$$\begin{aligned}\int_0^\infty \frac{1}{V}\left[Tr\left(e^{\frac{\Delta t}{a}}\right)\right] I_1(at)\, e^{-at} dt &= \int_0^\infty \frac{1}{V} Tr\left(e^{\Delta t}\right) e^{-at}\int_{-1}^{1} dx e^{atx}(at)\, dt\sqrt{1-x^2} \\ &= \int_0^\infty dt \frac{1}{V} Tr\left(e^{\Delta t}\right)\int_{-1}^{1} e^{-at(1-x)}(at)\sqrt{1-x^2}dx\end{aligned} \tag{3.113}$$

we choose $1-x=\xi$ so that we can get $\int_{-1}^{1} \longrightarrow \int_0^2 d\xi$.
Then the right hand side of (3.113) becomes,

$$\int_0^\infty dt \frac{1}{V} Tr\left(e^{\Delta t}\right) \int_0^2 e^{-at\xi} \sqrt{\xi}\sqrt{2-\xi}\,(at)\,d\xi \tag{3.114}$$

Poisson Formula does not allow $\int_0^\infty dt$ and $\sum\limits_q$ to commute, unless we cut off some of the integrals. For this purpose, we choose the integral over ξ:

$$\begin{aligned}\int_0^\infty dt \frac{1}{V} Tr\left(e^{\Delta t}\right) \int_0^2 e^{-at\xi} \sqrt{\xi}\sqrt{2-\xi}\,(at)\,d\xi \\ = \int_0^\infty dt \left[\frac{1}{V} Tr\left(e^{\Delta t}\right)\right] \left[\int_{V^{-\alpha}}^2 d\xi + \int_0^{V^{-\alpha}} d\xi\right] e^{-at\xi}\,(at)\,\sqrt{\xi}\sqrt{2-\xi}\end{aligned} \tag{3.115}$$

For the first part we use Poisson sum and we estimate the second piece

$$= \int_0^\infty dt \left[\int_{V^{-\alpha}}^2 \left[\frac{1}{\sqrt{4\pi t}} + \sum_{q\neq 0} \frac{e^{\frac{-\pi q^2 L^2}{t}}}{\sqrt{4\pi t}}\right]^3 + \int_0^{V^{-\alpha}} \left[\frac{1}{V} Tr\left(e^{\Delta t}\right)\right]\right] e^{-at\xi} \sqrt{2-\xi}\sqrt{\xi}\,(at)\,d\xi \tag{3.116}$$

$$\begin{aligned}= \int_0^\infty dt \int_{V^{-\alpha}}^2 \left(\frac{1}{(4\pi t)^{3/2}} + 12 \sum_{\substack{q_1=1\\ q_2,q_3=0}} \frac{e^{\frac{-\pi q^2 L^2}{t}}}{(4\pi t)^{3/2}} + 12 \sum_{\substack{q_1,q_2=1\\ q_3=0}} \frac{e^{-\pi \frac{q_1^2 L^2}{t} - \frac{q_2^2 L^2}{t}}}{(4\pi t)^{3/2}} + 8\left(\sum \frac{e^{\frac{-\pi q^2 L^2}{t}}}{(4\pi t)^{1/2}}\right)^3\right) \\ \times e^{-at\xi}\sqrt{2-\xi}\sqrt{\xi} d\xi (at) + \int_0^\infty \int_0^{V^{-\alpha}} \frac{1}{V} Tr\left(e^{\Delta t}\right) e^{-at\xi} (at) \sqrt{2-\xi}\sqrt{\xi} d\xi\end{aligned} \tag{3.117}$$

Let us estimate the double integral term in (3.117):

$$\begin{aligned}\int_0^\infty \int_0^{V^{-\alpha}} \frac{C}{t^{3/2}} (at) e^{-at\xi} \sqrt{2-\xi}\sqrt{\xi} d\xi &\leq C \int_0^\infty \int_0^{V^{-\alpha}} \frac{a}{\sqrt{t}} e^{-at\xi} \sqrt{2}\sqrt{\xi} dt d\xi \\ &\leq \left(C\sqrt{2}a\right) \int_0^\infty \int_0^{V^{-\alpha/2}} e^{-a\eta^2 s^2} \frac{\eta d\eta}{\eta} \\ &\leq \left(C\sqrt{2}a\right) \int_0^\infty \int_0^{V^{-\alpha/2}} e^{-a\eta^2 s^2} s^2 ds d\eta \\ &\leq \left(C\sqrt{2}a\right) \int_0^{V^{-\alpha/2}} \frac{s^2}{as} ds = C' s^2|_0^{V^{-\alpha/2}} = C' V^{-\alpha}\end{aligned} \tag{3.118}$$

And now we will control the other terms. For the first term,

$$\begin{aligned}\int_{V^{-\alpha}}^{2}\int_{0}^{\infty}\frac{at}{(4\pi t)^{3/2}}e^{-at\xi}\sqrt{2-\xi}\sqrt{\xi}d\xi &= \frac{a}{(4\pi)^{3/2}}\int_{0}^{2}d\xi\int_{0}^{\infty}e^{-at\xi}\sqrt{2-\xi}\sqrt{\xi}\frac{dt}{\sqrt{t}}\\ &= \frac{1}{(4\pi)^{3/2}}\int_{0}^{2}d\xi\sqrt{2-\xi}\frac{1}{\sqrt{\xi}}\sqrt{\xi}\\ &= \frac{1}{(4\pi)^{3/2}}\int_{0}^{2}d\xi\sqrt{2-\xi}\end{aligned} \tag{3.119}$$

the error is also of the same order. Now looking at the cross term,

$$\begin{aligned}\int_{V^{-\alpha}}^{2}d\xi\sum_{q_1=1}^{\infty}\int_{0}^{\infty}\frac{e^{(-\pi q^2L^2/t)-at\xi}}{\sqrt{t}}dt\sqrt{2-\xi}\sqrt{\xi} &= \int_{V^{-\alpha}}^{2}\sum_{\substack{q_1\\ q_2,q_3=0}}^{\infty}\frac{e^{-qL\sqrt{a\xi}}}{\sqrt{a\xi}}\sqrt{2-\xi}\sqrt{\xi}d\xi\\ &= \int_{V^{-\alpha}}^{2}\frac{1}{e^{L\sqrt{a\xi}}-1}\sqrt{2-\xi}d\xi\\ &= \int_{V^{-\alpha}L^2}^{2L^2}\frac{1}{e^{\sqrt{a\bar{\xi}}}-1}\sqrt{2-\bar{\xi}/L^2}\frac{d\bar{\xi}}{L^2}\\ &= \frac{1}{L^2}\int_{V^{-\alpha}L^2}^{2L^2}\frac{\sqrt{2}}{e^{\sqrt{a\bar{\xi}}}-1}\left[1-\frac{\bar{\xi}}{4L^2}+\frac{\bar{\xi}^2}{16L^4}...\right]d\bar{\xi}\\ &= \frac{1}{L^2}\int_{1}^{2L^2}\frac{\sqrt{2}}{e^{\sqrt{a\bar{\xi}}}-1}\left[1-\frac{\bar{\xi}}{4L^2}...\right]d\bar{\xi}\end{aligned} \tag{3.120}$$

Note that we choose $V^{-\alpha}L^2 = 1$ to get a finite lower bound and we approximate (3.120) to be:

$$\approx \frac{1}{L^2}\int_{1}^{\infty}\frac{\sqrt{2}}{e^{\sqrt{a\bar{\xi}}}-1}\left[1-\frac{\bar{\xi}}{4L^2}...\right]d\bar{\xi} = \frac{1}{L^2}\int_{1}^{\infty}\frac{\sqrt{2}}{e^{\sqrt{a\xi}}-1}d\xi + O\left(\frac{1}{L^4}\right) \tag{3.121}$$

This now implies that (3.118) behaves as $C'V^{-2/3}$, of the same order as those terms. And finally, for the third term,

$$\int_{V^{-\alpha}}^{2}d\xi\int_{0}^{\infty}dt\sum_{\substack{q_1,q_2=1\\ q_3=0}}\frac{e^{(-(q_1^2+q_2^2)L^2/t)-at\xi}}{\sqrt{t}}\sqrt{2-\xi}\sqrt{\xi} \tag{3.122}$$

and noting that $\sqrt{q_1^2+q_2^2} \geq \frac{q_1+q_2}{2}$, we can show that:

$$\int_{V^{-\alpha}}^{2} d\xi \sum_{q_1,q_2} \frac{e^{-\sqrt{q_1^2+q_2^2}L\sqrt{a\xi}}}{\sqrt{a\xi}} \sqrt{\xi}\sqrt{2-\xi} \;\leq\; \int_{V^{-\alpha}}^{2} d\xi \sqrt{2-\xi} \sum_{q_1} e^{-q_1 \frac{L}{2}\sqrt{a\xi}} \sum_{q_2} e^{-q_2 \frac{L}{2}\sqrt{a\xi}} \tag{3.123}$$

Thus we find the above expression to be:

$$\begin{aligned}
&\leq \int_{V^{-\alpha}}^{2} d\xi \sqrt{2-\xi} \frac{1}{(e^{\frac{L}{2}\sqrt{a\xi}}-1)^2} = \frac{1}{L^2} \int_{V^{-\alpha}L^2}^{2L^2} d\xi' \sqrt{2-\frac{\xi'}{L^2}} \frac{1}{(e^{\frac{\sqrt{a\xi'}}{2}}-1)^2} \\
&\leq \frac{1}{L^2} \int_{1}^{\infty} d\xi' \sqrt{2} \left(1 - \frac{\xi'}{4L^2} + \frac{\xi'^2}{16L^4} \ldots\right) \frac{1}{(e^{\frac{\sqrt{a\xi'}}{2}}-1)^2} \\
&\leq \frac{1}{L^2} \int_{1}^{\infty} \frac{d\xi'\sqrt{2}}{(e^{\frac{\sqrt{a\xi'}}{2}}-1)^2} + O\left(\frac{1}{L^4}\right)
\end{aligned} \tag{3.124}$$

And finally, for the fourth term:

$$\int_{V^{-\alpha}}^{2} d\xi \sum_{q_1=1,q_2=1,q_3=1}^{\infty} \int_{0}^{\infty} dt \frac{e^{(-(q_1^2+q_2^2+q_3^2)L^2/t)-at\xi}}{\sqrt{t}} \sqrt{2-\xi}\sqrt{\xi} \tag{3.125}$$

We will make use of the inequality:

$$\sqrt{q_1^2+q_2^2+q_3^2} \geq \frac{q_1+q_2+q_3}{3} \tag{3.126}$$

This inequality can be proved with symmetry: Adding separately the right and the left hand sides of the following inequalities,

$$\begin{aligned}
\sqrt{q_1^2+q_2^2+q_3^2} &\geq \frac{q_1}{2} + \frac{q_2+q_3}{4} \\
\sqrt{q_1^2+q_2^2+q_3^2} &\geq \frac{q_2}{2} + \frac{q_1+q_3}{4} \\
\sqrt{q_1^2+q_2^2+q_3^2} &\geq \frac{q_3}{2} + \frac{q_1+q_2}{4}
\end{aligned}$$

One can easily obtain (3.126). So having (3.126) at hand, it is possible to bound the fourth term as well:

$$\int_{V^{-\alpha}}^{2} d\xi \sum_{q_1=1,q_2=1,q_3=1}^{\infty} \int_0^{\infty} dt \frac{e^{(-(q_1^2+q_2^2+q_3^2)L^2/t)-at\xi}}{\sqrt{t}} \sqrt{2-\xi}\sqrt{\xi}$$
$$= \int_{V^{-\alpha}L^2}^{2L^2} \frac{d\xi'}{L^2} \sqrt{2-\frac{\xi'}{L^2}} \left[\sum_{q_1=1}^{\infty} e^{-\sqrt{q_1^2+q_2^2+q_3^2}\sqrt{a\xi'}}\right]^3$$
$$\leq \frac{1}{L^2} \int_1^{2L^2} d\xi' \sqrt{2-\frac{\xi'}{L^2}} \left[\sum_{q=1}^{\infty} e^{-q\frac{\sqrt{a\xi'}}{3}}\right]^3$$
$$\leq \frac{1}{L^2} \int_1^{2L^2} \sqrt{2}\left(1-\frac{\xi'}{4L^2}+\frac{\xi'^2}{16L^4}\right) \frac{d\xi'}{\left(e^{-\frac{\sqrt{a\xi'}}{3}}-1\right)^3}$$
$$\leq \frac{1}{L^2}\sqrt{2} \int_1^{\infty} \frac{d\xi' e}{\left(e^{-\frac{\sqrt{a\xi'}}{3}}-1\right)^3} + O\left(\frac{1}{L^4}\right) \tag{3.127}$$

Hence $n_e^{(0)}(T=0) + \underbrace{n_e^{(1)}(T=0)}_{=0} + \underbrace{n_e^{(2)}(T=0)}_{O(1/L^2)}$ can be found.

Hence, we see that the depletion coefficient at $T = 0°K$ will not get finite size corrections of order $\frac{1}{V^{1/3}}$.

3.4. Corrections to the Ground State Energy at T=0°K by Scaling Analysis for the Heat Kernel

The method we use in this section is more general than the previous ones and valid for arbitrary domain. Now taking back from the ground state expression in (3.84), we rewrite,

$$\Delta E_g = \frac{aV}{2\pi} \int_0^{\infty} dt \int_0^{1} dx \sqrt{1-x^2} \left[(1-e^{-t(1-x)}) + (1-e^{-t(1+x)})\right] \frac{1}{V} \mathrm{Tr} e^{\Delta t/a} \tag{3.128}$$

Changing the variable t such that $t \to at$

$$\Delta E_g = \frac{a^2}{2\pi} \int_0^\infty dt \int_0^1 dx \sqrt{1-x^2} \left[(1 - e^{-at(1-x)}) + (1 - e^{-at(1+x)}) \right] \mathrm{Tr} e^{\Delta t} \tag{3.129}$$

The integral over t lies from 0 to ∞. We divide the integral over t into two pieces:

$$\Delta E_g = \frac{a^2}{2\pi} \int_0^1 dx \left[\int_0^{V^{\frac{2}{3}-}} dt + \int_{V^{\frac{2}{3}-}}^\infty dt \right] \sqrt{1-x^2} \left[(1 - e^{-at(1-x)}) + (1 - e^{-at(1+x)}) \right] \mathrm{Tr} e^{\Delta t} \tag{3.130}$$

where we choose

$$V^{\frac{2}{3}-} = V^{\frac{2}{3}} / ln(kV^{\frac{2}{3}}) \tag{3.131}$$

with k being some multiple of σ_s^{-2}. Inside the logarithm we can not have any dimensions and hence k should be cancelling out the dimension of $V^{2/3}$. Since the ground state energy is already given in terms of σ_s, we picked the natural length scale to be σ_s. By (3.131), we guaranteed that we have a small number at hand which can serve as the upper limit of the first integral.

$$\Delta E_g = \frac{a^2}{2\pi} \int_0^1 dx \left[\int_0^{V^{\frac{2}{3}-}} dt + \int_{V^{\frac{2}{3}-}}^\infty dt \right] F(t,x) \mathrm{Tr} e^{\Delta t} \tag{3.132}$$

$$\Delta E_g = \frac{a^2}{2\pi} \int_0^1 dx \left[\underbrace{\int_0^{V^{\frac{2}{3}-}} dt F(t,x) \mathrm{Tr} e^{\Delta t}}_{\text{(I)}} + \underbrace{\int_{V^{\frac{2}{3}-}}^\infty dt F(t,x) \mathrm{Tr} e^{\Delta t}}_{\text{(II)}} \right] \tag{3.133}$$

We consider flat space and $d = 3$. Part II is the regular integration over t and already has a well known expression for the flat space. For that we excluded the $0 \to V^{\frac{2}{3}-}$ part

from the integration:

$$(\mathrm{II}) \leq \int_{V^{\frac{2}{3}-}}^{\infty} dt F(t,x) \frac{C}{(4\pi t)^{3/2}} V \tag{3.134}$$

We will now be scaling the part (I). But before that, we should recall a point about the heat equation: If one desires to make a change of variables for the parameters of the heat equation while still preserving its original form:

$$u_t = \alpha u_{xx} \tag{3.135}$$

then, there should be a relation between the old and the new variables. Remarking that the equation keeps its form under the change of variables:

$$t \to s = kt \tag{3.136}$$

$$x \to y = \sqrt{k}x \tag{3.137}$$

Then it is obvious that the form will remain the same as long as the ratio

$$\frac{x}{\sqrt{t}} \tag{3.138}$$

remains the same for the new set of variables. This will permit us to rescale our heat kernel, the fundamental solution of the heat equation.

In a more general setting, the scaling of x corresponds to the scaling of the metric. So defining the initial metric to be g, we have

$$\int d_g(\mathbf{x}) = V \tag{3.139}$$

and

$$\int d_g(\mathbf{x}) K_t(x, x \mid g) = \mathrm{Tr} e^{\Delta t} \tag{3.140}$$

We want to scale the trace in (I) as t is very small within the region in question. But obviously we need the form of the heat equation to remain intact; this immediately brings along the necessity of both the space and time variables being transformed simultaneously. Setting a new metric $\tilde{g}$ as

$$g = V^{2/3} \tilde{g} \tag{3.141}$$

with

$$\int d_{\tilde{g}}(\mathbf{x}) = 1 \tag{3.142}$$

We know that the ratio $\frac{x}{\sqrt{t}}$ needs to remain constant for whatever variable transformation we make. So, since from (3.141) we see

$$x' = V^{-1/3} x \tag{3.143}$$

and define some

$$t' = \xi \tag{3.144}$$

Then, since

$$\frac{x}{\sqrt{t}} = \frac{x'}{t'} = \frac{V}{\sqrt{\xi t}} \tag{3.145}$$

we find

$$\xi = V^{-2/3} \tag{3.146}$$

Because a change of space variables has occured, it is more convenient to use the symbol of ∇_g instead of Δ for the Laplacian, for it is now important to emphasize its dependence on the basis/metric. Finally, making the convenient change of variables within the heat equation we can write:

$$\begin{aligned}\int d_g(\mathbf{x})K_t(x,x \mid g) &= \mathrm{Tr}(e^{t\nabla_g}) \\ &= \int d_{\tilde{g}}(\mathbf{x})K_{V^{-\frac{2}{3}}t}(x,x \mid \tilde{g}) \\ &= \mathrm{Tr}(e^{V^{-\frac{2}{3}}t\nabla_{\tilde{g}}})\end{aligned} \tag{3.147}$$

Going back to part (I) in (3.133), we now can write:

$$\Delta E_g = \frac{a^2}{2\pi}\int_0^1 dx \left[\int_0^{V^{\frac{2}{3}-}} dtF(t,x)\mathrm{Tr}(e^{V^{-\frac{2}{3}}t\nabla_{\tilde{g}}}) + \int_{V^{\frac{2}{3}-}}^{\infty} dtF(t,x)\mathrm{Tr}e^{\Delta t}\right] \tag{3.148}$$

where the bound of the second integral was already mentioned in (3.134). We will focus on the bounds of the first part, now that the trace is scaled for small t. The good thing is that small t asymptotics for the trace of the heat kernel are already present [36]: As $t \to 0^+$ and $V \to \infty$,

$$\mathrm{Tr}(e^{V^{-\frac{2}{3}}t\nabla_{\tilde{g}}}) \sim \frac{V_{\tilde{g}(\Omega)}}{(4\pi t V^{-\frac{2}{3}})^{\frac{3}{2}}} + \frac{A_{\tilde{g}}(\partial\Omega)}{16\pi t V^{-\frac{2}{3}}} + \ldots \tag{3.149}$$

So,

$$\begin{aligned}\Delta E_g \leq \frac{a^2}{2\pi}\Bigg(&\int_0^1 dx \left[\int_0^{V^{\frac{2}{3}-}} dtF(t,x)\left(\frac{V_{\tilde{g}}(\Omega)}{(4\pi t V^{-\frac{2}{3}})^{\frac{3}{2}}} + \frac{A_{\tilde{g}}(\partial\Omega)}{16\pi t V^{-\frac{2}{3}}} + \ldots\right)\right] \\ &+ \int_0^1 dxV \int_{V^{\frac{2}{3}-}}^{\infty} dtF(t,x)\frac{C'}{t^{3/2}}\Bigg)\end{aligned} \tag{3.150}$$

where $C' = C/(4\pi)^{3/2}$.

Remarking that for $V \to \infty$,

$$\lim_{V\to\infty} \frac{V_{\tilde{g}}(\Omega)}{(4\pi t V^{-\frac{2}{3}})^{\frac{3}{2}}} = \frac{V}{(4\pi t)^{3/2}} \tag{3.151}$$

we recover the flat space result, only with a difference of coefficient. So based on (3.134) and (3.151), we can write:

$$\Delta E_g \sim \frac{a^2}{2\pi}\Bigg\{\left[\int_0^1 dx \int_0^{V^{\frac{2}{3}-}} dt F(t,x)\frac{V}{(4\pi t)^{\frac{3}{2}}}\right] + \left[\int_0^1 dx \int_0^{V^{\frac{2}{3}-}} dt F(t,x)\frac{A_{\tilde{g}}(\partial\Omega)}{16\pi t V^{-\frac{2}{3}}}\right] + \left[\int_0^1 dx V \int_{V^{\frac{2}{3}-}}^{\infty} dt F(t,x)\frac{C}{4\pi t^{3/2}}\right]\Bigg\} \tag{3.152}$$

from which we can deduce that,

$$E_g = E_g^{\text{flat}} + O(V^{-\lambda}) \tag{3.153}$$

where $O(V^{-\lambda})$ is all of the corrections to the flat space ground state energy (or equally for our purposes, corrections onto the $V \to \infty$ limit.) Now considering the area term, we write

$$O_{area} = \frac{a^2}{2\pi}\int_0^1 dx \int_0^{V^{\frac{2}{3}-}} dt F(t,x)\frac{A(\partial\Omega)}{16\pi t} \tag{3.154}$$

while defining $A(\partial\Omega) = A_{\tilde{g}}(\partial\Omega)\, V^{\frac{2}{3}}$ to be a function of the area. Our aim will be to figure out whether the area term of the finite size correction will turn out to be negligible or not. Noting that

$$F(t,x) \leq \sqrt{1-x^2}\left[1 - e^{-at} + 1 - e^{-2at}\right] \tag{3.155}$$

$$\leq 2\sqrt{1-x^2}\left[1 - e^{-2at}\right] \tag{3.156}$$

And remarking the presence of the identity:

$$\int_0^{2a} e^{-\eta t} t d\eta = 1 - e^{-2at} \tag{3.157}$$

Hence, the area term,

$$O_{area} \leq \underbrace{\frac{a^2}{16\pi^2} \int_0^{\infty} dx\sqrt{1-x^2}}_{\equiv a^2 B'} \int_0^{V^{\frac{2}{3}-}} \int_0^{2a} e^{-\eta t} t \frac{dt}{t} A(\partial\Omega) \tag{3.158}$$

$$O_{area} \leq a^2 B' A(\partial\Omega) \int_0^{2a} \left[\frac{1 - e^{V^{-\eta\frac{2}{3}-}}}{\eta}\right] d\eta \tag{3.159}$$

Scaling the integral with

$$\eta' = \eta V^{\frac{2}{3}-} \tag{3.160}$$

and getting

$$O_{area} \leq B'(a^2 V) \left(\frac{A(\partial\Omega)}{V}\right) \left[\underbrace{\int_0^{\infty} (\frac{1 - e^{-\eta'})}{\eta'} d\eta'}_{(1)} + \int_1^{2aV^{\frac{2}{3}-}} \frac{d\eta'}{\eta'} - \underbrace{\int_1^{2aV^{\frac{2}{3}-}} \frac{e^{-\eta'} d\eta'}{\eta'}}_{(2)}\right] \tag{3.161}$$

Clearly (1) results in a finite number, whereas for (2) it is possible to say that:

$$\mid (2) \mid \leq \int_0^{\infty} e^{-\eta'} d\eta' = 1 \tag{3.162}$$

So for the expression (3.161), we end up with

$$O_{area} \leq B'(a^2V)\left(\frac{A(\partial\Omega)}{V}\right)\left[\text{const} + \ln(aV^{\frac{2}{3}-})\right] \tag{3.163}$$

Now we will consider the remaining part:

$$R = \frac{a^2}{2\pi}\int_0^\infty dx \int_{V^{\frac{2}{3}-}}^\infty dt\, F(t,x)\left(\frac{C'}{t^{\frac{3}{2}}}\right)V \tag{3.164}$$

Then

$$R \ \leq \frac{a^2C'V}{2\pi}\int_{V^{\frac{2}{3}-}}^\infty \int_0^\infty dx\sqrt{1-x^2}(1-e^{-2at})\frac{dt}{t^{3/2}} \tag{3.165}$$

Referring to identity (3.157),

$$R \ \leq \frac{a^2C'V}{2\pi}\int_{V^{\frac{2}{3}-}}^\infty \int_0^\infty dx\sqrt{1-x^2}\left[\int_0^{2a} d\eta e^{-\eta t}\right]\frac{dt}{t^{3/2}} \tag{3.166}$$

$$\leq \frac{a^2VC^*}{2\pi}\int_{V^{\frac{2}{3}-}}^\infty \int_0^{2a} d\eta e^{-\eta t}\frac{dt}{t^{3/2}} \tag{3.167}$$

Rearranging (3.167),

$$\frac{a^2VC^*}{2\pi}\int_{V^{\frac{2}{3}-}}^\infty \int_0^{2a} d\eta e^{-\eta t}\frac{dt}{t^{3/2}} = \frac{a^2C^*}{2\pi}\int_{V^{\frac{2}{3}-}}^\infty \int_0^{2a} e^{-\eta t}\frac{dt}{t^{3/2}}d\eta V \tag{3.168}$$

Again keeping up, changing and rescaling the integral parameters:

$$\frac{a^2C^*}{2\pi}\int_{V^{\frac{2}{3}-}}^\infty \int_0^{2a} e^{-\eta t}\frac{dt}{t^{3/2}}d\eta V \leq \frac{a^2VC^*}{2\pi}\int_0^{2a} d\eta \int_{V^{\frac{1}{3}-}}^\infty e^{-\eta u^2}du \tag{3.169}$$

$$\leq \frac{a^2 VC^*}{2\pi} \int_0^{2a} d\eta \int_0^{\infty} e^{-\eta(V^{\frac{1}{3}-}+v)^2} dv \tag{3.170}$$

$$\leq \frac{a^2 VC^*}{2\pi} \int_0^{2a} d\eta e^{-\eta V^{\frac{2}{3}-}} \int_0^{\infty} e^{-\eta v^2} dv \tag{3.171}$$

$$\leq \frac{a^2 VC^*}{2\sqrt{\pi}} \int_0^{2a} d\eta \frac{e^{-\eta V^{\frac{2}{3}-}}}{\sqrt{\eta}} \tag{3.172}$$

Now looking at (3.172), at present we can not estimate this part. Apart from this one, we had found the order to be $1/L$; but for this one, all we can say is that it is smaller than $\frac{a^2}{V^{1/3}}$. Trying a limit where $a \to 0$ makes unintended quantities disappear as well, so it seems that we need a more elaborate analysis; this one has not yielded the desired accuracy in our results.

4. CONCLUSION

The usage of the Poisson summation method is advantegous in many ways, although constrained to cuboidal geometries and periodic boundary conditions. By this method, we have seen that the condensate term arises naturally without being artificially implemented, along with a complete finite size effects term which is an infinite sum. We have analysed some steps of the Poisson summation method in greater detail. By applying the Poisson summation method to the interacting systems, we managed to get an idea about the order of correction that the depletion coefficient would get at $T = 0^{\circ}K$ and the finite temperature case for the same problem will be investigated for future treatments. Concerning the correction of the ground state energy at $T = 0^{\circ}K$, it seems that we might need more detailed expressions for the heat kernel to obtain a more accurant result.

APPENDIX A: ON THE PAIR CORRELATION FUNCTION

While following the systematic mathematical steps of the Section 2.2, their physical meanings from other points of view should be considered as well. For this, we'll basically follow the same steps in Section 2.2, yet look at the subject at hand from a slightly different stand, which will clarify our understanding of the expressions considered in Section 2.2. Knowing that N_0/N is directly related to the diagonal elements of the density matrix [2], another concept which is related to the off-diagonal elements of the density matrix is the pair correlation function: $\rho_1(\mathbf{r}, \mathbf{r'})$. The pair correlation function is the measure of the overlap between the given wave function of a system and the new wave function that would be formed after moving one of the particles from the position $\mathbf{r}$ to the position $\mathbf{r'}$. For this reason, the pair correlation function is taken to be some sort of measure for the long range order of the system [2]. Our aim is now to get an expression of the pair correlation function, of which we can make use in the Section 2.2.

Starting with

$$\rho_1(\mathbf{r}, \mathbf{r'}) = \rho_1(\mid \mathbf{r} - \mathbf{r'} \mid) = \left\langle \hat{\psi}^\dagger \hat{\psi} \right\rangle \tag{A.1}$$

and the field operator,

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{r}} \hat{a}_{\mathbf{k}} \tag{A.2}$$

and the number operator:

$$\hat{n}_{\mathbf{k}} = \hat{a}^+_{\mathbf{k}} \hat{a}_{\mathbf{k}} \tag{A.3}$$

We get,

$$\rho_1(|\ \mathbf{r}-\mathbf{r'}\ |) = \frac{1}{V}\sum_{\mathbf{kk'}} e^{i(\mathbf{k'.r'}-\mathbf{k.r})}\left\langle a_{\mathbf{k}^+} a_{\mathbf{k'}}\right\rangle = \frac{1}{V}\sum_{\mathbf{k}} e^{-i\mathbf{k.(r-r')}}\left\langle \hat{a}^+_{\mathbf{k}}\hat{a}_{\mathbf{k}}\right\rangle \tag{A.4}$$

$$= \frac{1}{V}\sum_{\mathbf{k}} n_{\mathbf{k}} e^{-i\mathbf{k.(r-r')}} \tag{A.5}$$

Clearly, the pair correlation function is the Fourier transform of the particle number density. And of course as,

$$n_{\mathbf{k}} = \frac{1}{e^{(\alpha+\beta\varepsilon(\mathbf{k}))}-1} = \sum_{j=1}^{\infty} e^{-j(\alpha+\beta\epsilon(\mathbf{k}))} \tag{A.6}$$

and

$$\epsilon(\mathbf{k}) = \frac{\hbar^2}{2m}(k_1^2+k_2^2+k_3^2) \text{ with } k_i = \frac{2\pi n_i}{L_i} \tag{A.7}$$

we get,

$$\rho_1(|\ \mathbf{r}-\mathbf{r'}\ |) = \frac{1}{V}\sum_{\mathbf{k}}\sum_{j=1}^{\infty} e^{-j\alpha\beta} e^{-j\beta\epsilon(\mathbf{k})} e^{-i\mathbf{k.(r-r')}} \tag{A.8}$$

$$\begin{aligned} &= \frac{1}{V}\sum_{j=1}^{\infty} e^{-j\alpha\beta}\sum_{k_1} e^{-ik_1.(x_1'-x_1)} e^{-j\lambda^2 {k_1}^2/4\pi}\sum_{k_2} e^{-ik_2.(x_2'-x_2)} e^{-j\lambda^2 {k_2}^2/4\pi} \\ &\times \sum_{k_3} e^{-ik_3.(x_3'-x_3)} e^{-j\lambda^2 {k_3}^2/4\pi} \end{aligned} \tag{A.9}$$

$$= \frac{1}{V}\sum_{j=1}^{\infty} e^{-j\alpha\beta} \sum_{n_1=-\infty}^{\infty} e^{-\frac{2\pi i n_1(x_1-x_1')}{L_1}} - j\pi {n_1}^2 \left(\frac{\lambda}{L_1}\right)^2 \sum_{n_2=-\infty}^{\infty} e^{-\frac{2\pi i n_2(x_2-x_2')}{L_2}} - j\pi {n_2}^2 \left(\frac{\lambda}{L_2}\right)^2$$
$$\times \sum_{n_3=-\infty}^{\infty} e^{-\frac{2\pi i n_3(x_3-x_3')}{L_3}} - j\pi {n_3}^2 \left(\frac{\lambda}{L_3}\right)^2 \tag{A.10}$$

Applying the Poisson summation method to the n-sum in (A.10) we get,

$$\sum_{n=-\infty}^{\infty} e^{-jwn^2} e^{-i\frac{2\pi n}{L}(x-x')} = \sum_{q=-\infty}^{\infty} e^{-\pi\left(\frac{L}{\lambda}\right)^2 \frac{(\tilde{x}/L-q)^2}{j}} \tag{A.11}$$

with

$$\tilde{x} = x - x' \tag{A.12}$$

Now defining,

$$a_i = \frac{\tilde{x}}{L_i} \tag{A.13}$$

and

$$\gamma(\mathbf{q}) = \pi \left[\left(\frac{L_1}{\lambda}\right)^2 (q_1 - a_1)^2 + \left(\frac{L_2}{\lambda}\right)^2 (q_2 - a_2)^2 + \left(\frac{L_3}{\lambda}\right)^2 (q_3 - a_3)^2 \right] \tag{A.14}$$

we obtain

$$\rho_1(|\ \mathbf{r} - \mathbf{r'}\ |) = \frac{1}{\lambda^3} \sum_{j=1}^{\infty} j^{-3/2} \sum_{q_{1,2,3}=-\infty}^{\infty} e^{-j\alpha} e^{-\gamma(\mathbf{q})j} \tag{A.15}$$

which is exactly the same expression with (2.24), only with the difference of a factor of $\frac{1}{L^3}$. But for the present treatment, there is even a more crucial difference: this time we take the long range order into consideration as well, by defining $\mathbf{a} \neq 0$.

Once again, adding the non contributing $j = 0$ term into the sum and applying (2.26),

we get the same result as (2.36), except the L^3 factor:

$$\rho_1(|\ \mathbf{r}-\mathbf{r'}\ |) = \frac{1}{\lambda^3}\sum_{\mathbf{q}}\sum_{l=-\infty}^{\infty}\sqrt{\frac{\pi}{\gamma(\mathbf{q})}}e^{-2\sqrt{\gamma(\mathbf{q})}(\alpha-2\pi il)^{1/2}} \tag{A.16}$$

(A.16) is extremely critical also for our calculations in Section 2.2. This is a complicated expression to keep up with and we should try to get a legitimate approximation instead; that would be of great help for our calculations in Section 2.2 as well. To simplify (A.16), the easiest way is to divide the sum into different parts and evaluate each part separately.

We will now write down three different sums which form the expression (A.16) when added altogether. Those are:

(i) A, sum for all q values ranging from $-\infty$ to ∞ & $l = 0$

(ii) B, sum for $q = 0$ & $l \neq 0$

(iii) C, sum for $q \neq 0$ & $l \neq 0$

Defining

$$y_i = \pi^{1/2}\alpha^{1/2}\frac{L_i}{\lambda} \tag{A.17}$$

the first part is obvious and easy:

$$A = \frac{\pi^{1/2}\alpha^{1/2}}{\lambda^3}\sum_{\mathbf{q}}\frac{e^{-2[y_1^2(q_1-a_1)^2+y_2^2(q_2-a_2)^2+y_3^2(q_3-a_3)^2]^{1/2}}}{[y_1^2(q_1-a_1)^2+y_2^2(q_2-a_2)^2+y_3^2(q_3-a_3)^2]^{1/2}} \tag{A.18}$$

The second part, B ($q = 0$ and $l \neq 0$) is more tricky and needs to be handled with more care.

For the sum does not include the non zero q values, we have

$$q = 0 \longrightarrow \gamma(0) = \frac{\pi}{\lambda^2}(L_1^2a_1^2 + L_2^2a_2^2 + L_3^2a_3^2) = \frac{\pi R^2}{\lambda^2} \tag{A.19}$$

with

$$R = (L_1^2 a_1^2 + L_2^2 a_2^2 + L_3^2 a_3^2)^{1/2} = (\tilde{x_1}^2 + \tilde{x_2}^2 + \tilde{x_3}^2)^{1/2} = \mid \mathbf{r} - \mathbf{r'} \mid \tag{A.20}$$

Then B becomes,

$$B = \pi^{1/2} \frac{1}{\lambda^3} \sum_l{}' \frac{e^{-2\sqrt{\gamma(0)}(\alpha - 2\pi i l)^{1/2}}}{\sqrt{\gamma(0)}} = \pi^{1/2} \frac{1}{\lambda^3} \sum_l{}' \frac{e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha - 2\pi i l)^{1/2}}}{\sqrt{\pi}\left(\frac{R}{\lambda}\right)} \tag{A.21}$$

$$= \frac{1}{R\lambda^2} \sum_l{}' e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha - 2\pi i l)^{1/2}} \tag{A.22}$$

Noticing that,

$$(\alpha - i2\pi l) = (\alpha^2 + 4\pi^2 l^2)^{1/2} e^{i\theta} \tag{A.23}$$

We rewrite B as,

$$\begin{aligned}
B &= \frac{1}{R\lambda^2} \sum_l{}' e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2 + 4\pi^2 l^2)^{1/4} e^{i\theta/2}} \\
&= \frac{1}{R\lambda^2} \sum_l{}' e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2 + 4\pi^2 l^2)^{1/4} [cos(\theta/2) + isin(\theta/2)]} \\
&= \frac{1}{R\lambda^2} \sum_l{}' e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2 + 4\pi^2 l^2)^{1/4} cos(\theta/2)} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2 + 4\pi^2 l^2)^{1/4} isin(\theta/2)} \\
&= \frac{1}{R\lambda^2} \sum_{l=1}^{\infty} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2 + 4\pi^2 l^2)^{1/4} cos(\theta/2)} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2 + 4\pi^2 l^2)^{1/4} isin(\theta/2)} \\
&+ \frac{1}{R\lambda^2} \sum_{l=-\infty}^{l=-1} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2 + 4\pi^2 l^2)^{1/4} cos(\theta/2)} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2 + 4\pi^2 l^2)^{1/4} isin(\theta/2)}
\end{aligned} \tag{A.24}$$

Here, sums over positive l and negative l's cover the fourth and the first quadrants; hence span the complex space with opposite signed θ's. The only part of that depend on the sign of l is $e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2 + 4\pi^2 l^2)^{1/4} isin(\theta/2)}$ and the rest is same for both. Thus, we

can write,

$$B = \frac{1}{R\lambda^2}\{\sum_{l=1}^{l=\infty} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2+4\pi^2l^2)^{1/4}cos(\theta/2)} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2+4\pi^2l^2)^{1/4}isin(\theta/2)} + \sum_{l=1}^{l=\infty} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2+4\pi^2l^2)^{1/4}cos(\theta/2)} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2+4\pi^2l^2)^{1/4}(-isin(\theta/2))}\} \quad \text{(A.25)}$$

$$= \frac{1}{R\lambda^2}\sum_{l=1}^{l=\infty} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2+4\pi^2l^2)^{1/4}cos(\theta/2)}\{e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2+4\pi^2l^2)^{1/4}isin(\theta/2)} + e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2+4\pi^2l^2)^{1/4}(-isin(\theta/2))}\} \quad \text{(A.26)}$$

$$= \frac{1}{R\lambda^2}\sum_{l=1}^{l=\infty} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2+4\pi^2l^2)^{1/4}cos(\theta/2)}\left[2cos\left(-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(\alpha^2+4\pi^2l^2)^{1/4}sin(\theta/2)\right)\right] \quad \text{(A.27)}$$

(A.27) is far too messy for us to proceed with its exact form. We will try to approximate B or to be more clear, get an upper bound for B that will give us an idea about the highest order that it can have. Within the expression $(\alpha^2 + 4\pi^2l^2)$, α is a finite value for a configuration of the system, while summation over l spans to infinity; so α term can be neglegted.

$$B = \frac{2}{R\lambda^2}\sum_{l=1}^{l=\infty} e^{-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(4\pi^2l^2)^{1/4}cos(\theta/2)}\left[cos\left(-2\sqrt{\pi}\left(\frac{R}{\lambda}\right)(4\pi^2l^2)^{1/4}\right)\right]$$
$$= \frac{2}{R\lambda^2}\sum_{l=1}^{l=\infty} e^{-2^{3/2}\pi\left(\frac{R}{\lambda}\right)l^{1/2}cos(\theta/2)}\left[cos\left(-2^{3/2}\pi\left(\frac{R}{\lambda}\right)l^{1/2}\right)\right] \quad \text{(A.28)}$$

The terms within the brackets on the right is a cosine term, so it is bounded between -1 and 1. 1 being the value contributing the most, we will ignore this part altogether. For the exponential, we look for the smallest power that will make the overall expression the largest. Looking at

$$\sum_{l=1}^{\infty} e^{-2^{3/2}\pi\left(\frac{R}{\lambda}\right)l^{1/2}cos(\theta/2)} \quad \text{(A.29)}$$

we see that the $cos(\theta/2)$ should get its minimum value. The imaginary number of which θ is the phase is $(\alpha + 2\pi il)$, so

$$cos(\theta) = \frac{\alpha}{\sqrt{\alpha^2 + 4\pi^2 l^2}} \tag{A.30}$$

Then

$$cos(\theta/2) = \sqrt{\left[\frac{1}{2} + \frac{\alpha}{2\sqrt{\alpha^2 + 4\pi^2 l^2}}\right]^{1/2}} \tag{A.31}$$

The term

$$\frac{\alpha}{2\sqrt{\alpha^2 + 4\pi^2 l^2}} \tag{A.32}$$

will never get a value larger than $\frac{1}{2}$ which occurs for the $l = 0$ case. For any l other than zero, it will get a smaller value and finally converge to 0 as $l \to \infty$. Whatever the case, it is larger than or equal to zero. Then we are left with:

$$cos(\theta/2) \geq \frac{1}{\sqrt{2}} \tag{A.33}$$

and

$$e^{-2^{3/2}\pi\left(\frac{R}{\lambda}\right)l^{1/2}cos(\theta/2)} \leq e^{-2\pi\left(\frac{R}{\lambda}\right)l^{1/2}} \tag{A.34}$$

Omitting the factor of 2π as well, we will try to get a bound for the expression

$$\sum_{l=1}^{\infty} e^{-\frac{R}{\lambda}\sqrt{l}} \tag{A.35}$$

Defining some $\kappa = \frac{R}{\lambda}$ and using the Euler-Maclaurin summation formula [11], we can write

$$\sum_{n=1}^{\infty} e^{-\kappa\sqrt{n}} = \frac{f(1)}{2} + \int_1^{\infty} e^{-\kappa\sqrt{x}}dx + \int_1^{\infty} (e^{-\kappa\sqrt{x}})' \left(x - [x] - \frac{1}{2}\right) dx \tag{A.36}$$

The first term on the right hand side of (A.36) is of order $e^{-\frac{R}{\lambda}}$.
Now for the second on the right hand side of (A.36), we write:

$$\int_1^{\infty} e^{-\kappa\sqrt{x}}dx = \int_1^{\infty} e^{-\kappa\frac{\sqrt{x}}{2}} e^{-\kappa\frac{\sqrt{x}}{2}} dx \tag{A.37}$$

The maximum value which $e^{-\kappa\frac{\sqrt{x}}{2}}$ can have for the possible x values is $e^{-\frac{\kappa}{2}}$. Making use of that to get a bound for (A.37):

$$\int_1^{\infty} e^{-\kappa\frac{\sqrt{x}}{2}} e^{-\kappa\frac{\sqrt{x}}{2}} dx \leq e^{-\frac{\kappa}{2}} \int_1^{\infty} e^{-\kappa\frac{\sqrt{x}}{2}} dx \leq e^{-\frac{\kappa}{2}} \int_0^{\infty} e^{-\kappa\frac{\sqrt{x}}{2}} dx \tag{A.38}$$

Changing the variables as $\eta \equiv \frac{\sqrt{x}}{2}$,

$$\int_1^{\infty} e^{-\kappa\frac{\sqrt{x}}{2}} e^{-\kappa\frac{\sqrt{x}}{2}} dx \leq e^{-\frac{\kappa}{2}} \left(\int_0^{\infty} e^{-\kappa\eta} \eta d\eta \right) \tag{A.39}$$

and solving the Gaussian integral we get:

$$\int_1^{\infty} e^{-\kappa\frac{\sqrt{x}}{2}} e^{-\kappa\frac{\sqrt{x}}{2}} dx \leq 8\frac{e^{-\frac{\kappa}{2}}}{\kappa^2} \tag{A.40}$$

It turns out that the second term of the right hand side of (A.36) is of exponential order too, which is $e^{-\frac{R}{2\lambda}}$. And the last term:

$$\begin{aligned}
&\int_1^\infty (e^{-\kappa\sqrt{x}})' \left(x - [x] - \frac{1}{2}\right) dx = \int_1^\infty \left[\frac{\kappa}{\sqrt{x}}\right] (e^{-\kappa\sqrt{x}}) \left(x - [x] - \frac{1}{2}\right) dx \\
&= \int_1^2 \left[\frac{\kappa}{\sqrt{x}}\right] (e^{-\kappa\sqrt{x}}) \left(x - [x] - \frac{1}{2}\right) + \int_2^3 \left[\frac{\kappa}{\sqrt{x}}\right] (e^{-\kappa\sqrt{x}}) \left(x - [x] - \frac{1}{2}\right) + ... \\
&= \int_1^2 (...) + \int_2^3 (...) + \int_3^4 (...) + \int_4^5 (...) + ... \qquad \text{(A.41)}
\end{aligned}$$

Shifting the variable x to the left as $x \to x + k$ for each $k = 1, 2, 3, ...$; it becomes possible to write:

$$\int_1^\infty (e^{-\kappa\sqrt{x}})' \left(x - [x] - \frac{1}{2}\right) dx = \sum_{k=1}^\infty \int_0^1 \frac{\kappa}{\sqrt{x+k}} e^{-\kappa\sqrt{x+k}} \left(x - \frac{1}{2}\right) dx \qquad \text{(A.42)}$$

For

$$\frac{\sqrt{x} + \sqrt{k}}{2} > \sqrt{x+k} \qquad \text{(A.43)}$$

and noticing that

$$\frac{\kappa}{\sqrt{x}} > \frac{\kappa}{\sqrt{x+k}} \qquad \text{(A.44)}$$

We can bound (A.42) as:

$$\begin{aligned}
\sum_{k=1}^\infty \int_0^1 \frac{\kappa}{\sqrt{x+k}} e^{-\kappa\sqrt{x+k}} \left(x - \frac{1}{2}\right) dx &< \sum_{k=1}^\infty \int_0^1 \frac{\kappa}{\sqrt{x}} e^{-\kappa\frac{\sqrt{x}}{2}} e^{-\kappa\frac{\sqrt{k}}{2}} \left(x - \frac{1}{2}\right) dx \\
&= \sum_{k=1}^\infty e^{-\kappa\frac{\sqrt{k}}{2}} \int_0^1 \frac{\kappa}{\sqrt{x}} e^{-\kappa\frac{\sqrt{x}}{2}} \left(x - \frac{1}{2}\right) dx \qquad \text{(A.45)}
\end{aligned}$$

The integral in (A.45) will obviously result in some polynomial expression dependent on the parameter κ. Then,

$$\sum_{k=1}^{\infty} e^{-\kappa\frac{\sqrt{k}}{2}} \int_0^1 \frac{\kappa}{\sqrt{x}} e^{-\kappa\frac{\sqrt{x}}{2}} \left(x - \frac{1}{2}\right) dx < e^{-\frac{\kappa}{2}} P(\kappa) \tag{A.46}$$

From (A.46), we finally see that the third term on the right hand side of (A.36) is also of order $e^{-\frac{R}{2\lambda}}$. Eventually we deduce that B is at most of order $e^{-\frac{R}{\lambda}}$. The last part C (having $q \neq 0$ and $l \neq 0$) is the generalization of the second part, with R being replaced with $[L_1^2(q_1 - a_1)^2 + L_2^2(q_2 - a_2)^2 + L_3^2(q_3 - a_3)^2]^{1/2}$.
So,

$$C = \frac{2}{\lambda^2} {\sum_{\mathbf{q}}}' \sum_{l=1}^{l=\infty} \frac{e^{-2^{3/2}\pi\frac{l^{1/2}}{\lambda}[L_1^2(q_1-a_1)^2+L_2^2(q_2-a_2)^2+L_3^2(q_3-a_3)^2]^{1/2}}}{[L_1^2(q_1 - a_1)^2 + L_2^2(q_2 - a_2)^2 + L_3^2(q_3 - a_3)^2]^{1/2}}$$
$$\times \left[cos\left(\frac{-2^{3/2}\pi l^{1/2}}{\lambda}[L_1^2(q_1 - a_1)^2 + L_2^2(q_2 - a_2)^2 + L_3^2(q_3 - a_3)^2]^{1/2}]\right)\right] \tag{A.47}$$

The steps to obtain the highest possible order of C are exactly the same with the ones of B. Similarly, we find that C is at most of order $e^{-\frac{L}{\lambda}}$. Finally when all these parts are summed, we get: $A + B + C = \rho_1(|\ \mathbf{r} - \mathbf{r'}\ |)$ It would be wise to check each of these three parts to see whether any of them are small enough to be neglegted. Obviously for systems within the interest of statistical physics, $L_i/\lambda >> 1$. And when it's the long range correlations that one is interested in, $R/\lambda >> 1$ is also a valid condition. So in this case, B and C terms turn out to be negligible, with an error order of $e^{(-R/\lambda)}$ and $e^{(-L/\lambda)}$ respectively:

$$B \sim O(e^{-R/\lambda}) \text{ and } C \sim O(e^{-L/\lambda}) \tag{A.48}$$

Now that we have seen the orders of the pieces the pair correlation function consists of, we will go back to the step before opening up the sum. Now adopting the convention of $G(\mathbf{R})$ for the pair correlation function of the ideal Bose gas; we will obtain a useful

quantity that is directly related to the order of the system: The correlation length [1].

$$G(\mathbf{R}) = \frac{1}{V}\sum_{\mathbf{k}} \frac{e^{i\mathbf{k}.\mathbf{R}}}{e^{\alpha+\beta\epsilon(\mathbf{k})}-1} \tag{A.49}$$

Replacing the sum by integration and keeping the ground state aside:

$$G(\mathbf{R}) = \frac{N_0}{V} + \frac{1}{(2\pi)^d}\int \frac{e^{i\mathbf{k}.\mathbf{R}}}{e^{\alpha+\beta\hbar^2k^2/2m}-1} d^dk \tag{A.50}$$

For the evaluation of an integral of the form

$$I(\mathbf{r}) = \int f(k) e^{i\mathbf{r}.\mathbf{k}} d^nk \tag{A.51}$$

where $d^nk = k^{n-1}(sin\theta_1)^{n-2}...(sin\theta_{n-2})^1 dk d\theta_1 ... d\theta_{n-2} d\phi$ is the unit n dimensional volume in spherical polar coordinates, we know that another equivalent form is the following [1]

$$I(\mathbf{r}) = (2\pi)^{n/2}\int_0^\infty f(k)\left(\frac{1}{rk}\right)^{(n-2)/2} J_{(n-2)/2}(rk) k^{n-1} dk \tag{A.52}$$

where $J_\nu(x)$ is the ordinary Bessel function. For

$$f(k) = \frac{1}{e^{\alpha+\beta\hbar^2k^2/2m}-1} \tag{A.53}$$

$$\begin{aligned} G(\mathbf{R}) &= \frac{N_0}{V} + \frac{1}{(2\pi)^d}(2\pi)^{d/2}\int_0^\infty \frac{1}{e^{\alpha+\beta\hbar^2k^2/2m}-1}\left(\frac{1}{kR}\right)^{(d-2)/2} J_{(d-2)/2}(kR)\, k^{d-1} dk \\ &= \frac{N_0}{V} + \frac{1}{(2\pi)^{d/2}}\left(\frac{1}{R}\right)^{(d-2)/2}\sum_{j=1}^\infty e^{-j\alpha}\int_0^\infty e^{-j\beta\hbar^2k^2/2m} J_{(d-2)/2}(kR) k^{d/2} dk \end{aligned}$$

From [12],

$$\int_0^\infty x^{\nu+1} e^{-\alpha x^2} J_\nu(\gamma x) dx = \frac{\gamma^\nu}{(2\alpha)^{\nu+1}} e^{-\gamma^2/4\alpha} \quad \text{for Re } \alpha > 0, \text{ Re } \nu > -1 \tag{A.54}$$

For $\nu = \frac{d-2}{2}$ and $\alpha = \frac{j\beta\hbar^2}{2m} = \frac{\lambda^2 j}{4\pi}$

$$G(\mathbf{R}) = \frac{N_0}{V} + \frac{1}{(2\pi)^{d/2}} \left(\frac{1}{R}\right)^{(d-2)/2} \sum_{j=1}^{\infty} e^{-j\alpha} \frac{R^{(d-2/2)}}{2^{d/2}} \left(\frac{4\pi}{j\lambda^2}\right)^{(d/2)} e^{-\frac{R^2\pi}{\lambda^2 j}} \tag{A.55}$$

$$G(\mathbf{R}) = \frac{N_0}{V} + \frac{1}{\lambda^d} \sum_{j=1}^{\infty} e^{-j\alpha - \frac{\pi R^2}{j\lambda^2}} j^{-d/2} \tag{A.56}$$

As the $j = 0$ term is 0 for nonzero R values, so it can be added into the sum:

$$\begin{aligned} G(\mathbf{R}) &= \frac{N_0}{V} + \frac{1}{\lambda^d} \sum_{j=0}^{\infty} e^{-j\alpha - \frac{\pi R^2}{j\lambda^2}} j^{-d/2} \\ &= \frac{N_0}{V} + \frac{2\alpha^{(d-2)/4}}{\lambda^{(d+2)/2} \pi^{(d-2)/4} R^{(d-2)/2}} K_{(d-2)/2} \left[\frac{R 2\pi^{1/2} \alpha^{1/2}}{\lambda}\right] \end{aligned}$$

Here our variable is R. So it seems logical to gather the rest of the quantities within the Bessel function in one single quantity. This would give us the possibility to compare it to R and observe the asymptotic behaviour of the Bessel function more clearly. For this reason we define the correlation length as,

$$\xi = \frac{\lambda}{2\pi^{1/2}\alpha^{1/2}} \tag{A.57}$$

We then write,

$$G(\mathbf{R}) = \frac{N_0}{V} + \frac{2}{\lambda^2 (2\pi\xi R)^{(d-2)/2}} K_{(d-2)/2} \left(\frac{R}{\xi}\right) \tag{A.58}$$

To proceed further, we need to know about the behaviour of α. While approaching the critical temperature from above ($T \gtrsim T_{cr}$), α behaves as [1]

$$\alpha \backsim t^{2/(d-2)} \tag{A.59}$$

where

$$t = (T - T_{cr})/T_{cr} \text{ and, } 0 < t << 1 \tag{A.60}$$

For such an α, the correlation length then becomes,

$$\xi \sim \lambda \left(\frac{1}{t}\right)^{1/(d-2)} \tag{A.61}$$

and so obviously $\xi >> \lambda$, which means that only at distances much larger than the thermal wavelength the system can grasp order. Eventually, if for our purposes we take $R >> \xi$, the final approximated form of the pair correlation function ends up to be:

$$G(\mathbf{R}) \approx \frac{1}{\lambda^2 (2\pi\xi^{(d-3)/2}) R^{(d-1)/2}} e^{-R/\xi} \tag{A.62}$$

APPENDIX B: A SHORT REVIEW ON HEAT KERNELS

We will make a very short review about the heat kernels, 'the fundamental solution of the heat equation'. The solution to the one dimensional homogeneous heat equation with Neumann boundary conditions is a subject treated in most of the introductory differential equations texts, so we will skip the intermediate steps and just mention the well known results. The heat equation in d-dimensions is:

$$\frac{\partial u}{\partial t} = \alpha \Delta u \tag{B.1}$$

where α is the thermal diffusivity. To simplify things, we will take α to be 1 throughout the treatment and solve the equation in just one dimension:

$$u_t(x,t) = u_{xx}(x,t),\ x \in M \tag{B.2}$$

$$u_x(x,t) = 0,\ x \in \partial M \tag{B.3}$$

$$u(x,0) = \phi(x)\ x \in M \tag{B.4}$$

where M is an open and bounded set: (-L,L) $\subset \mathbb{R}$ The solution can be written as:

$$u(x,t) = \sum_{-\infty}^{\infty} a_n e^{\frac{in\pi x}{2L}} e^{-\left(\frac{n\pi}{2L}\right)^2 t} \tag{B.5}$$

with the initial value problem

$$u(x,0) = \phi(x) = \sum_{-\infty}^{\infty} \left[\frac{1}{4L} \int_{-L}^{L} \phi(y) e^{-\frac{in\pi y}{2L}} dy \right] e^{\frac{in\pi x}{2L}} \tag{B.6}$$

$$u(x,t) = \phi(x)e^{-k^2t} \tag{B.7}$$

where

$$k_n = \frac{n\pi}{2L} \tag{B.8}$$

Fourier transforming the heat equation gives:

$$\tilde{u_t}(k,t) = \alpha\tilde{u_{xx}}(k,t) = -\alpha k^2\tilde{u}(k,t) \tag{B.9}$$

Solving this equation now gives as solution:

$$\tilde{u}(k,t) = \tilde{\phi}(k)e^{-\alpha k^2t} \tag{B.10}$$

We write $u(x,t)$ as the inverse Fourier transform of $\tilde{u}(k,t)$:

$$\begin{aligned} u(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\tilde{u}(k,t)dk \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\tilde{\phi(k)}e^{-\alpha k^2t}dk \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-iky}\phi(y)dy\right]e^{-\alpha k^2t}dk \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dy\phi(y)\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ik(y-x)}e^{-\alpha k^2t}dk\right] \end{aligned} \tag{B.11}$$

It is seen that the term in brackets is the Fourier transform of $e^{-\alpha k^2t}$. Defining $h(y-x)$ to be the inverse Fourier transform of $\tilde{h} = e^{-\alpha k^2t}$, we write

$$u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dy\,\phi(y)\,h(y-x) \tag{B.12}$$

Calculating the integral

$$h(y-x) = \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik(y-x)} e^{-\alpha k^2 t} dk \right] \tag{B.13}$$

we find

$$h(y-x) = \frac{1}{\sqrt{2\alpha t}} e^{-\frac{(y-x)^2}{4\alpha t}} \tag{B.14}$$

Solution to the one dimensional heat equation for Neumann boundary conditions is then found to be:

$$u(x,t) = \frac{1}{\sqrt{4\pi\alpha t}} \int_{-\infty}^{\infty} \phi(y) e^{-\frac{(x-y)^2}{4\alpha t}} dy \tag{B.15}$$

Generalizing this to the d-dimensional case,

$$u(\mathbf{x},t) = \frac{1}{\sqrt{4\pi\alpha t}} \int_{\mathbb{R}^d} \phi(\mathbf{y}) e^{-\frac{|x-y|^2}{4\alpha t}} d(\mathbf{y}) \tag{B.16}$$

and also (B.14)

$$H(\mathbf{x},\mathbf{y},t) = \frac{1}{(4\pi\alpha t)^{d/2}} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4\alpha t}} \tag{B.17}$$

Now we define

$$K_t(\mathbf{x},\mathbf{y}) \equiv \begin{cases} H(\mathbf{x},\mathbf{y},t), & t > 0 \\ 0, & t < 0 \end{cases} \tag{B.18}$$

And by using the convolution, we can write

$$u(\mathbf{x},t) = [K_t * \phi](x) = \int_{\mathbb{R}^d} K_t(\mathbf{x},\mathbf{y}) \phi(\mathbf{y}) d(\mathbf{y}) \tag{B.19}$$

Looking at (B.19) we see that the t depence of the heat equation's solution is all loaded upon $J_t(\mathbf{x}, \mathbf{y})$. And especially if it is possible to write such that (if there exists such a function $J(\mathbf{x}, \mathbf{y})$ for some operator $\hat{J}$):

$$\int J(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d(\mathbf{y}) = \hat{J} f(\mathbf{x}) \tag{B.20}$$

then $J(\mathbf{x}, \mathbf{y})$ is called the kernel of the operator $\hat{J}$. It is highly probable that this may not be the case for an operator $\hat{J}$: The kernel of an operator might not exist. Luckily, apparently for our case, what we have just called to be 'the heat kernel' is the kernel of the operator $e^{\Delta t}$:

$$e^{\Delta t} f(\mathbf{x}) = \int_M K_t(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d(\mathbf{y}) \tag{B.21}$$

Detailed properties for the heat kernel can be found in [36]. We have a very useful theorem at hand, which is extremely critical and indispensible for us. It it this theorem that permits us to use the introduce the concept of heat kernel into our work. The work by Dodziuk states [37]:

$$K_t(\mathbf{x}, \mathbf{y}) = \sum_{i=0} e^{-\lambda_i t} \psi_i(\mathbf{x}) \psi_i(\mathbf{y}) \tag{B.22}$$

Throughout all our work, the applicability conditions of this theorem [37] will be satisfied. With the help of this theorem, and the fact that the eigenvalues of the Laplacian can be chosen to be all real [27], we are able to write

$$\int_M K_t(\mathbf{x}, \mathbf{x}) d(\mathbf{x}) = \int \sum_{i=0} e^{-\lambda_i t} \mid \psi_i(\mathbf{x}) \mid^2 d(\mathbf{x}) = \sum_{i=0} e^{-\lambda_i t} = \mathrm{Tr} e^{\Delta t} \tag{B.23}$$

By this theorem, it is clear that the heat equation and the heat kernel are inarguably related to the eigenvalues and the eigenfunctions of the Laplacian.

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