

BOSE-EINSTEIN CONDENSATION ON A RIEMANNIAN MANIFOLD WITH  
NONNEGATIVE RICCI CURVATURE

by

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*To my family*

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## ABSTRACT

### **BOSE-EINSTEIN CONDENSATION ON A RIEMANNIAN MANIFOLD WITH NONNEGATIVE RICCI CURVATURE**

In this thesis, the properties of the Bose-Einstein condensation in flat spaces are reviewed. Three dimensional weakly interacting Bose systems are examined by using the Bogoliubov approximation. The heat kernel of the Laplace operator is introduced. The Bose-Einstein condensation for an ideal gas and for a weakly interacting gas in the nonrelativistic limit on a Riemannian manifold with nonnegative Ricci curvature is studied using the heat kernel and eigenvalue estimates of the Laplace operator. The Bose gas is assumed to obey the Neumann boundary conditions. Behaviour of the chemical potential at low temperatures is described. Bounds for the depletion of the condensate and for the critical temperature of an ideal Bose system are derived in the thermodynamic limit. We observed that the condensation does not take place in two dimensions, however it is formed in three dimensions which is consistent with the flat space results. In the case of dilute gases on a compact Riemannian manifold, Bogoliubov theory is applied. The ground state of a dilute Bose system is analyzed using the heat kernel methods. Specifically, the depletion of the condensate is estimated at absolute zero temperature. For finite volumes, we concluded that the condensate exists in two dimensions for weakly interacting gases. We also analyzed the depletion of the condensate at finite temperatures. Inconsistency of the Bogoliubov approximation in the thermodynamic limit is shown using heat kernel methods. Justification of the  $c$ -number substitution on a manifold is given.

## ÖZET

# NEGATİF OLMAYAN RICCI EĞRİLİĞİNE SAHİP BİR RIEMANN ÇOKKATLISINDA BOSE-EINSTEIN YOĞUNLAŞMASI

Bu tezde, düz uzaylarda Bose-Einstein yoğunlaşmasının özellikleri gözden geçirilmiştir. Bogoliubov yaklaşımı kullanılarak üç boyutta zayıf etkileşimli Bose sistemleri incelenmiştir. Laplace operatörünün ısı çekirdeği takdim edilmiştir. Negatif olmayan Ricci eğriliğine sahip bir Riemann çokkathısında klasik limitte (parçacık hızlarının ışık hızından çok küçük olduğu durum) ideal gazlar ve zayıf etkileşimli gazlar için Laplace operatörünün ısı çekirdeği ve özdeğer tahminleri kullanılarak Bose-Einstein yoğunlaşması incelenmiştir. Bu incelemede Bose gazının Neumann sınır şartlarını sağladığı varsayılmıştır. Düşük sıcaklıklarda kimyasal potansiyelin davranışı tasvir edilmiştir. İdeal Bose gazları için yoğunluğun tükenimine ve kritik sıcaklığa sınırlar türetilmiştir. Düz uzaylardaki çözümle tutarlı olarak yoğunlaşmanın iki boyutlu çokkathılarda gerçekleşmediği fakat üç boyutlu çokkathılarda gerçekleştiği gözlenmiştir. Seyreltik gazlar durumunda Bogoliubov teorisi kullanılmıştır. Zemin hali ısı çekirdeği metotları yardımıyla analiz edilmiştir. Özel olarak, mutlak sıfır sıcaklığında Bose-Einstein yoğunluğunun tükenimi tahmin edilmiştir. Zayıf etkileşimli gazlar için sonlu hacimlerde yoğunlaşmanın iki boyutlu çokkathılarda gerçekleştiği gözlenmiştir. Ayrıca sonlu sıcaklıklarda yoğunluğun tükenimi analiz edilmiştir. Isı çekirdeği metotları kullanılarak termodinamik limitte Bogoliubov yaklaşımının tutarsızlığı gösterilmiştir. Bir çokkathıda sabit sayı ikamesinin gerekçelendirilmesi verilmiştir.

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## LIST OF SYMBOLS

$\mathcal{G}$	Grand partition function
$\hbar$	Reduced Planck constant
$\hat{H}$	Hamiltonian operator
$g$	Coupling constant
$k$	Boltzmann constant
$n$	Number density
$O$	Order
$T_c$	Critical temperature
Tr	Trace
$\beta$	Temperature parameter
$\lambda_{dB}$	de Broglie wavelegth
$\mu$	Chemical potential
$\sigma$	Single-particle state

## LIST OF ACRONYMS/ABBREVIATIONS

BE	Bose-Einstein
<i>e.g.</i>	Exempli gratia (“for example”)
<i>et al.</i>	Et alii (“and others”)
<i>i.e.</i>	Id est (“that is”)
ODE	Ordinary Differential Equations
PDE	Partial Differential Equations

# 1. INTRODUCTION

## 1.1. Definition

Bose-Einstein (BE) condensation is a remarkable feature of quantum mechanical characteristics of particles. It is described as a phenomenon of macroscopic occupation of single-particle states. Bose gas, which is comprised of Bose particles (bosons), displays a phase change as the de Broglie wavelength,  $\lambda_{dB} = (2\pi\hbar^2/mkT)^{1/2}$ , is comparable to the interatomic separation. In this limit, bosons lose their identities and do not behave like individual particles. It can be observed that, de Broglie wavelength rises as the temperature of the system falls, leading to a dense “quantum soup” phase which is a mixture of non-localized bosons. From the classical point of view, this feature is incomprehensible as the classical mechanics is not able to predict such a phenomenon due to over-generalization of classical nature of particles to low temperatures. However, the wave-particle duality (postulating that all particles exhibit both wave and particle properties) and quantum statistics which classifies bosons as identical - indistinguishable - particles introduces a new viewpoint.

A phase transition is the transformation of a thermodynamic system from one state of matter to another. A certain phase of a thermodynamic system has uniform physical properties. During a phase transition, some properties of the system may change abruptly. Near the critical point between phases, which is a unique combination of the pressure and the temperature for ideal gases, distinction between the phases is almost non-existent.

Standard Model of particle physics introduces particle classification as bosons and fermions, which have integer spins and half-integer spins, respectively. The very nature of bosons permits numerous occupation of single-particle states, which can not be generalized including fermions. As noted above, when the smooth condition of de Broglie wavelength is satisfied, bosons pile up into the single-particle ground state, where quantum effects become apparent on a macroscopic scale. Considering

non-interacting free particle case, this *dense* state should be understood as *dense in the momentum space*. However, trapping potentials lead to a condensation in the coordinate space as well, regardless of interparticle interaction potentials.

## 1.2. A Brief Historical Background

Bose-Einstein condensation was initially a fictitious phenomenon first predicted by Einstein in 1925, on the basis of a paper by Satyendra Nath Bose on the quantum statistics of photons (which are massless bosons) [1]. Einstein then extended Bose's ideas to massive bosons. The result was a special statistics including bosons called Bose-Einstein statistics, which describes the statistical distribution of bosons as being identical particles.

After the discovery of Superfluid  $^4\text{He}$  by Pyotr Kapitsa, John Frank Allen and Don Misener [2, 3] in 1937, BE condensation concept is considered as an underlying mechanism by Fritz London [4]. Later, several debates are conducted for decades [5] concluding superfluidity in  $^4\text{He}$  is closely related to BE condensation [6].

Studies on creating a dilute BE condensate in an atomic gas is reached a level that spin-polarized hydrogen would be a great candidate for producing a BE due to its theoretical prediction asserting it would remain a gas down to absolute zero temperature. Originators of this idea are Hecht [7], Stwalley and Nosanov [8]. Some experimental groups are attracted to test this prediction in the early 1980s [9, 10]. In these experiments, general method was first cooling atoms in dilution refrigerator, then trapping them in a strong magnetic field and lastly cooling further by evaporation. Following these steps, spin-polarized hydrogen is first stabilized in 1980 by Silvera and Walvaren [11].

Developments in the cooling mechanisms, especially laser cooling process allowed trapped gases for cooling further to ultra cold temperatures, resulting in a higher density [12]. Reasonably enough, this achievement led speculations that BE condensate can be produced by laser cooling mechanisms and trapping.

Finally, in the 1995, Cornell and Wieman reached temperatures required to observe BE condensate in vapours of  $^{87}\text{Rb}$  and  $^{23}\text{Na}$  by laser cooling to extract heat from the samples until the temperature is  $\sim 2\mu\text{K}$  [13, 14]. This was the first experimental realization and production of the BE condensate.

### 1.3. Motivation

The main purpose here is to analyze the depletion coefficient of the Bose-Einstein condensate on a Riemannian manifold with a nonnegative Ricci curvature using global heat kernel and eigenvalue estimates for the Laplacian on the manifold. More precisely, these estimates will be used to bound the depletion coefficient.

We will consider both the ideal gas and the gas with a weak hard-core repulsion [15–18]. The latter case will be analyzed using the curved space version of the Bogoliubov theory. A key ingredient of the Bogoliubov approach is the replacement of the ground state creation and annihilation operators by c-numbers. That this is an exact procedure and not merely an approximation was proven by several authors [19–22]. In particular, Lieb *et al.* [20], have shown that the c-number substitution is a general property of second quantization. The generalization of this property to the Riemannian manifolds will be discussed in the appendix.

The use of the Neumann boundary conditions for the Bose gas implies that the single-particle ground state wave function is constant. Since the ideal gas is non-interacting, the thermodynamic properties are sensitive to the boundary conditions imposed, in a sense all the interaction comes from the boundary. The use of Neumann boundary condition is equally acceptable as the Dirichlet condition, the former would mean that the particle flux from the boundary is zero. In our approach the Neumann boundary condition is more natural. The homogeneity of the ground state allows us to carry the flat space proof to the curved case. For an extensive review of the Bogoliubov theory in flat space see Zagrebnov and Bru [23] and references therein (for a curved space version see Rivas *et al.* [24]), and for a mathematically rigorous account of Bose-Einstein condensation in flat space see Lieb *et al.* [25].

For an ideal gas in a flat manifold the behavior of the chemical potential  $\mu$  is crucial for the understanding of the Bose-Einstein condensation. The chemical potential is determined by requiring the constancy of the total number density of the Bose gas. Below a critical temperature  $T_c$  the chemical potential is of the order of  $V^{-1}$  where  $V$  is the volume of the gas. This is a direct consequence of the fact that for  $0 < T \leq T_c$

$$n_0 = \lim_{V \rightarrow \infty} \frac{1}{V} \frac{1}{e^{-\beta\mu} - 1} = \lim_{V \rightarrow \infty} \frac{1}{V\beta|\mu|} > 0. \quad (1.1)$$

Here we assumed that the ground state energy was zero. In the flat space, when we consider a box of typical dimensions given by  $L = O(V^{1/3})$ , we have

$$\epsilon_\sigma = O(L^{-2}), \quad \text{for } \sigma \neq 0, \quad (1.2)$$

since the momentum operator is in the order of  $L^{-1}$ . Here  $\sigma$ 's are the quantum numbers of the gas, with  $\sigma = 0$  denoting the ground state, and  $\epsilon_\sigma$ 's are the corresponding energies. Therefore, we see that for  $T < T_c$ , for  $\sigma \neq 0$

$$n_\sigma \leq \lim_{V \rightarrow \infty} \frac{1}{V} \frac{1}{e^{\beta\epsilon_\sigma} - 1} = 0. \quad (1.3)$$

So in the thermodynamic limit the ground state is occupied macroscopically, while the excited states are not. As we will see, thanks to eigenvalue bounds on manifolds, this argument remains correct for macroscopically admissible volumes, which we define to be a domain inside the manifold, such that the diameter  $D_M$  is also  $O(V^{1/d})$ , where  $d$  is the dimension of the manifold. More precisely, on a Riemannian manifold  $S$  with a non-negative Ricci curvature the eigenvalues of the Laplacian obey precisely (1.2) [26,27] if  $L$  is interpreted as the geodesic diameter  $D_M$  of the confining box which is abstracted as a submanifold  $M \subset S$  with boundary. We will assume that the gas obeys Neumann boundary conditions on  $\partial M$ .

Our main observation is that the number density of the excited particles can be expressed in terms of the trace of the heat kernel on  $S$ . This is obvious in the case

of an ideal gas, but is more involved in the case of a weakly interacting gas. Once we establish this result, we will use the heat kernel and eigenvalue bounds of the Laplacian to discuss the Bose-Einstein condensation on  $S$ .

First, we will introduce ideal Bose gas and Bose-Einstein condensation in flat manifolds, which will actually be a brief review [28–30]. Then we will introduce Bogoliubov theory to explain the behaviour of dilute gases, specifically the depletion of the condensate at absolute zero temperature (for finite temperatures, see Abrikosov *et al.* [31]). Also, an overview on the heat equation and the connection between the geometry of a Riemannian manifold and the heat kernel will be given. Finally, we will analyse Bose-Einstein condensation on a Riemannian manifold with nonnegative Ricci curvature using the heat kernel. Here, we choose Ricci curvature to be nonnegative in order to use estimates given by Li and Yau [26].

We will not attempt any comparison with the existing bounds on the depletion coefficient in flat space [32–37]. Our bounds, which are very geometric in character, seem to provide a whole new class of constraints on the depletion of the condensate. We also note the following alternative approaches to the Bose-Einstein condensation in curved spaces [38, 39].

This thesis is essentially based on the joint study of L. Akant, O. T. Turgut, F. Tapramaz and E. Ertuğrul with the title “*Bose-Einstein Condensation on a Manifold with Nonnegative Ricci Curvature*” [40].

## 2. FREE IDEAL BOSE GAS IN FLAT MANIFOLDS

### 2.1. Introductory Remarks

Perfect classical gas, that is a gas of non-interacting<sup>1</sup> distinguishable particles, has the property that in any single-particle state there is at most one particle in general, *i.e.*, it is very unlikely that any single-particle state is crowded by two or more particles. This situation will occur if the number of single particle states in any energy region is excessively large compared to the number of particles possessing that sort of energy (continuous spectrum). This is called the *classical regime*. Considering this, mean occupation numbers  $n_\sigma$  for any single-particle state  $\sigma (= 0, 1, 2, \dots)$  are much smaller than unity

$$n_\sigma \ll 1, \quad \text{for all } \sigma \in \mathbb{N}^0. \quad (2.1)$$

This is not the case when quantum effects become important, *i.e.*, de Broglie wavelength of particles

$$\lambda_{dB} = (2\pi\hbar^2/mkT)^{1/2}, \quad (2.2)$$

is comparable to the interatomic separation (when the temperature is very low or the gas is very dense, or both). Thus, a modification of classical statistics is required to explain the behaviour of the ideal Bose gas<sup>2</sup> especially at low temperatures. This modification leads naturally to quantum statistics.

Taking into consideration that a system consisting of non-interacting bosons in their gaseous phase, discrete single-particle states are enumerated with  $\sigma (= 0, 1, 2, \dots)$ .

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<sup>1</sup>Non-interacting particles is an idealization in which the potential energy of interaction between particles is negligible compared to their kinetic energy of motion.

<sup>2</sup>By the ideal Bose gas, we mean a one-component system comprised of non-interacting free bosons. Moreover, we are in the non-relativistic limit.

Corresponding energy levels for these states are given as

$$\epsilon_0 \leq \epsilon_1 \leq \dots \leq \epsilon_\sigma \leq \dots \quad (2.3)$$

Considering a gas of  $N$  particles, state of the system is specified exactly by giving occupation numbers for each single-particle state

$$n_0, n_1, \dots, n_\sigma, \dots \quad (2.4)$$

since the energy states are already determined by the volume  $V$  of the container. Occupation of a single-particle state by any numbers of bosons is valid, *i.e.*,

$$n_\sigma = 0, 1, 2, \dots, \quad \text{for all } \sigma \in \mathbb{N}^0. \quad (2.5)$$

This is due to the symmetry property of the wave function describing a system of bosons. Unlike fermions, bosons can crowd a single-particle state in greater amounts.

Summarizing above introduction with another enumeration of single-particle states is going to play the key role in further derivations in this chapter. Gathering the same single-particle energy levels under a label:

$$\epsilon_0 < \epsilon_1 < \dots < \epsilon_i < \dots \quad (2.6)$$

where for each energy level  $\epsilon_i$ , there are  $g_i$  numbers of distinguishable single-particle states contributing to it, and there are  $n_i$  indistinguishable particles in each single-particle energy level  $\epsilon_i$  ( $i \in \mathbb{N}^0$ ).

For applying BE statistics to a system of ideal Bose gas in a large reservoir of constant temperature  $T$  (heat bath), and finding its equilibrium properties, realizing the fact that single-particle energy levels are actually very close to each other even in the

microscopic point of view, *i.e.*, for a single-particle energy level  $\epsilon$ , there are excessive amount of single-particle states distributed as continuum within the interval  $(\epsilon, \epsilon + \delta\epsilon)$ , is of utmost importance. In this manner, any single-particle energy level is many-fold degenerate. We can call the degeneracy of any single-particle energy level  $\epsilon_i$  as  $g_i \gg 1$  for all  $i \in \mathbb{N}^0$ . Notice that, (2.6) loses its meaning in the continuum limit as the difference between two neighboring single-particle energy levels become infinitesimally small and therefore vanishes. Discrete enumeration in this case is problematic. However, dividing energy levels into small intervals still permits grouping single-particle energy levels as in the perfect classical gas.

## 2.2. Mean Occupation Numbers of Single-Particle States

To obtain mean occupation numbers of single-particle states for our isolated system ( $N$ ,  $V$ , and total energy  $E$  of the system<sup>3</sup> are given and constants, as in the microcanonical ensemble) in equilibrium, microcanonical partition function (statistical weight  $\Omega$ ) will be maximized according to the constraints

$$N = \sum_i n_i, \quad \text{and} \quad E = \sum_i n_i \epsilon_i, \quad \text{for all } i \in \mathbb{N}^0 \quad (2.7)$$

where  $N$  and  $E$  denotes total number of particles in the system and total energy of the system, respectively. We choose  $N$  to be a large number so that  $n_i \gg 1$  for all  $i \in \mathbb{N}^0$ . Moreover, we totally isolate our system instead of putting it in a heat bath. The results for the mean occupation numbers will be equivalent however, as we will see later in this section.

According to Boltzmann, equilibrium state of an isolated system is the state with maximum entropy ( $S = k \ln \Omega$ ). Assuming equilibrium, we should maximize  $\Omega$  then. Here  $\Omega = \Omega(n_0, n_1, \dots)$ .

To calculate  $\Omega$ , we have to consider all distinct ways that  $N$  particles can be

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<sup>3</sup>This is the total internal energy of the system actually. In the frame which the system is at rest macroscopically, these two becomes equivalent.

distributed to the single-particle energy levels  $\epsilon_i$ . Thus  $\Omega$  can be written as

$$\Omega = \prod_i \frac{(n_i + g_i - 1)!}{n_i!(g_i - 1)!}. \quad (2.8)$$

This is the correct way to write the number of different arrangements, since in an energy level  $\epsilon_i$ , all  $g_i$  substates are distinguishable, whereas  $n_i$  particles are indistinguishable.

Now, instead of  $\Omega$ , logarithm of  $\Omega$  will be maximized due to its better convergence rate. Using Lagrange multipliers  $\alpha$  and  $\beta$ , we introduce  $Q$ :

$$Q(n_0, n_1, \dots; \alpha, \beta) = \ln \Omega + \alpha \left[ N - \sum_i n_i \right] + \beta \left[ E - \sum_i n_i \epsilon_i \right]. \quad (2.9)$$

Since  $n_i \gg 1$ , we use Stirling's approximation

$$\ln x! \approx x \ln x - x, \quad \text{for } x \gg 1, \quad (2.10)$$

to simplify  $Q$  as

$$\begin{aligned} Q \approx \sum_i \{ & (n_i + g_i - 1) \ln (n_i + g_i - 1) - (n_i + g_i - 1) - n_i \ln (n_i) \\ & + n_i - \ln [(g_i - 1)!] - \alpha n_i - \beta n_i \epsilon_i \} + \alpha N + \beta E. \end{aligned} \quad (2.11)$$

It follows that

$$\frac{\partial Q}{\partial n_i} = \ln (n_i + g_i - 1) - \ln (n_i) - \alpha - \beta \epsilon_i, \quad \text{for all } i. \quad (2.12)$$

We then set this equation to zero and solve for  $n_i$ , which yields

$$n_i = \frac{g_i}{e^{(\alpha + \beta \epsilon_i)} - 1}, \quad \text{for all } i, \quad (2.13)$$

since  $g_i \gg 1$  for all  $i$ . Here, note the symmetry between the substates of any single-

particle energy level  $\epsilon_i$ . This leading to the mean occupation number of each substate, *i.e.*, for each single-particle state of  $\sigma$  is

$$n_\sigma = \frac{1}{e^{(\alpha+\beta\epsilon_\sigma)} - 1}, \quad \text{for all } \sigma. \quad (2.14)$$

At first,  $\alpha$  and  $\beta$  appeared as merely constants, but they actually have thermodynamical meanings as

$$\alpha = -\frac{\mu}{kT} \quad \text{and} \quad \beta = \frac{1}{kT}, \quad (2.15)$$

where  $\mu$  and  $k$  are the chemical potential and the Boltzmann's constant, respectively. Thus we have

$$n_\sigma = \frac{1}{e^{\beta(\epsilon_\sigma - \mu)} - 1}, \quad \text{for all } \sigma.^4 \quad (2.16)$$

Now we substitute  $n_i$  into (2.11) and simplify as

$$\begin{aligned} Q = \ln \Omega &\approx \sum_i (n_i + g_i) \ln (n_i + g_i) - n_i \ln n_i - g_i \ln g_i \\ &= \alpha N + \beta E - \sum_i g_i \ln (1 - e^{-(\alpha+\beta\epsilon_i)}). \end{aligned} \quad (2.17)$$

Therefore, we have

$$\begin{aligned} -\sum_i g_i \ln (1 - e^{-(\alpha+\beta\epsilon_i)}) &= \frac{TS + \mu N - E}{kT} \\ &= \frac{PV}{kT}, \end{aligned} \quad (2.18)$$

where  $G = \mu N = E - TS + PV$  is the grand potential. For the left hand side of this equation, we will sum over single-particle states  $\sigma$  instead of summing over single-

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<sup>4</sup>This is also true locally for subsystems in equilibrium, even if the system as a whole is not in equilibrium.

particle energy levels  $i$ . Hence we obtain

$$\frac{PV}{kT} = \ln \mathcal{G}(T, V, \mu) \quad (2.19)$$

where  $\mathcal{G} = \mathcal{G}(T, V, \mu)$  is the grand partition function given by [29]

$$\mathcal{G} = \prod_{\sigma} \frac{1}{1 - e^{-\beta(\epsilon_{\sigma} - \mu)}} \quad (2.20)$$

from which complete thermodynamics of this system can be derived.

Coming back to the mean occupation numbers of single-particle states given by (2.16) we see taking the zero of the energy scale so that,  $\epsilon_0 = 0$  implies  $\mu < 0$  for the sake of  $n_{\sigma} \geq 0$  for all  $\sigma$ .

The very same result for the mean occupation numbers of single-particle states is also valid for systems in a heat bath. Although the condition of constant total energy is not satisfied for these systems, small fluctuations around the mean total energy are very small (in the order of  $N^{-1/2}$ ) compared to the mean total energy. Hence, the total energy can be approximated as if it is constant for a system in a heat bath.

In (2.16), it seems like  $n_{\sigma}$  are determined completely by  $T$  and  $\epsilon_{\sigma}$ , since  $\mu = \mu(T, V)$  and  $\beta = \beta(T)$ . Nevertheless, there exist statistical fluctuations around  $n_{\sigma}$ , which is the reason  $n_{\sigma}$  is called as the ‘*mean*’ occupation number of single particle states  $\sigma$ . Actually, these statistical fluctuations are inevitable, but their amplitudes remain insignificant compared to the mean in the large  $N$  limit.

Before concluding this section we will establish physical meanings of  $\alpha$  and  $\beta$  in (2.15). The generalization of the fundamental thermodynamic relation for a one-component system whose particle number  $N$  is not kept fixed, is given as

$$dE = TdS - PdV + \mu dN \quad (2.21)$$

where  $\mu$  is the chemical potential of the system, which is the energy required to add one particle to the system under fixed entropy and fixed volume. Using this relation, we have

$$\frac{1}{T} = \left( \frac{\partial S}{\partial E} \right)_{N,V}. \quad (2.22)$$

Let our system has fixed volume  $V$ , therefore fixed single-particle energy levels  $\epsilon_i$ . Also assume without loss of generality that  $dn_j = -dn_k \neq 0$ , and  $dn_i = 0$  for  $i \neq j, k$ . Using (2.7), (2.8) and (2.13), we get

$$\frac{1}{kT} = \frac{\partial \ln \Omega}{\partial n_j} \frac{\partial n_j}{\partial E} = \frac{(\alpha + \beta \epsilon_j) - (\alpha + \beta \epsilon_k)}{\epsilon_j - \epsilon_k} = \beta. \quad (2.23)$$

For the chemical potential, we have

$$\mu = \left( \frac{\partial E}{\partial N} \right)_S = - \frac{\left( \frac{\partial S}{\partial N} \right)_E}{\left( \frac{\partial S}{\partial E} \right)_N} \quad (2.24)$$

for fixed  $V$ . To increase the number of particles in the system by one without changing the total energy of the system, we have to add an extra particle to the ground state of the system. Thus

$$\left( \frac{\partial S}{\partial N} \right)_E = k \frac{\partial \ln \Omega}{\partial n_0} \frac{\partial n_0}{\partial N} = k\alpha \quad (2.25)$$

where  $dn_0 \neq 0$ , and  $dn_i = 0$  for  $i \neq 0$ . Hence we have  $\alpha = -\mu/kT$ .

In order to derive the mean occupation number of single-particle states, we benefited from two different probability distributions of microscopic states at the same time, which are microcanonical ensemble (fixed  $E, V, N$ ), and grand canonical ensemble<sup>5</sup> (fixed  $T, V, \mu$ ). This may seem contradictory. However, for the system in equilibrium with the reservoir, with respect to particle and energy exchange, fluctuations around the means are negligible in the large  $N$  limit. In this sense, our system in a heat bath

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<sup>5</sup>Whereas the particle number is fixed in the canonical ensemble, in the grand canonical ensemble particle number fluctuates statistically as it has been traded for a fixed chemical potential  $\mu$ .

behaves like an isolated system, therefore the distribution (2.16) applies in general. Additionally, our system in a heat bath is assumed to be weakly connected with the reservoir so that its single-particle energy states are not perturbed by proximity to the reservoir, *i.e.*,  $\epsilon_i$  are determined only by the volume  $V$ .

### 2.3. The Density of States

We can always force the energy levels of a thermodynamic system to be a discrete set rather than a continuum, by putting the system in a box and that, furthermore, if the box is large enough the surface effects introduced by the box cannot effect the physical properties of the system [28]. This means the discrete states of our system must lie very close together, so that the discrete number of states in an infinitesimal volume in the phase space of the system will be indistinguishable from a continuum of states. Thus, we use integrals instead of sums for counting of states.

We will find the normal modes of the three dimensional wave equation

$$\nabla^2\psi(\mathbf{r}) + k^2\psi(\mathbf{r}) = 0, \quad (2.26)$$

which describes standing or progressive waves depending on the boundary conditions. Here,  $k$  is the magnitude of the three dimensional wave vector  $\mathbf{k}$ .

We consider waves in a cubic enclosure with sides  $L$ . Imposing vanishing boundary conditions

$$\psi(\mathbf{r}) = 0, \quad \text{on all faces of the cube,} \quad (2.27)$$

then using separation of variables, we get standing waves with solutions

$$\psi_{n_1 n_2 n_3}(\mathbf{r}) = C \sin\left(\frac{n_1\pi}{L}x\right) \sin\left(\frac{n_2\pi}{L}y\right) \sin\left(\frac{n_3\pi}{L}z\right), \quad (2.28)$$

where  $C$  is a constant and  $n_i \in \mathbb{N} - \{0\}$ ,  $i = 1, 2, 3$ . And for the wavevectors

$$\mathbf{k} = \frac{\pi}{L}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z}). \quad (2.29)$$

In the wavevector space, where the components of  $\mathbf{k}$  become like cartesian axes, there is a volume of  $(\pi/L)^3$  per normal mode. To get the number of such normal modes of standing waves, we actually count the number of the cubes with sides  $\pi/L$  in a volume between two spherical shells with radii  $k$  and  $k + dk$  in the positive octant, and the result is

$$f(k)dk = \frac{\frac{1}{8}(4\pi k^2 dk)}{(\pi/L)^3} = \frac{V}{2\pi^2}k^2 dk, \quad (2.30)$$

where  $V$  is introduced as the volume of the cubic enclosure.

On the other hand, the periodic boundary conditions suggest progressive waves with wavevectors

$$\mathbf{k} = \frac{2\pi}{L}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z}), \quad n_i \in \mathbb{Z}, i = 1, 2, 3 \quad (2.31)$$

by which a volume of  $(2\pi/L)^3$  is left for each mode. In the counting, the sum is over whole sphere, leading to the same result. Of course there is an error dividing the spherical shell by cubic volumes. But this fractional error is of the order of  $(Lk)^{-1}$ , which is practically much smaller than one and therefore, can be ignored [28].

Each mode of the standing wave corresponds to an energy  $\epsilon$  as

$$\epsilon = \frac{\hbar^2 k^2}{2m}. \quad (2.32)$$

So the number of states (modes) between energies  $\epsilon$  and  $\epsilon + d\epsilon$  is

$$f(\epsilon)d\epsilon = 2\pi V \left( \frac{\sqrt{2m}}{h} \right)^3 \epsilon^{1/2} d\epsilon, \quad (2.33)$$

where  $f(\epsilon)$  is the energy density of states.

It may seem strange that the Planck constant  $h$  appears all of a sudden in the counting of states, however this is essential considering non-locality of particles in the momentum space as well as in the coordinate space. This can be observed as a result of the uncertainty principle.

#### 2.4. The Concept of Critical Temperature

The total particle number is

$$N = \sum_{\sigma} n_{\sigma} = \sum_{\sigma} \frac{1}{e^{\beta(\epsilon_{\sigma} - \mu)} - 1}, \quad (2.34)$$

where the sum is over all  $\sigma$ . Note that with this normalization condition, chemical potential is determined uniquely as  $\mu = \mu(V, T)$ . To rewrite this normalization equation as an integral, we require the energy density of single-particle states. Number of particles between single-particle energies  $(\epsilon, \epsilon + d\epsilon)$  is then

$$N(\epsilon)f(\epsilon)d\epsilon = \frac{V}{h^3} 2\pi(2m)^{3/2} \frac{\epsilon^{1/2}d\epsilon}{e^{\beta(\epsilon - \mu)} - 1}, \quad (2.35)$$

where  $f(\epsilon)$  is the energy density of states and,  $N(\epsilon)$  is the number of particles with energy  $\epsilon$ . Integrating this, we have

$$\frac{N_e}{V} = \frac{N - N_0}{V} = \frac{2\pi(2m)^{3/2}}{h^3} \int_0^{\infty} \frac{\epsilon^{1/2}d\epsilon}{e^{\beta(\epsilon - \mu)} - 1}, \quad (2.36)$$

where  $N_0$  is the number of particles in the ground state and  $N_e$  is the number of particles in the excited states. We had to exclude  $N_0$  from the total number of particles  $N$ , since in the counting we inadvertently gave zero weight to the zeroth energy level, so the integral does not *see* the particles in the ground state in some sense. Note that except the ground state, counting the density of states is not problematic.

$N_0$  can be written as

$$N_0 = \frac{1}{e^{-\beta\mu} - 1}, \quad (2.37)$$

using  $\epsilon_0 = 0$ . Using this relation, we can determine the chemical potential as

$$\mu = kT \ln \left( \frac{N_0}{1 + N_0} \right), \quad (2.38)$$

which is smaller than zero.

As the temperature goes to zero,  $N_0$  increases rapidly (diverges) for nonvanishing  $\mu$ . This contradicts with the constant number of particles in the system as  $N_0$  must be less than given  $N$ . Therefore, there must be a critical temperature  $T_c$  where at  $\mu$  is extremely close to zero -not equal to zero in any case- so that  $N_0 < N$ . Even if less than  $N$ , towards this critical temperature  $N_0$  becomes macroscopically significant (above that critical temperature  $N_0$  remains insignificant). This accumulation of particles into the ground state as the temperature falls below the critical temperature, hence reaching a macroscopic fracture of the system is known as Bose-Einstein Condensation. For temperatures lower than the critical temperature we see  $\mu$  is practically zero, since  $N_0 = O(N) \gg 1$ .

We considered our system in a heat bath with allowed particle exchange. Below the critical temperature  $T_c$ , two phases<sup>6</sup> coexist *i.e.*, a *condensed* phase, consisting of  $N_0$  particles accumulated in the ground state, and a *normal* phase, consisting of  $N_e$

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<sup>6</sup>By a phase, we mean a homogeneous part of a system bounded by surfaces across which the thermodynamic properties change discontinuously.

particles distributed over the excited states. We may also consider these two phases as two different thermodynamical systems in equilibrium, where their chemical potentials must be equal to each other along with their pressures and temperatures. Let's put these systems together in an isolated reservoir without loss of generality. For low temperatures, we see adding an extra particle from excited particles to the condensate requires no energy, therefore the chemical potential vanishes. On the other hand, if we add another particle to the isolated reservoir we require an energy of  $\epsilon_\sigma$  to release the particle in a single-particle state  $\sigma$ , which also vanishes on the average, since  $N_0$  dominates  $N_e$ . For weakly repulsively interacting systems, we will see in Section 3.3 that, whereas the chemical potential of the condensate vanishes, the chemical potential of the system comprised of two phases is greater than zero.

### 2.5. Discontinuity in $\partial C_v/\partial T$

Using the grand canonical partition function  $\mathcal{G} = \mathcal{G}(T, V, \mu)$  given by (2.19) for our system, [29]

$$\frac{PV}{kT} = \ln \mathcal{G} = - \sum_{\sigma} \ln (1 - ze^{-\beta\epsilon_{\sigma}}) \quad (2.39)$$

is obtained, where  $z = e^{\mu/kT}$  is the *fugacity* of the gas, which is an intensive thermodynamic variable of the system. Using  $z$ , we rewrite this sum as an integral

$$\frac{P}{kT} = -\frac{2\pi}{h^3}(2m)^{3/2} \int_0^{\infty} \ln(1 - ze^{-\beta\epsilon})\epsilon^{1/2}d\epsilon - \frac{1}{V} \ln(1 - z). \quad (2.40)$$

Here we extracted  $\epsilon = 0$  case out of the sum as we did previously for  $N/V$ . This is not problematic as the integral does not see  $\epsilon = 0$  case already. Notice that, using (2.38), the last term in the right-hand side of (2.40) becomes

$$-\frac{1}{V} \ln(1 - z) = \frac{1}{V} \ln(1 + N_0) \leq n \frac{\ln(1 + N)}{N}, \quad (2.41)$$

therefore can be neglected in the large  $N$  limit. Here  $n$  is the number density, which is finite.

Evaluating integrals for  $P/kT$  and  $N/V$  using de Broglie wavelength  $\lambda \equiv \lambda_{dB}$ , and Bose-Einstein functions<sup>7</sup>

$$g_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1} dx}{z^{-1}e^x - 1} = z + \frac{z^2}{2^\nu} + \frac{z^3}{3^\nu} + \dots \quad (2.42)$$

we get

$$\frac{P}{kT} = \frac{1}{\lambda^3} g_{5/2}(z), \quad (2.43)$$

and

$$\frac{N_e}{V} = \frac{1}{\lambda^3} g_{3/2}(z). \quad (2.44)$$

Note that, the concentration of particles in the excited states depends only on the temperature. If we know the number of particles in the excited states  $N_e$  we can determine the exact value of  $z$  by using the last equation. Here  $g_\nu(z)$  is a monotonically increasing function with increasing  $z$ , and is bounded by its extremal value

$$g_\nu(z) \leq g_\nu(1) = \zeta(\nu). \quad (2.45)$$

where,  $\zeta$  denotes the Riemann zeta function. Therefore,

$$g_{3/2}(z) \leq \zeta\left(\frac{3}{2}\right), \quad \text{for all } z. \quad (2.46)$$

Now, if the total number of particles given exceeds this limiting value for the particles

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<sup>7</sup>For the behaviour and the values at critical point of these functions, see [25]

in the excited states, BE condensation begins:

$$N_0 = N - \frac{V}{\lambda^3} \zeta\left(\frac{3}{2}\right), \quad (2.47)$$

where we can conclude that the capacity of single-particle ground state is unlimited. Equating  $N_0$  to zero gives us the critical temperature:

$$T_c = \frac{2\pi\hbar^2}{mk} \left[ \frac{N/V}{\zeta(3/2)} \right]^{2/3}. \quad (2.48)$$

Below the critical temperature, an unusual phase is observed along with the normal phase consisting of particles in the excited states. Number of particles in the ground state reaches a greater amount, creating the condensed phase. In terms of the critical temperature, the ratio  $N_0/N$  can be written as

$$\frac{N_0}{N} = 1 - \left( \frac{T}{T_c} \right)^{3/2}, \quad \text{for } T < T_c. \quad (2.49)$$

As  $T$  gets close to  $T_c$ , the right hand side goes down to zero implying the insignificance of  $N_0$  with respect to  $N$ . We see the critical temperature marks the last value for the temperature where  $N_0$  remains insignificant coming down to zero point.

For the pressure below the critical temperature, we again use the extremal value of  $z$ , and we get

$$P = \zeta\left(\frac{5}{2}\right) \frac{kT}{\lambda^3}, \quad \text{for } T < T_c, \quad (2.50)$$

which does not depend on  $V$ . Therefore, the isothermal compressibility given as

$$\kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_T \quad (2.51)$$

for the condensate is infinite. We say the condensed state has *infinite compressibility*.

The total energy of the system is given by

$$E = - \left( \frac{\partial \ln G}{\partial \beta} \right)_{z,V} = \frac{3}{2} \frac{kT}{\lambda^3} V g_{5/2}(z). \quad (2.52)$$

Replacing (2.43) gives

$$E = \frac{3}{2} PV. \quad (2.53)$$

Thus the heat capacity under constant volume of the system  $C_v = \left( \frac{\partial E}{\partial T} \right)_{N,V}$  is written for low temperatures ( $T < T_c$ ) as

$$\begin{aligned} C_v &= \frac{3}{2} \left( \frac{\partial(PV)}{\partial T} \right)_{N,V} = \frac{3}{2} \zeta \left( \frac{5}{2} \right) kV \frac{\partial}{\partial T} \left( \frac{T}{\lambda^3} \right)_{N,V} \\ &= \frac{15}{4} \zeta \left( \frac{5}{2} \right) \frac{kV}{\lambda^3}, \quad \text{for } T < T_c. \end{aligned} \quad (2.54)$$

Notice that, as  $T \rightarrow T_c^-$ ,  $C_v$  converges to

$$\frac{15}{4} \frac{\zeta(5/2)}{\zeta(3/2)} Nk. \quad (2.55)$$

Here we used (2.44) for substituting  $\lambda$  in the limit  $N_e \rightarrow N$ . For high temperatures ( $T > T_c$ ), we rewrite the internal energy of the system using (2.44), and for the heat capacity we get

$$C_v = \frac{3}{2} Nk \frac{\partial}{\partial T} \left( T \frac{g_{5/2}(z)}{g_{3/2}(z)} \right)_{N,V}. \quad (2.56)$$

Using (2.44) again, we have the derivative of the Bose-Einstein function  $g_{3/2}(z)$  with respect to  $T$

$$\left( \frac{\partial}{\partial T} g_{3/2}(z) \right)_{N,V} = -\frac{3}{2T} g_{3/2}(z) \quad (2.57)$$

since  $\lambda = O(T^{1/2})$ . Additionally, from (2.42), we get the derivatives

$$\frac{\partial}{\partial z} g_\nu(z) = \frac{1}{z} g_{\nu-1}(z). \quad (2.58)$$

Combining these results, we obtain

$$\left( \frac{\partial z}{\partial T} \right)_{N,V} = -\frac{3}{2T} z \frac{g_{3/2}(z)}{g_{1/2}(z)}. \quad (2.59)$$

Hence, differentiating (2.52) with respect to  $T$ , we get

$$C_v = Nk \left[ \frac{15}{4} \frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{9}{4} \frac{g_{3/2}(z)}{g_{1/2}(z)} \right], \quad \text{for } T > T_c. \quad (2.60)$$

In the large  $T$  limit,  $z$  converges to 0, since  $\mu < 0$ . And asymptotic forms of the Bose-Einstein functions imply  $g_\nu(z) \rightarrow z$ . Therefore

$$C_v = \frac{3}{2} Nk, \quad \text{for } T \gg T_c \quad (2.61)$$

which is equal to the heat capacity of the perfect classical gas under constant volume.

As  $T \rightarrow 0$ ,  $\mu$  is practically zero and  $z \rightarrow 1$ , we see that  $C_v$  approaches to the value in (2.55) both from above and below, since  $g_{1/2}(z)$  diverges in this limit. However, the first derivative of  $C_v$  with respect to  $T$  is discontinuous, *i.e.*,

$$\begin{aligned} \left( \frac{\partial C_v}{\partial T} \right)_{T \rightarrow T_c^-} - \left( \frac{\partial C_v}{\partial T} \right)_{T \rightarrow T_c^+} &= \frac{27}{16\pi} [\zeta(3/2)^2] \frac{Nk}{T_c} \\ &\simeq 3.66 \frac{Nk}{T_c}. \end{aligned} \quad (2.62)$$

## 2.6. Two Dimensional and One Dimensional Cases

In two dimensional flat spaces, using the same arguments in Section 2.3, the density of states can be written as

$$f(\epsilon)d\epsilon = \frac{2\pi mV}{h^2}d\epsilon, \quad (2.63)$$

where,  $f(\epsilon)d\epsilon$  is the number of single-particle states with energies between  $(\epsilon, \epsilon + d\epsilon)$ . Then, total number of particles in the excited states are

$$\begin{aligned} N - N_0 &= \frac{2\pi mV}{h^2} \int_0^\infty \frac{1}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon \\ &= \frac{2\pi mV\beta}{h^2} \int_0^\infty \frac{1}{z^{-1}e^x - 1} dx \\ &\propto g_1(z). \end{aligned} \quad (2.64)$$

As  $T$  goes down to zero, chemical potential  $\mu$  approaches to zero from below,  $z$  approaches to unity. Thus

$$N - N_0 \rightarrow g_1(1) \rightarrow \infty, \quad \text{for } T \rightarrow 0, \quad (2.65)$$

since  $g_1(1)$  is divergent. Conclusion is, there is no macroscopical piling up of particles into the ground state energy level for temperatures close to zero, since excited states can hold infinitely many particles at zero temperature. We say, BE condensation is not observable in two dimensional flat case.

For the one dimensional case, similar calculations lead to the same conclusion

$$f(\epsilon)d\epsilon = \frac{(2m)^{1/2}V}{2h} \epsilon^{-1/2} d\epsilon, \quad (2.66)$$

therefore, the number of particles in the excited states are

$$\begin{aligned}
N - N_0 &= \frac{(2m)^{1/2}V}{2h} \int_0^\infty \frac{\epsilon^{-1/2}}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon \\
&= \frac{V}{2h} \left(\frac{2m}{\beta}\right)^{1/2} \int_0^\infty \frac{x^{-1/2}}{z^{-1}e^x - 1} dx \\
&\propto g_{1/2}(z).
\end{aligned} \tag{2.67}$$

The last term diverges even faster than  $g_1(z)$  as  $T \rightarrow 0$ , concluding there is no BE condensation in one dimensional flat space too.

## 2.7. Generalization to d-Dimensional Case

The energy density of states for a free system in a  $d$ -dimensional flat space with volume  $V$  can be calculated by the standard method as

$$f(\epsilon) = \frac{V}{2} R(d) \left(\frac{\sqrt{2m}}{h}\right)^d \epsilon^{\frac{d}{2}-1}, \tag{2.68}$$

where  $R(d)$  depends only on the spatial dimension of the system.<sup>8</sup>

Then the number of particles in the excited states can be written as

$$\frac{N_e}{V} = \frac{1}{2} R(d) \left(\frac{\sqrt{2m}}{h}\right)^d \int_0^\infty \frac{\epsilon^{\frac{d}{2}-1} d\epsilon}{e^{\beta(\epsilon-\mu)} - 1} \equiv S(d) \frac{1}{\beta^{d/2}} \Gamma\left(\frac{d}{2}\right) g_{d/2}(z), \tag{2.69}$$

where all the constants are included in the density of states factor  $S(d)$ , which is the density of states factor in  $\mathbb{R}^d$ .

To obtain the concentration of particles with nonzero momenta below the critical

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<sup>8</sup> $R(d) = 4\pi, 2\pi, 1$  for  $d = 3, 2, 1$ , respectively.

temperature, we take the limit  $\mu \rightarrow 0^-$ , then  $z \rightarrow 1$ , and the result is

$$n_e^{flat} := \frac{N_e}{V} = S(d) \frac{1}{\beta^{d/2}} \Gamma\left(\frac{d}{2}\right) \zeta\left(\frac{d}{2}\right), \quad \text{for } \beta \geq \beta_c = \frac{1}{kT_c}. \quad (2.70)$$

Here, we can observe the divergence of the number density of particles in the excited states directly from the Riemann zeta function. In fact,  $n_e$  in a  $d$ -dimensional flat space converges only for  $d > 2$ . For the critical temperature  $T_c$ , we equate  $n_e^{flat}$  to  $n$  and we obtain

$$T_c = \frac{1}{k} \left[ \frac{S(d)\Gamma(d/2)\zeta(d/2)}{n} \right]^{-2/d}. \quad (2.71)$$

It can be easily checked that for  $d = 3$ , we get (2.48).

### 3. BOGOLIUBOV THEORY OF WEAKLY INTERACTING BOSE GAS ON THREE DIMENSIONAL FLAT MANIFOLDS

#### 3.1. Introduction

In the absence of interparticle forces, BE condensation occurs in flat manifolds in three dimensions due to infinite compressibility. Heuristically, effect of particle-particle interaction seems a candidate to reduce the condensate or to completely destroy it even for weakly interacting (weakly non-ideal) dilute gases. Bogoliubov approached this problem with a new perturbative technique including only two-particle interaction potentials [15]. As we will see, even in the weakly interacting system, the Bose gas has the capacity to form a BE condensate.

This is an approximation under the context of many-body theory especially working very effectively for dilute gases, where the effective interparticle distance for particle-particle interactions to show up is much less than mean interparticle separation. While the underlying physical laws for each particle is very simple to describe, a sample containing large numbers of particles may be extremely complex to investigate further. A perturbative picture here, with the exclusion of three or more particle-particle interactions gives results good enough to understand major effects of interaction. For simplicity, we assume that the particles have spin zero, which makes the states of the gas spin independent.

To describe a deeper picture of an ideal Bose gas with inter-particle potentials here, a brief review of second quantization will be given in order to present a microscopic justification of the Bose gas. Then a Hamiltonian in the second quantized form will be introduced, which is the main tool to study Bose systems. Finally, we will discuss the Bogoliubov theory.

### 3.2. Method of Second Quantization

Second quantization describes many-particle systems by quantizing the fields using a basis, known as *occupation number basis* which spans the Fock space, that describes the number of particles occupying each state in a complete set of single-particle states. It is based on Hamiltonian formulation on quantum mechanics<sup>9</sup>. In the first quantization, single-particle states are used as a basis which spans the Hilbert space. Unlike the classical field, which is indexed by position, second quantization indexes the field by enumerating the single-particle quantum states.

In the classical electrodynamics, electromagnetic fields can be described in terms of modes with wavevector  $\mathbf{k}$ , each behaving as an oscillator of frequency  $\omega = ck$ , where  $c$  is the speed of light. Each of these modes, annihilation ( $\hat{a}_k$ ) and creation ( $\hat{a}_k^\dagger$ ) operators are introduced, which annihilate and create a photon of wavevector  $\mathbf{k}$ , respectively. Usage of these operators extends from electromagnetic field propagators (photons, which are massless bosons) to massive bosons if the particle number in the sample need not be conserved, as in the grand canonical ensemble. Commutation relations between these operators are given as

$$[\hat{a}_k, \hat{a}_{k'}] = 0, \quad [\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger] = 0, \quad [\hat{a}_k, \hat{a}_{k'}^\dagger] = \delta_{kk'} \quad (3.1)$$

where  $\delta_{kk'}$  is the *kronecker delta*, and

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (3.2)$$

is the commutator of two operators  $\hat{A}, \hat{B}$ .

In the first quantization formalism we deal with quantum states of single particles. The states of many-body particles are also written as a combination of single particle states, *i.e.*, wavefunction for  $N$  identical bosons is completely symmetric and

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<sup>9</sup>For another approach, see the Feynman path-integral method, which is based on a Lagrangian formulation.

can be written as a combination of single-particle wavefunctions which gives Slater determinant

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_1(\mathbf{x}_1) & \chi_2(\mathbf{x}_1) & \cdots & \chi_N(\mathbf{x}_1) \\ \chi_1(\mathbf{x}_2) & \chi_2(\mathbf{x}_2) & \cdots & \chi_N(\mathbf{x}_2) \\ \vdots & \vdots & & \vdots \\ \chi_1(\mathbf{x}_N) & \chi_2(\mathbf{x}_N) & \cdots & \chi_N(\mathbf{x}_N) \end{vmatrix}, \quad (3.3)$$

where  $\chi_k(\mathbf{x}_i)$  denotes the single particle wavefunction as  $i$ th particle is in the  $k$ th single particle state, and  $\mathbf{x}_i$  are spatial coordinate vectors of particles ( $i, k \in [1, N] \subset \mathbb{Z}$ ).

A little confusion may arise, since we labeled ‘*identical*’ bosons by numbering them. But notice that, total wavefunction includes a labeled boson in any of the  $N$  single-particle states, therefore is non-committal as to which particle in which state.

In the second quantization formalism, quantum states are described in terms of the occupation numbers in basis states of definite one-particle occupation. In this notation, particle indistinguishability is automatically included. And the statistics of particles is contained in the commutation rules. A state vector in this basis is written as:

$$|n_1, n_2, \dots, n_k, \dots\rangle, \quad (3.4)$$

which means  $n_1$  particles are in the first single-particle state,  $n_2$  are in the second, and so on.<sup>10</sup>

The creation operator acts on the state vector as

$$\hat{a}_k^\dagger |n_1, n_2, \dots, n_k, \dots\rangle = \sqrt{n_k + 1} |n_1, n_2, \dots, n_k + 1, \dots\rangle, \quad (3.5)$$

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<sup>10</sup>First single-particle state here means the one with the lowest energy, instead of the first excited state.

increasing  $n_k$  by unity and multiplying the state vector by  $\sqrt{n_k + 1}$ .

Similarly, the annihilation operator acts on the state vector as

$$\hat{a}_k |n_1, n_2, \dots, n_k, \dots\rangle = \sqrt{n_k} |n_1, n_2, \dots, n_k - 1, \dots\rangle, \quad (3.6)$$

decreasing  $n_k$  by unity<sup>11</sup> and multiplying the state vector by  $\sqrt{n_k}$ . Although these operators appeared first in the algebraic approach to quantum harmonic oscillators, extensive use of them is possible in the second quantization.

Notice that

$$\hat{a}_k^\dagger \hat{a}_k |n_1, n_2, \dots, n_k, \dots\rangle = n_k |n_1, n_2, \dots, n_k, \dots\rangle. \quad (3.7)$$

This operator,  $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$  is called the occupation number operator, having occupation numbers in  $k$ th single-particle state,  $n_k$ , as eigenvalues.

Now we can define field operators that create or annihilate a particle at a certain point in space. They can be defined through the single-particle states  $\chi_k(\mathbf{x})$  with quantum number  $k$  as

$$\hat{\psi}(\mathbf{x}) = \sum_k \hat{a}_k \chi_k(\mathbf{x}) \quad (3.8)$$

Picking single-particle states  $\chi_k(\mathbf{x})$  as the momentum eigenstates in a box of volume  $V$  with periodic boundary conditions

$$\chi_k(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{x}} \quad (3.9)$$

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<sup>11</sup>if the number of particles in the  $k$ th single-particle state is zero already, the annihilation operator  $\hat{a}_k$  acting on the state vector yields zero, *i.e.*,  $\hat{a}_k |0, 0, \dots, n_k = 0, \dots\rangle = 0$ . This is different than the vacuum state with no bosons present,  $|0\rangle \equiv |0, 0, \dots, 0, \dots\rangle$  and in particular  $\langle 0|0\rangle = 1$ .

suggests that we can construct field operators by applying the Fourier transform to the creation and annihilation operators for single-particle states which are enumerated in terms of their momenta

$$\hat{\psi}^\dagger(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_k e^{-i\mathbf{k}\cdot\mathbf{x}} \hat{a}_k^\dagger, \quad \text{and} \quad \hat{\psi}(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_k e^{i\mathbf{k}\cdot\mathbf{x}} \hat{a}_k, \quad (3.10)$$

where  $\hat{\psi}^\dagger(\mathbf{x})$  and  $\hat{\psi}(\mathbf{x})$  are the quantum fields which create and annihilate a particle in a position eigenstate, respectively. Here the summations are over  $\mathbf{k}$  as a vector.

We can show that these bosonic field operators obey the same commutation relations between the creation and annihilation operators

$$\left[ \hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{x}') \right] = 0, \quad \left[ \hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}') \right] = 0, \quad \left[ \hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}') \right] = \delta^3(\mathbf{x} - \mathbf{x}') \quad (3.11)$$

Although the field operators and the single-particle wavefunctions are commonly denoted with the same symbol, they are not the same thing. Field operators act on the Fock space, and the single-particle wavefunctions are quantum mechanical amplitudes for finding a particle in a position. However, they are closely related as can be observed from (3.8).

The second quantization procedure relies crucially on particles being identical (indistinguishable). From the classical point of view, indistinguishability of particles sounds a little strange. But in the world of quantum mechanics, there are particles in no way different except their positions in space (we say ‘*an*’ electron instead of ‘*the*’ electron, as electrons are fermions). This is a fact and many physicists prefer to explain indistinguishability of particles in the context of Quantum Field Theory [41].

### 3.3. Bogoliubov Hamiltonian

Let's say we have a Hamiltonian of a system with a space representation, interacting through the pair potential  $U$  and immersed in the external potential  $V$

$$\hat{H}' = \sum_i \left( -\frac{\hbar^2}{2m} \Delta_i + V(\mathbf{x}_i) \right) + \sum_{i < j} U(\mathbf{x}_i - \mathbf{x}_j) \quad (3.12)$$

where  $i$  and  $j$  run over all particles. Then, the field theory Hamiltonian of a system of spinless bosons in the non-relativistic limit is given in the second quantization by [15–18],

$$\begin{aligned} \hat{H}' = & \int \hat{\Psi}^\dagger(\mathbf{x}) \left( -\frac{\hbar^2}{2m} \Delta + V(\mathbf{x}) \right) \hat{\Psi}(\mathbf{x}) d^3\mathbf{x} \\ & + \frac{1}{2} \int \int \hat{\Psi}^\dagger(\mathbf{x}_2) \hat{\Psi}^\dagger(\mathbf{x}_1) U(\mathbf{x}_1 - \mathbf{x}_2) \hat{\Psi}(\mathbf{x}_1) \hat{\Psi}(\mathbf{x}_2) d^3\mathbf{x}_1 d^3\mathbf{x}_2. \end{aligned} \quad (3.13)$$

Exact diagonalization of this Hamiltonian is practically not possible due to the size of the Hilbert space of the system. However, the main interest is the ground state of the system in the case of weak particle-particle interactions, that is, our aim is to determine how the ground state and spectrum of elementary excitations are affected by weak interaction. In the case of macroscopic occupation of the ground state of the system, we can expect to use a mean field approach which relies on substitution of the bosonic operator  $\hat{\psi}(\mathbf{x})$  with a classical field  $\hat{\phi}_0(\mathbf{x})$ .<sup>12</sup>

For a system of bosons confined in a large volume, the energy is minimized by a configuration where many momentum modes are macroscopically occupied. The resulting in our case Gross-Pitaevskii equation reveals a homogeneous stationary solution [42, 43],

$$\hat{\phi}_0(\mathbf{x}) = \frac{1}{\sqrt{V}}, \quad (3.14)$$

---

<sup>12</sup>The mean-field theory, which describes the behaviour of the classical field  $\hat{\phi}_0(\mathbf{x})$ , and ignores the fluctuations  $\hat{\eta}(\mathbf{x})$  is contained in the Gross-Pitaevskii theory. This assumption is legal only in small systems with finite volume.

which is the condensate wavefunction. Quantum fluctuations around the mean field solution can be described within the Bogoliubov theory. We will use this method on a compact Riemannian manifold in chapter five.

To get a use of the second quantization formalism, we would like to write the Hamiltonian of the system in terms of bosonic creation and annihilation operators as in (3.10). The kinetic energy operator becomes

$$\hat{T} = \int d^3 \mathbf{x} \sum_{k,k'} \frac{1}{V} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \hat{a}_{k'}^\dagger \epsilon_k \hat{a}_k = \sum_{k,k'} \delta_{kk'} \epsilon_k \hat{a}_{k'}^\dagger \hat{a}_k \quad (3.15)$$

resulting

$$\hat{T} = \sum_k \hat{n}_k \epsilon_k = \epsilon_0 \hat{n}_0 + \sum_{k \neq 0} \hat{n}_k \epsilon_k, \quad (3.16)$$

where  $\epsilon_k$  are single-particle state energies. The expectation value of the kinetic energy operator is thus,

$$\langle \hat{T} \rangle = \sum_{k \neq 0} \langle \hat{n}_k \rangle \epsilon_k, \quad (3.17)$$

where  $\langle \hat{n}_k \rangle$  are mean occupation numbers for single-particle states.

If the gas is dilute and cold, then two-body potential can be replaced by the pseudopotential

$$U(\mathbf{x} - \mathbf{x}') = g \delta(\mathbf{x} - \mathbf{x}') \quad (3.18)$$

which is fixed by a single parameter, the s-wave scattering length  $a$ , through the coupling constant

$$g = \frac{4\pi\hbar^2 a}{m}. \quad (3.19)$$

The basic idea involved in making this simplification is, in the ground state, the particles of an ideal Bose gas occupy the lowest level with zero energy (the condensate). In a dilute gas, because of the weakness of interactions, the ground state will differ only slightly from the ground state of an ideal gas, *i.e.*, the number of particles in the condensate will still greatly exceed the number of particles in other levels, so that  $N \sim N_0$ . This approximation is expected to be valid for scattering processes in the limit of extremely small momentum transfer so that the magnitude of the wavevector  $\mathbf{k}$  is taken as constant during collisions (the first Born approximation). Also we assume the interaction between every pair of particles is identical, and the scattering amplitude does not depend on angle (s-wave scattering). Scatterings under these approximations are known as low energy hard sphere scattering in the quantum scattering theory. Another approximation can be seen through the appearance of dirac delta as a distribution, which is, bosons are taken as massive but volumeless particles (point particles). By these approximations, interaction term in the Hamiltonian can be written as

$$\hat{U} = \frac{g}{2} \int d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \hat{\psi}(\mathbf{x}), \quad (3.20)$$

and in the momentum representation it becomes

$$\hat{U} = \frac{g}{2} \sum_{k_1, k_2, k_3, k_4} \int d^3\mathbf{x} \frac{1}{V^2} e^{-i((\mathbf{k}_1 + \mathbf{k}_2) - (\mathbf{k}_3 + \mathbf{k}_4)) \cdot \mathbf{x}} \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_3} \hat{a}_{k_4} \quad (3.21)$$

which is equal to

$$\hat{U} = \frac{g}{2V} \sum_{k_1, k_2, k_3, k_4} \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_3} \hat{a}_{k_4} \delta_{k_1 + k_2, k_3 + k_4}. \quad (3.22)$$

These combinations of creation and annihilation operators can be viewed as the operator  $\hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_3} \hat{a}_{k_4}$  annihilates two particles at  $\mathbf{k}_4$  and  $\mathbf{k}_3$  each in the momentum space, then creates two particles at  $\mathbf{k}_2$  and  $\mathbf{k}_1$  each in the momentum space ( $\mathbf{p} = \hbar\mathbf{k}$ ). By each of these operations, particle number does not change,  $\hat{H}'$  is a number preserving

operator, thus commutes with the total particle number operator  $\hat{N} = \sum_k \hat{n}_k$ . Also the momentum is conserved since  $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$  by the kronecker delta.

Another approach to the interaction term in the Hamiltonian is taking Fourier transforms of the interaction potential  $U(\mathbf{x})$ , which depends on the separation of the interacting particles. The total interaction potential of the system is then,

$$U \equiv \frac{1}{2} \sum_{i \neq j} U(\mathbf{x}_i - \mathbf{x}_j) = \frac{1}{2} \sum_q U_q \left( \rho_q^* \rho_q - \frac{N}{V} \right) \quad (3.23)$$

where

$$U_q = \int d^3\mathbf{x} U(\mathbf{x}) e^{-i\mathbf{q}\cdot\mathbf{x}} \quad (3.24)$$

which is equal to  $g$ , since  $U(\mathbf{x}) = g \delta(\mathbf{x})$ , and

$$\rho_q = \frac{1}{\sqrt{V}} \int d^3\mathbf{x} \nu(\mathbf{x}) e^{-i\mathbf{q}\cdot\mathbf{x}}, \quad (3.25)$$

and the particle density

$$\nu(\mathbf{x}) = \sum_i \delta(\mathbf{x} - \mathbf{x}_i). \quad (3.26)$$

Here,  $U_q$  is the Fourier transform of  $U(\mathbf{x})$ ,  $\rho_q$  is the Fourier transform of the particle density  $\nu(\mathbf{x})$ , and sum is over  $\mathbf{q}$  as a vector. To get the second quantized form of the potential energy, we replace  $\nu(\mathbf{x})$  by the operator

$$\hat{\nu}(\mathbf{x}) = \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}), \quad (3.27)$$

then we get,

$$\hat{\rho}_q^\dagger = \frac{1}{\sqrt{V}} \sum_k \hat{a}_{k+q}^\dagger \hat{a}_k, \quad \text{and} \quad \hat{\rho}_q = \frac{1}{\sqrt{V}} \sum_{k'} \hat{a}_{k'-q}^\dagger \hat{a}_{k'}. \quad (3.28)$$

Here the operator  $\hat{a}_{k+q}^\dagger \hat{a}_k$  annihilates a particle at  $\mathbf{k}$  and creates another particle at  $\mathbf{k}+\mathbf{q}$ , and the operator  $\hat{a}_{k'-q}^\dagger \hat{a}_{k'}$  annihilates a particle at  $\mathbf{k}'$  and creates another particle at  $\mathbf{k}' - \mathbf{q}$ . As the case before, these operations does not change the particle number. However, each changes the momentum by  $\pm\hbar\mathbf{q}$ . The sum of such operators over all  $\mathbf{k}$  represents a collective mode, *i.e.*, a density fluctuation. Using these density operators and the commutation rules, we get the interaction potential operator in second quantized form as

$$\begin{aligned}
\hat{U} &= \frac{g}{2} \sum_q \left( \hat{\rho}_q^\dagger \hat{\rho}_q - \frac{\hat{N}}{V} \right) \\
&= \frac{g}{2V} \sum_q \left[ -\hat{N} + \sum_{k \neq k'-q} \hat{a}_{k+q}^\dagger \hat{a}_k \hat{a}_{k'-q}^\dagger \hat{a}_{k'} + \sum_{k=k'-q} \hat{a}_{k+q}^\dagger \hat{a}_k \hat{a}_{k'-q}^\dagger \hat{a}_{k'} \right] \\
&= \frac{g}{2V} \sum_q \left[ -\hat{N} + \sum_{k,k'} \hat{a}_{k+q}^\dagger \hat{a}_{k'-q}^\dagger \hat{a}_{k'} \hat{a}_k + \sum_{k=k'-q} \hat{a}_{k+q}^\dagger \hat{a}_{k'} \right] \\
&= \frac{g}{2V} \sum_{k,k',q} \hat{a}_{k+q}^\dagger \hat{a}_{k'-q}^\dagger \hat{a}_{k'} \hat{a}_k. \tag{3.29}
\end{aligned}$$

Picking  $g = 0$  in the Hamiltonian leads to the simplest BE condensate state in which all particles are in the same single-particle eigenstate,  $\phi_0$  ( $k = 0$  state). The density of particles in the ground state is then just the total density  $n = N/V$  at zero temperature. For small  $g$ , the ground state of the Bose system can be well approximated by a coherent state, for which the total number of particles is not fixed (as in the grand canonical ensemble).  $N_0$  in this case is less than  $N$ , but still macroscopic ( $N_0 \gg 1$ ).

Now we will apply Bogoliubov approximation, which is for small  $g$ ,  $N_0 \gg 1$  permits effective commutation of the creation and annihilation operators of the ground state, since the difference between  $N_0$  and  $N_0 + 1$  is insignificant. Therefore,

$$\hat{a}_0^\dagger |\Psi\rangle \rightarrow \sqrt{N_0} |\Psi\rangle, \quad \text{and} \quad \hat{a}_0 |\Psi\rangle \rightarrow \sqrt{N_0} |\Psi\rangle, \tag{3.30}$$

so we can approximate the bosonic creation and the annihilation operators as c-

numbers, *i.e.*,

$$\hat{a}_0 \sim \sqrt{N_0}, \quad \text{and} \quad \hat{a}_0^\dagger \sim \sqrt{N_0}. \quad (3.31)$$

Since  $N_0$  is a very large number, we are justified in regarding the operators  $\hat{a}_0, \hat{a}_0^\dagger$  as c-numbers, replacing them by  $\sqrt{N_0}$ . Using the c-number substitution for  $\hat{a}_0^\dagger$  and  $\hat{a}_0$  means that, from the whole sum in the interaction, it is sufficient to keep only those terms which involve interaction with the condensate itself.

In this limit,  $|\Psi\rangle$  becomes an eigenstate of both creation and annihilation operators, and hence is a coherent state. Thus, the density operator can be approximated as (keeping just the dominating terms as  $N_0 \rightarrow \infty$ )

$$\hat{\rho}_q^\dagger \simeq \frac{1}{\sqrt{V}} (\hat{a}_q^\dagger \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_{-q}) = \sqrt{\frac{N_0}{V}} (\hat{a}_q^\dagger + \hat{a}_{-q}). \quad (3.32)$$

This is an example of the random phase approximation [44]. It is interesting that, a density creation operator in this case reduces to an equal superposition of a particle creation and particle annihilation operators in the small  $g$  approximation.

Now, we will apply c-number substitution in the case of macroscopic occupation of  $k = 0$  mode. We pull out the zero mode to inspect it closely,

$$\begin{aligned} \hat{U} = \frac{g}{2V} & \left[ \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 + \sum_{k \neq 0} 4 \hat{a}_k^\dagger \hat{a}_0^\dagger \hat{a}_k \hat{a}_0 + \sum_{k \neq 0} \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_0 \hat{a}_0 + \sum_{k \neq 0} \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_k \hat{a}_{-k} \right. \\ & \left. + \sum_{k, k' \neq 0} 2 \hat{a}_k^\dagger \hat{a}_{k'}^\dagger \hat{a}_{k+k'} \hat{a}_0 + \sum_{k, k' \neq 0} 2 \hat{a}_{k+k'}^\dagger \hat{a}_0^\dagger \hat{a}_k \hat{a}_{k'} + \sum_{k, k', k'' \neq 0} \hat{a}_k^\dagger \hat{a}_{k'}^\dagger \hat{a}_{k''} \hat{a}_{k+k'-k''} \right], \quad (3.33) \end{aligned}$$

then using Bogoliubov approximation, we get

$$\begin{aligned} \hat{U} = \frac{g}{2V} & \left[ N_0^2 + 4N_0 \sum_{k \neq 0} \hat{a}_k^\dagger \hat{a}_k + N_0 \sum_{k \neq 0} \left( \hat{a}_k^\dagger \hat{a}_{-k}^\dagger + \hat{a}_k \hat{a}_{-k} \right) \right. \\ & \left. + 2\sqrt{N_0} \sum_{k, k' \neq 0} \left( \hat{a}_{k+k'}^\dagger \hat{a}_k \hat{a}_{k'} + \hat{a}_k^\dagger \hat{a}_{k'}^\dagger \hat{a}_{k+k'} \right) + \sum_{k, k', k'' \neq 0} \hat{a}_k^\dagger \hat{a}_{k'}^\dagger \hat{a}_{k''} \hat{a}_{k+k'-k''} \right]. \end{aligned} \quad (3.34)$$

Define  $n_0 = N_0/V$ . In the thermodynamic limit ( $V \rightarrow \infty$ , as  $n = N/V$  is constant) the last two sums vanish. Then the Hamiltonian with only the terms surviving the thermodynamic limit is

$$\hat{H}'_{eff} = \frac{1}{2} n_0^2 g V + \sum_{k \neq 0} \left[ (\epsilon_k + 2gn_0) \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} gn_0 \left( \hat{a}_k^\dagger \hat{a}_{-k}^\dagger + \hat{a}_k \hat{a}_{-k} \right) \right]. \quad (3.35)$$

Notice that by c-number substitution, (3.29) also reduces to this form of the interaction term in the effective Hamiltonian. Terms involving the excited states of the ideal gas have the following physical interpretation:

- $g \left( \hat{a}_k^\dagger \hat{a}_k \right)$  represents the ‘*Hartree-Fock energy*’ of excited particles interacting with the condensate,
- $g \left( \hat{a}_k^\dagger \hat{a}_{-k}^\dagger + \hat{a}_k \hat{a}_{-k} \right)$  represents creation and annihilation of excited particles from the condensate. Note that interaction energies among particles in the excited states are automatically excluded. In this present approximation, total number of particles is not conserved,  $\hat{H}'_{eff}$  is not a number preserving operator, hence it does not commute with the total number operator  $\hat{N}$ .

Note that, there are no spin indices included in the field operators, just the spacial coordinates are present. Thus, Hamiltonian we have is missing spin states. Including spin indices makes this relevant to the Gross-Pitaevskii and Bogoliubov theories for superfluids [15].

Observing the Hamiltonian in (3.35), we see the kinetic energy operator is diag-

onal in the single-particle operators, whereas the potential energy operator is diagonal in the density operators. To diagonalize the full Hamiltonian, we should transform the  $\hat{H}'_{eff}$  matrix.

We see that, with the substitution of c-numbers, the Hamiltonian reduces to a quadratic form in the single-particle operators that can be diagonalized by a linear transformation from the starting Bose operators  $(\hat{a}_k^\dagger, \hat{a}_k)$  to new Bose operators  $(\hat{b}_k^\dagger, \hat{b}_k)$ , which are named as quasiparticle creation and annihilation operators, respectively. They are assumed to obey the same bosonic commutation rules as the original Bose operators given by (3.1),

$$[\hat{b}_k, \hat{b}_{k'}] = 0, \quad [\hat{b}_k^\dagger, \hat{b}_{k'}^\dagger] = 0, \quad [\hat{b}_k, \hat{b}_{k'}^\dagger] = \delta_{kk'}. \quad (3.36)$$

With this canonical transformation, an excited state can be described in terms of elementary excitations with number density  $\hat{b}_k^\dagger \hat{b}_k$  and energy  $\omega_k$ . The aim is to find the new Bose operators and the new excitation energy in terms of the parameters of the Hamiltonian. This is done by the procedure of Bogoliubov transformation.

As a remark, since the occupation number of the excited states with  $k \neq 0$  is small in a dilute and cold gas, in the lowest-order approximation the ground state energy takes the form

$$E'_0 = \frac{g}{2V} N_0^2 \simeq \frac{g}{2V} N^2. \quad (3.37)$$

It is convenient to include the chemical potential in the Hamiltonian and define

$$\hat{H} = \hat{H}' - \mu \hat{N}, \quad (3.38)$$

where,  $\mu$  is the chemical potential of the whole system, the ground state energy becomes

$$E_0 \simeq \frac{g}{2V} N_0^2 - \mu N_0. \quad (3.39)$$

Until now, we have used the total number of particles in the system as the independent variable, since to set up our perturbation theory formalism, we had to start from the characteristics of an ideal Bose gas, for which there is no condensation when the chemical potential is finite. In fact, we have seen that the chemical potential of an ideal Bose gas converges to zero below the critical temperature  $T_c$ . However, for a system of interacting particles, the chemical potential is nonzero, and hence can be chosen as a thermodynamic variable as well. As usual, the value of  $\mu$  can be found from the condition that the average number of particles in the system is equal to the given actual number of particles  $N$ . Therefore, the transformation from the variable  $N$  to the variable  $\mu$  can be accomplished by replacing the total Hamiltonian of the system, by  $\hat{H}' - \mu \hat{N}$ . Then, we shall assume  $\mu$  as the independent thermodynamic variable.

For the system in equilibrium, the chemical potential of the condensate,  $\mu_c$ , is taken to be zero at zero temperature in the lowest order approximation. Therefore using thermodynamic formula for the chemical potential of the condensate gives

$$\mu_c = \left( \frac{\partial E_0}{\partial N_0} \right)_{S,V} = gn_0 - \mu = 0, \quad (3.40)$$

which suggests that the chemical potential of the system as a whole is taken as

$$\mu = gn_0. \quad (3.41)$$

Notice that  $\mu \rightarrow \mu_c = 0$  as  $g$  is small and  $n_0$  is finite. This result is interesting since the chemical potential for the condensate is always negative (zero is its boundary value in the low temperature limit) for the noninteracting Bose system. In the first order approximation, where the particles in the ground state dominates the system,

*i.e.*,  $N_0 \simeq N$ , this result suggests a positive chemical potential for the whole system of weakly interacting bosons. Actually, in a system of ideal Bose gas, populating the ground state (the condensate) lowers the total energy of the system. In the repulsively interacting particles case, however, an extra energy is required to add one particle to the ground state due interactions between particles, and its given as  $\mu = gn_0$  in the lowest order approximation. In the limit  $g \rightarrow 0$ ,  $\mu$  also converges to zero as in the ideal Bose gas.

For the pressure of the condensate we write

$$P_0 \equiv - \left( \frac{\partial E_0}{\partial V} \right)_{S,N} = \frac{g}{2} n_0^2 \quad (3.42)$$

therefore, the speed of sound in the condensate is

$$c = \sqrt{\left( \frac{\partial P_0}{\partial \rho_0} \right)_S} = \sqrt{\frac{gn_0}{m}} \quad (3.43)$$

where,  $\rho_0 = mn_0$  is the particle mass density in the condensate. Also we observe that the isothermal compressibility of the condensate turns out to be finite

$$\kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial P_0} \right)_T = \frac{1}{gn_0^2} \quad (3.44)$$

Note that this result is different from the one in the case of the ideal Bose gas, which has infinite compressibility. The thermodynamic stability requires that the compressibility to be positive. This leads to an important conclusion that a dilute BE condensate can stably exist only if the system has a repulsive interaction ( $g > 0$ ).

### 3.4. Bogoliubov Transformation and Depletion of the Condensate

In writing the original Hamiltonian  $H'$  of weakly interacting Bose system, we considered the system having statistical properties of a canonical ensemble, which has

fixed number of particles. Including the chemical potential to the Hamiltonian gives

$$\hat{H} = \hat{H}' - \mu \hat{N}, \quad (3.45)$$

which is the Hamiltonian of a grand canonical ensemble, where particle exchange is allowed. Using the chemical potential in the Hamiltonian (3.35) as  $\mu = gn_0$ , we have

$$\hat{H}_{eff} = -\frac{1}{2}gn_0^2V + \left[ \sum_{k \neq 0} (\epsilon_k + gn_0) \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2}gn_0 (\hat{a}_k^\dagger \hat{a}_{-k}^\dagger + \hat{a}_k \hat{a}_{-k}) \right]. \quad (3.46)$$

Now we will put the Hamiltonian in a symmetric form up to a constant diagonal term

$$\hat{H}_{eff} = \frac{1}{2} \sum_{k \neq 0} \left[ (\epsilon_k + gn_0) (\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k} \hat{a}_{-k}^\dagger) + gn_0 (\hat{a}_k^\dagger \hat{a}_{-k}^\dagger + \hat{a}_k \hat{a}_{-k}) \right]. \quad (3.47)$$

We observe that  $\hat{H}_{eff}$  can be expressed as a matrix multiplication

$$\hat{H}_{eff} = \sum_{k \neq 0} \begin{bmatrix} \hat{a}_k^\dagger & \hat{a}_{-k} \end{bmatrix} \begin{bmatrix} \epsilon_k + gn_0 & gn_0 \\ gn_0 & \epsilon_k + gn_0 \end{bmatrix} \begin{bmatrix} \hat{a}_k \\ \hat{a}_{-k}^\dagger \end{bmatrix}. \quad (3.48)$$

Here onward, we will use the canonical Bogoliubov transformation, which is

$$\begin{bmatrix} \hat{a}_k \\ \hat{a}_{-k}^\dagger \end{bmatrix} = \begin{bmatrix} \cosh \theta_k & \sinh \theta_k \\ \sinh \theta_k & \cosh \theta_k \end{bmatrix} \begin{bmatrix} \hat{b}_k \\ \hat{b}_{-k}^\dagger \end{bmatrix}. \quad (3.49)$$

Here  $\hat{b}_k^\dagger$  and  $\hat{b}_k$  represent new Bose operators and are known as quasiparticle creation and annihilation operators, respectively. They are linear combinations (superpositions) of the particle creation and annihilation operators as can be seen exclusively by the inverse transformation

$$\begin{bmatrix} \hat{b}_k \\ \hat{b}_{-k}^\dagger \end{bmatrix} = \begin{bmatrix} \cosh \theta_k & -\sinh \theta_k \\ -\sinh \theta_k & \cosh \theta_k \end{bmatrix} \begin{bmatrix} \hat{a}_k \\ \hat{a}_{-k}^\dagger \end{bmatrix}. \quad (3.50)$$

Applying this to the Hamiltonian given by (3.35), we get

$$\begin{aligned}
\hat{H}_{eff} = & -\frac{1}{2}gn_0^2V + \sum_{k \neq 0} \left[ (\epsilon_k + gn_0) \sinh^2 \theta_k + \frac{1}{2}gn_0 \sinh 2\theta_k \right] \\
& + \sum_{k \neq 0} ((\epsilon_k + gn_0) \cosh 2\theta_k + gn_0 \sinh 2\theta_k) (\hat{b}_k^\dagger \hat{b}_k) \\
& + \frac{1}{2} \sum_{k \neq 0} ((\epsilon_k + gn_0) \sinh 2\theta_k + gn_0 \cosh 2\theta_k) (\hat{b}_k^\dagger \hat{b}_{-k}^\dagger + \hat{b}_k \hat{b}_{-k}), \quad (3.51)
\end{aligned}$$

where we used  $\theta_{-k} = \theta_k$ . For this form of the Hamiltonian to be diagonalized in the quasiparticle basis, we force terms in the third sum to be equal to zero for all  $\mathbf{k} \neq 0$

$$(\epsilon_k + gn_0) \sinh 2\theta_k + gn_0 \cosh 2\theta_k = 0, \quad (3.52)$$

solving for  $\theta_k$  gives

$$\begin{aligned}
\cosh 2\theta_k &= \frac{\epsilon_k + gn_0}{\omega_k}, \\
\sinh 2\theta_k &= \frac{-gn_0}{\omega_k}. \quad (3.53)
\end{aligned}$$

where

$$\omega_k = \sqrt{(\epsilon_k + gn_0)^2 - (gn_0)^2}. \quad (3.54)$$

Now the Hamiltonian is diagonalized by this canonical transformation as

$$\hat{H}_{eff} = E_0 + \sum_{k \neq 0} \omega_k \hat{b}_k^\dagger \hat{b}_k. \quad (3.55)$$

This is the famous dispersion law of the Bogoliubov excitation spectrum. In the limit of small momenta ( $\mathbf{k} \sim 0$ ), spectrum of low-energy excitations scales as

$$\epsilon_k \simeq \hbar ck \quad (3.56)$$

which corresponds to the phonon part of the spectrum of the Bose gas. Here,  $c = \sqrt{gn/m}$  is the speed of sound in the system. For large momenta, spectrum becomes free-particle like, *i.e.*,  $\omega_k \rightarrow \epsilon_k$ .

The ground state energy  $E_0$  of this Hamiltonian can be extracted from (3.51), and using (3.53), it simplifies as

$$E_0 = -\frac{1}{2}gn_0^2V - \frac{1}{2}\sum_{k \neq 0}(\epsilon_k + gn_0) - \omega_k. \quad (3.57)$$

Coming back to our original Hamiltonian  $H'_{eff}$  with fixed particle number  $N$ , and using the lowest order approximation  $n \sim n_0$ , the ground state energy is written as

$$E'_0 = E_0 + \mu N \sim \frac{1}{2}gn^2V - \frac{1}{2}\sum_{k \neq 0}(\epsilon_k + gn) - \omega_k. \quad (3.58)$$

It is obvious that the sum over  $\mathbf{k}$  in this expression diverges like  $\sum_k \frac{1}{k^2}$ , which is an ultraviolet divergence, hence non-physical. This is due to the fact that the energy cannot actually be expanded in powers of the coupling constant  $g$ . In fact, the presence of constant  $g$  forces the ground state energy to diverge. In the case being considered, it is essential that the scattering amplitude  $a$  should be finite and small, in order to expand the energy with respect to  $a$ . We modify the relationship between  $a$  and  $g$  (3.18) as [31, 45],

$$g - \frac{g^2}{2V}\sum_{k \neq 0}\frac{1}{\epsilon_k} \equiv \frac{4\pi\hbar^2 a}{m}, \quad (3.59)$$

using second order perturbation theory to examine the scattering of two particles of the condensate with a transition to the state  $\mathbf{k}$ ,  $-\mathbf{k}$ . With the first order term only, total interaction energy in the condensate diverges due to large amount of interparticle collisions in the condensate. However with the second order correction to  $g$ , substituting

(3.59) for  $g$ , we obtain

$$E'_0 = \frac{gn^2V}{2} - \frac{1}{2} \sum_{k \neq 0} \left[ \epsilon_k + gn - \omega_k - \frac{(gn)^2}{2\epsilon_k} \right] \quad (3.60)$$

which converges for large  $k$ . Integrating this expression with respect to  $k$  we get

$$E'_0 = \frac{gn^2V}{2} \left[ 1 + \frac{128}{15\sqrt{\pi}} (na^3)^{1/2} \right]. \quad (3.61)$$

Here  $a$  denotes the scattering amplitude of the interaction. The first term of this expression gives the mean-field energy and coincides with the result obtained from the Gross-Pitaevskii equation. The second term gives the correction to the ground state energy arising from the zero-point motion of the quasiparticles. The result is valid if the system is dilute, *i.e.*, if the gas parameter is small

$$na^3 \ll 1. \quad (3.62)$$

The chemical potential for the condensate in the first order correction can be derived by substituting the zeroth order chemical potential for the system as

$$\mu_c = \left( \frac{\partial E_0}{\partial N_0} \right)_{S,V} = \left( \frac{\partial (E'_0 - gn_0N)}{\partial N_0} \right)_{S,V} \simeq gn_0 \left[ \frac{32}{3\sqrt{\pi}} (n_0a^3)^{1/2} \right]. \quad (3.63)$$

Thus the chemical potential for the whole system becomes

$$\mu = gn_0 \left[ 1 + \frac{32}{3\sqrt{\pi}} (n_0a^3)^{1/2} \right], \quad (3.64)$$

coinciding with our previous result in the zeroth order.

Now, notice that the operator  $\hat{b}_k^\dagger \hat{b}_k$  corresponds to the number of elementary excitations of noninteracting quasiparticles, which satisfies the usual BE distribution

with zero chemical potential

$$\hat{b}_k^\dagger \hat{b}_k = \frac{1}{e^{\beta\omega_k} - 1}, \quad (3.65)$$

which converges to zero at zero temperature. For the mean occupation number of particles we have

$$\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k. \quad (3.66)$$

Using the canonical transformation in (3.49) yields

$$\hat{n}_k = \frac{\hat{b}_k^\dagger \hat{b}_k + \tanh^2 \theta_k (\hat{b}_k^\dagger \hat{b}_k + 1)}{1 - \tanh^2 \theta_k}. \quad (3.67)$$

This applies only for  $k \neq 0$ . At absolute zero temperature, quasiparticle occupation number vanishes. Therefore mean occupation number of particles simplifies as

$$n_k = \sinh^2 \theta_k = \frac{\epsilon_k + gn - \omega_k}{2\omega_k}, \quad (3.68)$$

where we used  $n \sim n_0$  again. Integrating with respect to  $\mathbf{k}$

$$\frac{N_e}{N} = \frac{1}{N} \sum_{k \neq 0} \sinh^2 \theta_k = \frac{1}{n} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \sinh^2 \theta_k = \frac{1}{3\pi^2 n} k_0'^3. \quad (3.69)$$

Here,  $k_0'$  is the magnitude of the single-particle ground state wavevector in the lowest order approximation

$$\frac{\hbar^2 k_0'^2}{2m} = \epsilon_0' \equiv \frac{E_0'}{N_0} \simeq \frac{gn}{2}. \quad (3.70)$$

Hence, we get

$$\frac{N_e}{N} = \frac{n_e}{n} = \frac{8}{3\sqrt{\pi}} (na^3)^{1/2}. \quad (3.71)$$

So the depletion coefficient, which is the number density of bosons out of the condensate is

$$n_e = \frac{8}{3\sqrt{\pi}}(na)^{3/2}. \quad (3.72)$$

Equivalently

$$N_0 = N \left[ 1 - \frac{8}{3\sqrt{\pi}} (na^3)^{1/2} \right]. \quad (3.73)$$

Notice that we used  $N$  and  $N_0$  interchangeably to get a first order correction to  $N_0$ , like in the Born series. This suggests that we can substitute eqn. (3.73) for  $N_0$ , and get a second order term, and so on. The same method applies for obtaining higher order terms of the chemical potential. However, the description of the effective Hamiltonian by the c-number substitution overshadows the physical meaning of higher order terms, *i.e.*, these terms appear not as corrections in higher orders.

Due to interactions, particles are pushed out of the condensate and a fraction of particles with nonzero momenta is present even at zero temperature. This phenomenon is called *quantum depletion of the condensate*. The same result is valid also in the dilute regime,  $na^3 \ll 1$ , in which the quantum depletion is small and Bogoliubov theory applies.

To conclude, we indicate that diagonalization of the Hamiltonian with the new Bose operators has a deep physical meaning. The original system of interacting particles can be described by the Hamiltonian for non-interacting quasiparticles. In this picture, a real particle  $\hat{a}_k$  is described as the superposition of the forward propagating many quasiparticles  $\cosh \theta_k \hat{b}_k$  and the backward propagating many quasiparticles  $\sinh \theta_k \hat{b}_{-k}^+$ . Looking at the limit cases of the momentum, we see

$$\cosh \theta_k \simeq \sinh \theta_k \gg 1, \quad \text{and} \quad \hat{a}_k \sim \cosh \theta_k (\hat{b}_k - \hat{b}_{-k}^+), \quad \text{for small } k \quad (3.74)$$

and

$$\cosh \theta_k \simeq 1, \quad \text{and} \quad \sinh \theta_k \simeq 0, \quad \text{for large } k. \quad (3.75)$$

In the large  $k$  limit, quasiparticle operators become indistinguishable from the real particle operators, *i.e.*,  $\hat{a}_k \sim \hat{b}_k$ .

## 4. A BRIEF OVERVIEW ON THE HEAT KERNEL IN A RIEMANNIAN MANIFOLD

In order to see the connection between the spectrum of the laplacian operator  $\Delta$  and the geometry of a smooth,  $d$ -dimensional, connected Riemann manifold  $M$  with boundary  $\partial M$ , and with metric  $g$ , we will first define what is meant by the heat kernel.

The heat equation is a parabolic PDE that describes the distribution of heat in a given region over time. In a  $d$ -dimensional manifold, the homogeneous heat equation without boundary conditions is

$$\frac{\partial u}{\partial t} = \alpha \Delta u, \tag{4.1}$$

where  $u = u(x, y, z, t)$  is a function with three spatial variables  $(x, y, z)$ , and the time variable  $t$ ,  $\alpha > 0$  is the thermal diffusivity. We will take  $\alpha = 1$ , and solve the homogeneous heat equation in one dimension for simplicity. Generalizations will be straightforward.

We will consider the initial value problem with the Neumann boundary condition

$$\begin{cases} u_t(x, t) = u_{xx}(x, t), & x \in M_1, t > 0 \\ u_x(x, t) = 0, & x \in \partial M_1 \\ u(x, 0) = \phi(x), & x \in M_1 \end{cases} \tag{4.2}$$

where, indices mean partial differentiation with respect to that variable. Here  $M_1 = (-L, L) \subset \mathbb{R}$  is an open, bounded set (interval). We will use separation of variables method to solve this boundary value problem. Assume simple solutions in the form

$$u(x, t) = X(x)T(t). \tag{4.3}$$

Substituting this into (4.2) and dividing both sides by  $X(x)T(t)$  gives

$$\frac{1}{T} \frac{dT}{dt} = \frac{1}{X} \frac{d^2X}{dx^2} = -\lambda \quad (4.4)$$

since, equivalence of these functions of different variables mean that they both must be a constant  $-\lambda$ , which is called a separation of variable constant. Notice that  $X(x) = T(t) = 0$  solves the initial value problem, but we look for nontrivial solutions. Solving for  $T$  yields

$$T(t) = Ce^{-\lambda t} \quad (4.5)$$

where,  $C$  is an arbitrary constant. Furthermore, the boundary condition gives

$$X'(-L)T(t) = 0, \quad \text{and} \quad X'(L)T(t) = 0, \quad \text{for all } t. \quad (4.6)$$

$T(t) \neq 0$  for nontrivial solutions, thus we have the eigenvalue problem with the Neumann boundary condition

$$-X''(x) = \lambda X(x), \quad \text{and} \quad X'(-L) = X'(L) = 0 \quad (4.7)$$

where  $\lambda$  being an eigenvalue of the operator  $-d^2/dx^2$  with eigenfunction  $X$ .

Now, we will find the eigenvalues and eigenfunctions. Multiply both sides of (4.7) by  $X$ . Integrating from  $x = -L$  to  $x = L$ , and using integration by parts with the boundary condition gives

$$\lambda \int_{-L}^L X^2 dx = - \int_{-L}^L X'' X dx = \int_{-L}^L X'^2 dx. \quad (4.8)$$

Therefore,

$$\lambda = \frac{\int_{-L}^L X'^2 dx}{\int_{-L}^L X^2 dx} \geq 0. \quad (4.9)$$

We conclude  $\lambda = 0$  or  $\lambda > 0$ . First, pick  $\lambda = 0$ . Then

$$X(x) = Ax + B, \quad (4.10)$$

where,  $A$  and  $B$  are arbitrary constants. Applying boundary conditions, we get  $A = 0$ . Hence  $\lambda_0 = 0$  is an eigenvalue with the constant eigenfunction  $\psi_0(x) = 1$ . Now pick  $\lambda = \kappa^2 > 0$ . Then we have solutions of the form

$$X(x) = Ae^{i\kappa x} + Be^{-i\kappa x} \quad (4.11)$$

and

$$X'(x) = i\kappa Ae^{i\kappa x} - i\kappa Be^{-i\kappa x}. \quad (4.12)$$

Applying boundary condition gives  $\sin 2\kappa L = 0$ , which implies  $\kappa = n\pi/2L$ . Therefore,

$$\lambda_n = \kappa_n^2 = \left(\frac{n\pi}{2L}\right)^2 \quad \text{with eigenfunctions} \quad \psi_n(x) = e^{\frac{in\pi x}{2L}}, \quad (4.13)$$

where  $n = \dots - 2, -1, 0, 1, 2, \dots$

Now, consider general eigenvalue problem for the Laplacian on an open, bounded set  $M$  in  $\mathbb{R}^d$  with the Neumann boundary condition

$$\begin{cases} -\Delta v(\mathbf{x}) = \lambda v(\mathbf{x}), & \mathbf{x} \in M \\ \hat{\mathbf{n}} \cdot \nabla v(\mathbf{x}) = 0, & \mathbf{x} \in \partial M \end{cases} \quad (4.14)$$

where  $\hat{\mathbf{n}}$  is the unit normal vector. In the Neumann boundary condition, flux through  $M$  vanishes in some sense. As in the one dimensional case, Laplacian for the Neumann boundary condition has pure point spectrum, *i.e.*,

$$\lambda_0 < \lambda_1 < \lambda_2 < \dots \quad (4.15)$$

There are infinitely many eigenvalues accumulating only at infinity [46]. For the connected manifolds with contact support, the zeroth (ground state) eigenvalue is zero,  $\lambda_0 = 0$ . This result is a simple generalization from one dimensional case (see [47] for details).

Eigenfunctions and eigenvalues of the Laplacian have certain properties [48] (not only for the Neumann boundary condition):

- (i) All eigenvalues are real.
- (ii) All eigenfunctions can be chosen to be real-valued.
- (iii) Eigenfunctions corresponding to distinct eigenvalues are real.
- (iv) All eigenfunctions can be chosen to be orthogonal by using Gram-Schmidt process.

Coming back to the solution of the homogeneous heat equation in one dimension, since any linear combination of solutions is also a solution, we write

$$u(x, t) = \sum_{-\infty}^{\infty} a_n e^{\frac{in\pi x}{2L}} e^{-\left(\frac{n\pi}{2L}\right)^2 t} \quad (4.16)$$

where  $a_n$  are constants, and the sum is over  $n$ . For the initial value problem, we have

$$u(x, 0) = \phi(x) = \sum_{-\infty}^{\infty} a_n e^{\frac{in\pi x}{2L}}, \quad (4.17)$$

Using Fourier's trick, we get

$$a_n = \frac{1}{4L} \int_{-L}^L \phi(x) e^{-\frac{in\pi x}{2L}} dx. \quad (4.18)$$

Hence, we can write

$$\phi(x) = \sum_{-\infty}^{\infty} \left[ \frac{1}{4L} \int_{-L}^L \phi(y) e^{-\frac{in\pi(y-x)}{2L}} dy \right]. \quad (4.19)$$

Substitute  $k = n\pi/2L$ . As  $L \rightarrow \infty$ , we can think of  $\Delta k \rightarrow dk$ , and the infinite sum becomes a Riemann integral. Then we write

$$\phi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi(y) e^{-i(y-x)k} dy dk. \quad (4.20)$$

This result motivates us to use the Fourier transform of the function  $\phi$  to solve the homogeneous heat equation on the whole real line, and more generally in  $\mathbb{R}^d$ .

For a function  $f \in L^1(\mathbb{R}^d)$ <sup>13</sup>, Fourier transform of  $f(\mathbf{x})$  at a point  $\mathbf{k} \in \mathbb{R}^d$  is defined as

$$\tilde{f}(\mathbf{k}) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}) d\mu_g(\mathbf{x}). \quad (4.21)$$

Here,  $d\mu_g(\mathbf{x})$  is the Riemannian volume element corresponding to the metric  $g$ . Under suitable conditions,  $f(\mathbf{x})$  is determined by  $\tilde{f}(\mathbf{k})$  via the inverse transform

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{i\mathbf{k}\cdot\mathbf{x}} \tilde{f}(\mathbf{k}) d\mu_g(\mathbf{k}). \quad (4.22)$$

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<sup>13</sup>  $f \in L^1(\mathbb{R}^d)$  if  $\int_{\mathbb{R}^d} |f(\mathbf{x})| d\mu_g(\mathbf{x}) < \infty$ .

Now, consider the initial value problem for the homogeneous heat equation on  $\mathbb{R}$ ,

$$\begin{cases} u_t = \alpha u_{xx}, & x \in \mathbb{R}, t > 0 \\ u(x, 0) = \phi(x). \end{cases} \quad (4.23)$$

Applying the Fourier transform to the heat equation, we have

$$\tilde{u}_t(k, t) = \alpha \widetilde{u_{xx}}(k, t) = -\alpha k^2 \tilde{u}(k, t), \quad (4.24)$$

where we used integration by parts to get the result. Solving this ODE with the initial condition, we have

$$\tilde{u}(k, t) = \tilde{\phi}(k) e^{-\alpha k^2 t}. \quad (4.25)$$

Hence,

$$\begin{aligned} u(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \tilde{u}(k, t) dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \left[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iky} \phi(y) dy \right] e^{-\alpha k^2 t} dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(y) \left[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik(y-x)} e^{-\alpha k^2 t} dk \right] dy \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(y) h(y-x) dy \end{aligned} \quad (4.26)$$

where,  $h(y-x)$  is the inverse Fourier transform of  $\tilde{h}(k) \equiv e^{-\alpha k^2 t}$ . By simple calculations, we have

$$h(y-x) = \frac{1}{\sqrt{2\alpha t}} e^{-\frac{(y-x)^2}{4\alpha t}}. \quad (4.27)$$

Finally, the solution of the initial value problem for the homogeneous heat equation on

$\mathbb{R}$  is given by

$$u(x, t) = \frac{1}{\sqrt{4\pi\alpha t}} \int_{-\infty}^{\infty} \phi(y) e^{-\frac{(x-y)^2}{4\alpha t}} dy. \quad (4.28)$$

Same analysis applies for solving the problem in higher dimensions. Consider the initial value problem for the homogeneous heat equation in  $\mathbb{R}^d$ ,

$$\begin{cases} u_t = \alpha \Delta u, & \mathbf{x} \in \mathbb{R}^d, t > 0 \\ u(\mathbf{x}, 0) = \phi(\mathbf{x}). \end{cases} \quad (4.29)$$

Using the Fourier transform as in the one dimensional case, we have

$$u(\mathbf{x}, t) = \frac{1}{(4\pi\alpha t)^{d/2}} \int_{\mathbb{R}^d} \phi(\mathbf{y}) e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4\alpha t}} d\mu_g(\mathbf{y}). \quad (4.30)$$

It is easy to verify that this solution actually satisfies the initial value problem, *i.e.*,  $\lim_{t \rightarrow 0^+} u(\mathbf{x}, t) = \phi(\mathbf{x})$ . Obviously, the function

$$H(\mathbf{x}, \mathbf{y}, t) := \frac{1}{(4\pi\alpha t)^{d/2}} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4\alpha t}} \quad (4.31)$$

satisfies the homogeneous heat equation for all  $t > 0$ . Now define

$$K_t(\mathbf{x}, \mathbf{y}) \equiv \begin{cases} H(\mathbf{x}, \mathbf{y}, t), & t > 0 \\ 0, & t < 0. \end{cases} \quad (4.32)$$

Using this function, solutions of (4.29) can be written as a convolution

$$u(\mathbf{x}, t) = [K_t * \phi](\mathbf{x}) = \int_{\mathbb{R}^d} K_t(\mathbf{x}, \mathbf{y}) \phi(\mathbf{y}) d\mu_g(\mathbf{y}). \quad (4.33)$$

Here,  $t$  dependence comes from  $K_t$ , which is called the *fundamental solution* of the heat equation, also known as the *heat kernel*.

Now we will give the definition of operator kernel

**Definition 4.1.** *Let  $A$  be an operator on  $L^2(M)$ . If there exists a function  $A(\mathbf{x}, \mathbf{y})$  such that*

$$A f(\mathbf{x}) = \int A(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mu_g(\mathbf{y}). \quad (4.34)$$

for all functions  $f$ , then we call  $A(\mathbf{x}, \mathbf{y})$  is the kernel of the operator  $A$ .

By this definition, we say the kernel of an operator does not exist in general. For instance, let  $\mathcal{B}$  be a Banach space, and let  $I$  be the identity map. Then the kernel of  $I$  does not exist. Nevertheless, the heat kernel exists in a Riemannian manifold with smooth boundary, which is the kernel of the operator  $e^{\Delta t}$ , and defined formally as [49]

**Definition 4.2.** *Let  $M$  be a complete Riemannian manifold. Then there exists heat kernel  $K_t(\mathbf{x}, \mathbf{y}) \equiv K(\mathbf{x}, \mathbf{y}, t) \in \mathbb{C}^\infty(M \times M \times \mathbb{R}^+)$  such that*

$$(e^{\Delta t} f)(\mathbf{x}) = \int_M K_t(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mu_g(\mathbf{y}). \quad (4.35)$$

for any square-integrable function  $f$ .

The heat kernel satisfies properties given below [49]:

- (i)  $K_t(\mathbf{x}, \mathbf{y}) = K_t(\mathbf{y}, \mathbf{x})$ ,
- (ii)  $\lim_{t \rightarrow 0^+} K_t(\mathbf{x}, \mathbf{y}) = \delta_{\mathbf{x}}(\mathbf{y})$ ,
- (iii)  $(\Delta - \frac{\partial}{\partial t}) K_t(\mathbf{x}, \mathbf{y}) = 0$ ,
- (iv)  $K_{t_1+t_2}(\mathbf{x}, \mathbf{y}) = \int_M K_{t_1}(\mathbf{x}, \mathbf{z}) K_{t_2}(\mathbf{y}, \mathbf{z}) d\mu_g(\mathbf{z})$ , for  $t_1, t_2 > 0$ .

For flat spaces, we can easily check that the heat kernel (4.31) satisfies these properties. The last property is called as the *self-reproduction property* of the heat kernel.

There exists a nice connection between the heat equation and eigenvalues and eigenfunctions of the laplacian  $-\Delta$ . Dodziuk states the following theorem [46]:

**Theorem 4.1.** *There exists a complete orthonormal basis  $\{\psi_\xi\}_{\xi=1}^\infty$  of  $L^2(M)$  consisting of eigenfunctions of  $-\Delta$ . If  $\lambda_i$  is the eigenvalue corresponding to  $\psi_i$ , then  $\lim_{i \rightarrow \infty} \lambda_i = \infty$ . Also*

$$K_t(\mathbf{x}, \mathbf{y}) = \sum_{i=0} e^{-\lambda_i t} \psi_i(\mathbf{x}) \psi_i(\mathbf{y}), \quad (4.36)$$

where the convergence is uniform in  $\bar{M} \times \bar{M} \times \mathbb{R}^+$  for all  $\epsilon > 0$ .

Using this theorem we obtain

$$\begin{aligned} \int_M K_t(\mathbf{x}, \mathbf{x}) d\mu_g(\mathbf{x}) &= \int_M \sum_i e^{-\lambda_i t} [\psi_i(\mathbf{x})]^2 d\mu_g(\mathbf{x}) \\ &= \sum_i e^{-\lambda_i t} \\ &\equiv \text{Tr } e^{\Delta t}, \end{aligned} \quad (4.37)$$

since  $\{\psi_i\}$  is an orthonormal set. Here,  $\text{Tr}$  denotes the trace.

We observe  $K_t$  as an infinite dimensional operator with matrix elements  $K_t(\mathbf{x}, \mathbf{y})$ . In this sense, we can write the integral of the heat kernel as

$$\begin{aligned} \int_M K_t(\mathbf{x}, \mathbf{x}) d\mu_g(\mathbf{x}) &\equiv \int_M \langle \mathbf{x} | K_t | \mathbf{x} \rangle d\mu_g(\mathbf{x}) \\ &= \text{Tr } K_t \end{aligned} \quad (4.38)$$

where  $|\mathbf{x}\rangle$  denotes eigenkets of  $K_t$ . Here appears the equivalence of  $K_t$  and  $e^{\Delta t}$ . Therefore, we can denote the heat kernel as

$$K_t(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x} | e^{\Delta t} | \mathbf{y} \rangle. \quad (4.39)$$

Also using (4.31) and setting  $\alpha = 1$ , we see

$$\mathrm{Tr} e^{\Delta t} = \mathrm{Vol}(M) \frac{1}{(4\pi t)^{d/2}}. \quad (4.40)$$

This result is true in  $d$ -dimensional flat spaces, where we get the form of the heat kernel in (4.31). On a more general manifold in  $\mathbb{R}^d$ , such an explicit formula is not generally possible. However, the heat kernel exists and is smooth for  $t > 0$  on any Riemann manifold with boundary, provided the boundary is sufficiently regular. We will introduce upper and lower bounds by Li and Yau [26] for the trace of the heat kernel on a Riemannian manifold in Section 5.1.

Now, we will present some results obtained in Riemannian geometry using the heat kernel methods. Before this, we will need several definitions [50].

**Definition 4.3.** *The Ricci curvature of a Riemannian manifold  $M$  with metric  $g$ ,  $(M, g)$ , is the trace of the endomorphism of  $T_m M$  given by  $v \mapsto R_m(x, v)y$ , where  $R$  is the curvature tensor.*

**Definition 4.4.** *The scalar curvature,  $c$ , of  $(M, g)$  is the trace of the Ricci curvature. Notice that this is a function on  $M$ .*

In the following theorem, we will see two asymptotic expansions for the heat kernel [49].

**Theorem 4.2.** *(Minakshisundaram-Pleijel Asymptotic Expansion) Let  $(M, g)$  be a  $d$ -dimensional Riemannian manifold. The following asymptotic expansions hold as  $t \rightarrow 0^+$ :*

$$(i) \quad K_t(\mathbf{x}, \mathbf{x}) \sim \frac{1}{(4\pi t)^{d/2}} \sum_{m=0}^{\infty} u_m(\mathbf{x}) t^m, \text{ and}$$

$$(ii) \quad \mathrm{Tr} e^{\Delta t} \sim \frac{1}{(4\pi t)^{d/2}} \sum_{m=0}^{\infty} a_m t^m.$$

*The functions  $u_m(\mathbf{x})$  are  $\mathbb{C}^\infty$  functions on  $M$  which can be expressed as universal polynomials in the components of the curvature tensor and its covariant derivatives.*

See [51], for a brief outline of the proof of this construction. Now we will state Weyl's asymptotic formula in the form given in Chavel [51]:

**Theorem 4.3.** (*Weyl's Asymptotic Formula*) *Let  $M$  be a compact Riemannian Manifold with eigenvalues  $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots$ , with each distinct eigenvalue repeated with its multiplicity. Define  $N(\lambda)$  to be the number of eigenvalues less than or equal to  $\lambda$ , and let  $\omega_d$  denote the volume of the unit disk in  $\mathbb{R}^d$ . Then*

$$N(\lambda) \sim \frac{\omega_d \text{Vol}(M) \lambda^{d/2}}{(2\pi)^d}, \quad (4.41)$$

as  $\lambda \rightarrow \infty$ . Additionally, as  $k \rightarrow \infty$ ,

$$(\lambda_k)^{d/2} \sim \frac{(2\pi)^d k}{\omega_d \text{Vol}(M)}. \quad (4.42)$$

Both theorems are examples of inverse problems. In both cases, if we assume some knowledge about the eigenvalue of  $\Delta$ , we are given specific geometrical information about  $M$ , *i.e.*, we can determine the dimension of  $M$ , the volume of  $M$ , and the integral of the scalar curvature.

We have seen that defining the Laplace operator on Riemannian manifolds and determining its eigenvalues and eigenfunctions allowed us to discover geometrical information about the manifolds. Specifically, we used the heat kernel to correlate the spectrum and the geometry of the manifolds. In the next chapter, we will use eigenvalue estimates given in the form of upper and lower bounds for the trace of the heat kernel to investigate Bose-Einstein condensation on a  $d$ -dimensional Riemannian manifold. For a brief review, see [52].

## 5. HEAT KERNEL ANALYSIS OF BOSE-EINSTEIN CONDENSATION ON A MANIFOLD WITH NONNEGATIVE RICCI CURVATURE

### 5.1. Heat Kernel and Eigenvalue Bounds

We will introduce our geometric setting as a  $d$ -dimensional Riemannian manifold with metric  $g$  and nonnegative Ricci curvature

$$\mathbf{Ric} = R_{ij} dx^i \otimes dx^j, \quad (5.1)$$

where

$$R_{ij} = R_{ikj}^k \quad (5.2)$$

is the contraction of the Riemann curvature tensor.

Define  $(S, g)$  as a  $d$ -dimensional Riemannian manifold with metric  $g$  and nonnegative Ricci curvature

$$\mathbf{Ric}_S \geq 0. \quad (5.3)$$

A symmetric covariant tensor field  $\hat{T}$  of rank 2 is bounded below if there exists a real number  $c$  such that

$$\hat{T}(X, X) \geq c \hat{g}(X, X). \quad (5.4)$$

for all vector fields  $X$  on  $S$  ( $\hat{g}$  is the metric tensor).

Let  $M$  be a connected open submanifold of  $S$  with compact support and smooth

convex boundary  $\partial M$ . Since  $M \subset S$ , the Ricci curvature of  $M$  is also nonnegative. Let  $\Delta$  be the Laplacian of the metric  $g$  and  $f_\sigma$  ( $\sigma = 0, 1, 2, \dots$ ) be a complete orthonormal set of real (standing wave) square-integrable eigenfunctions of  $-\Delta$  on  $M$  with the Neumann boundary conditions

$$-\Delta f_\sigma = \epsilon_\sigma f_\sigma, \quad \text{and} \quad \hat{\mathbf{n}} \cdot \nabla f_\sigma|_{\partial M} = 0. \quad (5.5)$$

Here  $\hat{\mathbf{n}}$  is the normal vector on the boundary directed outwards. In the previous chapter, we stated a relation between the eigenvalues of the Laplacian as:

$$\epsilon_0 < \epsilon_1 < \epsilon_2 < \dots \rightarrow \infty, \quad (5.6)$$

$\epsilon_0$  being the smallest eigenvalue (ground state eigenvalue). The ground state is

$$f_0 = \frac{1}{\sqrt{V}}, \quad (5.7)$$

with  $\epsilon_0 = 0$ . Here,  $V$  is the volume of  $M$ . Essentially, this ground state is unique by our picture of  $M$  being connected.

We know that the eigenfunctions of the laplacian are real. Therefore,

$$\int_M d\mu_g(\mathbf{x}) f_\sigma^*(\mathbf{x}) f_\rho(\mathbf{x}) = \int_M d\mu_g(\mathbf{x}) f_\sigma(\mathbf{x}) f_\rho(\mathbf{x}) = \delta_{\sigma\rho}. \quad (5.8)$$

Picking  $\rho = 0$  and  $\sigma \neq 0$ , we get

$$\int_M d\mu_g(\mathbf{x}) f_\sigma(\mathbf{x}) f_0(\mathbf{x}) = \frac{1}{\sqrt{V}} \int_M d\mu_g(\mathbf{x}) f_\sigma(\mathbf{x}) = 0 \quad (5.9)$$

For the Neumann problem, heat kernel on a manifold  $M$  with a nonnegative Ricci

curvature and diameter  $D_M$ , one has the following estimates of Li and Yau [26],

$$\frac{1}{(4\pi t)^{d/2}} V \leq \text{Tr } e^{\Delta t} \leq \tilde{C}(d)g(t). \quad (5.10)$$

Here  $\text{Tr}$  denotes the trace, and  $\tilde{C}(d)$  is a positive constant which depends only on the dimension  $d$  and

$$g(t) = \begin{cases} \left(\frac{D_M}{\sqrt{t}}\right)^d & \text{if } \sqrt{t} \leq D_M, \\ 1 & \text{if } \sqrt{t} \geq D_M. \end{cases}$$

Note the  $O(t^{-d/2})$  behaviour of the heat kernel. The diameter  $D_M$  of a manifold means the greatest geodesic distance between any two points in the manifold, *i.e.*,

$$D_M = \sup\{r(\mathbf{p}, \mathbf{q}) : \mathbf{p}, \mathbf{q} \in M\}, \quad (5.11)$$

where  $r$  is the geodesic distance defined by the metric  $g$  on  $M$ .

A consequence of the upper bound for the trace of the heat kernel is a lower bound for the eigenvalue  $\epsilon_\sigma$  [26],

$$\epsilon_\sigma \geq \frac{C(d)}{D_M^2} (\sigma + 1)^{2/d} \geq \frac{C(d)}{D_M^2} \sigma^{2/d}, \quad (5.12)$$

where  $C(d)$  is a positive constant which depends only on the dimension  $d$ .

On the other hand one also has the following upper bound of Colbois and Maerten [27] for the eigenvalues

$$\epsilon_\sigma \leq B(d) \left(\frac{\sigma}{V}\right)^{2/d}. \quad (5.13)$$

Here  $B(d)$  is a positive constant which depends only on the dimension.

Using the eigenvalue bounds we get the following bounds for  $\text{Tr}' e^{\Delta t}$  (prime denotes

the trace without the ground state),

$$\frac{1}{V} \sum_{\sigma=1}^{\infty} e^{-\frac{tB}{v^{2/d}} \sigma^{2/d}} \leq \frac{1}{V} \sum_{\sigma=1}^{\infty} e^{-t\epsilon_{\sigma}} \leq \frac{1}{V} \sum_{\sigma=1}^{\infty} e^{-\frac{tC}{D_M^2} \sigma^{2/d}}, \quad (5.14)$$

where  $B$  and  $C$  are substituted for  $B(d)$  and  $C(d)$  for simplicity. Now we will replace the sums bounding the trace with integrals. As the terms in sums decrease with increasing  $\sigma$ , for the lower bound we get

$$\frac{1}{V} \sum_{x=1}^{\infty} e^{-\frac{tB}{v^{2/d}} x^{2/d}} \geq \frac{1}{V} \int_1^{\infty} dx e^{-\frac{tB}{v^{2/d}} x^{2/d}}. \quad (5.15)$$

They become equal in the thermodynamic limit ( $V \rightarrow \infty$ ) as the sum becomes a Riemann integral. For the upper bound term we have

$$\frac{1}{V} \sum_{x=1}^{\infty} e^{-\frac{tC}{D_M^2} x^{2/d}} \leq \frac{D_M^d}{V} \int_0^{\infty} dx e^{-tC x^{2/d}}. \quad (5.16)$$

Showing our results compactly,

$$\frac{1}{V} \int_1^{\infty} dx e^{-\frac{tB}{v^{2/d}} x^{2/d}} \leq \frac{1}{V} \text{Tr}' e^{\Delta t} \leq \frac{D_M^d}{V} \int_0^{\infty} dx e^{-tC x^{2/d}}. \quad (5.17)$$

These integrals can be evaluated explicitly as

$$\frac{1}{B^{d/2}} \frac{d}{2} \Gamma\left(\frac{d}{2}, \frac{tB}{V^{2/d}}\right) \left(\frac{1}{t}\right)^{d/2} \leq \frac{1}{V} \text{Tr}' e^{\Delta t} \leq \frac{D_M^d}{V C^{d/2}} \Gamma\left(\frac{d}{2} + 1\right) \left(\frac{1}{t}\right)^{d/2}. \quad (5.18)$$

Here  $\Gamma(x, y)$  is the upper incomplete gamma function defined as

$$\Gamma(x, y) = \int_y^{\infty} s^{x-1} e^{-s} ds. \quad (5.19)$$

For  $y = 0$ , it becomes the ordinary gamma function

$$\begin{aligned}\Gamma(x, 0) &= \int_0^{\infty} s^{x-1} e^{-s} ds \\ &\equiv \Gamma(x).\end{aligned}\tag{5.20}$$

Here, (5.18) is an important result describing the behaviour of the trace of the heat kernel. We will mainly use the estimates given by (5.18) to investigate the BE condensate in this chapter.

Another upper bound for the trace of the heat kernel which holds for large  $t$  is [53],

$$\mathrm{Tr}' e^{\Delta t} \leq (\mathrm{Tr}' e^{\Delta t_0}) e^{-\epsilon_1(t-t_0)}, \quad \text{for } t \geq t_0.\tag{5.21}$$

Here  $t_0 > 0$  is some fixed time.

Before concluding this section, we will show how the upper bound for the eigenvalues (5.12) follow from the upper estimate for the trace of the heat kernel given in (5.10), and how one gets the long time behaviour (5.21) from the self-reproducing property of the heat kernel.

We observe that

$$(\sigma + 1)e^{-\epsilon_\sigma t} \leq \mathrm{Tr} e^{\Delta t} \leq \tilde{C}(d)g(t),\tag{5.22}$$

since

$$e^{-\epsilon_k t} \geq e^{-\epsilon_\sigma t}, \quad \text{for all } k \leq \sigma.\tag{5.23}$$

And using the upper bound

$$\mathrm{Tr} e^{\Delta t} \leq \tilde{C}(d)g(t) \quad (5.24)$$

we get

$$(\sigma + 1) \leq e^{\epsilon_\sigma t} \tilde{C}(d)g(t) \quad (5.25)$$

for all positive  $t$ . Minimizing the right hand side we get

$$\epsilon_\sigma g(t_0) + g'(t_0) = 0. \quad (5.26)$$

Since  $g'(t) = 0$  for  $\sqrt{t} > D_M$ , we see that  $\sqrt{t_0} < D_M$ . Then we get

$$t_0 = \frac{d}{2\epsilon_\sigma}. \quad (5.27)$$

Plugging this into (5.25) we get the desired bound

$$\epsilon_\sigma \geq \frac{C(d)}{D_M^2} (\sigma + 1)^{2/d} \geq \frac{C(d)}{D_M^2} \sigma^{2/d}. \quad (5.28)$$

For the upper bound in (5.21), let  $K_t(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x} | e^{\Delta t} | \mathbf{y} \rangle$  be the heat kernel for the Neumann problem on  $M$ . Clearly  $K_t(\mathbf{x}, \mathbf{y})$  is a self-reproducing kernel. It is convenient to define

$$\bar{K}_t(\mathbf{x}, \mathbf{y}) = K_t(\mathbf{x}, \mathbf{y}) - \frac{1}{V}. \quad (5.29)$$

Since  $V^{-1/2}$  is the eigenfunction of the Laplacian with zero eigenvalue we have

$$\frac{1}{\sqrt{V}} = \int_M d\mu_g(\mathbf{y}) K_t(\mathbf{x}, \mathbf{y}) \frac{1}{\sqrt{V}}. \quad (5.30)$$

Using this it is easy to see that  $\bar{K}_t$  is also self-reproducing

$$\bar{K}_{t_1+t_2}(\mathbf{x}, \mathbf{y}) = \int_M d\mu_g(\mathbf{z}) \bar{K}_{t_1}(\mathbf{x}, \mathbf{z}) \bar{K}_{t_2}(\mathbf{z}, \mathbf{y}). \quad (5.31)$$

Now note that [53],

$$\begin{aligned} \frac{\partial}{\partial t} \bar{K}_t(\mathbf{x}, \mathbf{x}) &= \frac{\partial}{\partial t} \int_M d\mu_g(\mathbf{z}) \bar{K}_{t/2}^2(\mathbf{x}, \mathbf{z}) \\ &= - \int_M d\mu_g(\mathbf{z}) \bar{K}_{t/2}(\mathbf{x}, \mathbf{z}) \hat{h} \bar{K}_{t/2}(\mathbf{x}, \mathbf{z}) \\ &\leq -\epsilon_1 \int_M d\mu_g(\mathbf{z}) \bar{K}_{t/2}^2(\mathbf{x}, \mathbf{z}) = -\epsilon_1 \bar{K}_t(\mathbf{x}, \mathbf{x}). \end{aligned} \quad (5.32)$$

Here,  $\hat{h} \equiv -\Delta$ . In the last line the variational inequality is used (see *e.g.* [51]). Integrating this inequality one finds that for  $t \geq t_0$

$$\bar{K}_t(\mathbf{x}, \mathbf{x}) \leq \bar{K}_{t_0}(\mathbf{x}, \mathbf{x}) e^{-\epsilon_1(t-t_0)}. \quad (5.33)$$

Fixing the value of  $t_0$  we see that the diagonal elements of  $\bar{K}_t$  decay exponentially in time. Integrating over  $\mathbf{x}$  we get

$$\text{Tr}' e^{\Delta t} \leq (\text{Tr}' e^{\Delta t_0}) e^{-\epsilon_1(t-t_0)}. \quad (5.34)$$

## 5.2. Ideal Bose Gas in a Riemannian Manifold

The single particle free Hamiltonian is taken as

$$\hat{h} = -\Delta. \quad (5.35)$$

The corresponding many-body Hamiltonian is

$$\hat{H}' = \int d\mu_g(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \hat{h} \hat{\psi}(\mathbf{x}), \quad (5.36)$$

where  $\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}(\mathbf{x})$  are quantum field operators.

The thermal averages in the grand-canonical ensemble are given by

$$\langle \hat{O} \rangle = \frac{\text{Tr} \hat{O} e^{-\beta \hat{H}}}{\text{Tr} e^{-\beta \hat{H}}}. \quad (5.37)$$

This is equivalent to writing  $\langle \hat{O} \rangle = \text{Tr} \hat{O} \hat{\rho}$ , which is one of the basic results of equilibrium statistical mechanics. Here  $\hat{O}$  is an observable and  $\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}$  is the density matrix, where  $Z = \text{Tr} e^{-\beta \hat{H}}$  is the partition function. Hamiltonian is  $\hat{H} = \hat{H}' - \mu \hat{N}$ . Here

$$\hat{H} = \int d\mu_g(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) (\hat{h} - \mu) \hat{\psi}(\mathbf{x}) \quad (5.38)$$

is the number preserving Hamiltonian,  $\mu$  is the chemical potential. Expanding  $\hat{H}$  in terms of creation-annihilation operators and normal ordering the result we get

$$\hat{H} = \sum_{\sigma} (\epsilon_{\sigma} - \mu) \hat{a}_{\sigma}^{\dagger} \hat{a}_{\sigma}. \quad (5.39)$$

Here the sum is over all single-particle states. Using this as a constraint for total energy of the free system  $E \equiv \langle \hat{H} \rangle$ , with the total number of particles

$$N \equiv \langle \hat{a}_{\sigma}^{\dagger} \hat{a}_{\sigma} \rangle, \quad (5.40)$$

we get the mean occupation numbers exactly as in the flat case

$$\langle \hat{N}_{\sigma} \rangle = \langle \hat{a}_{\sigma}^{\dagger} \hat{a}_{\sigma} \rangle = \frac{1}{e^{\beta(\epsilon_{\sigma} - \mu)} - 1}, \quad (5.41)$$

where we have taken, as usual,  $\mu < 0$ . Clearly,  $N_0$  is singular at  $\mu = 0$ . As in the flat case, fixing the total number of particles allows us to determine  $\mu$ . To maximize the occupation of each level, we should let  $\mu \rightarrow 0^-$ . However, that is a delicate limit, the chemical potential is not strictly zero, the macroscopic occupation of the ground state

leads to  $\mu = O(V^{-1})$  so that we find a well-defined thermodynamic limit.

Note that

$$N = \sum_{\sigma} \frac{1}{e^{\beta(\epsilon_{\sigma}-\mu)} - 1}, \quad (5.42)$$

does not scale in a simple way to determine the chemical potential even in the continuum limit (energy eigenvalues get infinitesimally close), since the density of states in curved manifolds may not be a simple expression in general. Now we will discuss finite volume case and the thermodynamic limit separately.

*Finite Volume:* First note that

$$n_{\sigma} = \frac{N_{\sigma}}{V} = \frac{1}{V} \frac{e^{-\beta(\epsilon_{\sigma}-\mu)}}{1 - e^{-\beta(\epsilon_{\sigma}-\mu)}} = \frac{1}{V} \sum_{k=1}^{\infty} e^{k\beta\mu} e^{-k\beta\epsilon_{\sigma}} \quad (5.43)$$

and consequently,

$$\begin{aligned} n_e &= \sum_{\sigma \neq 0} n_{\sigma} = \frac{1}{V} \sum_{\sigma \neq 0} \sum_{k=1}^{\infty} e^{k\beta\mu} e^{-k\beta\epsilon_{\sigma}} \\ &= \frac{1}{V} \sum_{k=1}^{\infty} e^{k\beta\mu} \text{Tr}' e^{-k\beta \hat{h}}. \end{aligned} \quad (5.44)$$

Here  $\text{Tr}'$  denotes the trace with the ground state omitted, and  $n_e = n_e(T)$  is the number density of bosons in the excited single-particle states.

We employ (5.21) to study the low temperature behavior of  $n_e$ . Fixing  $k\beta_0$  such that  $k\beta > k\beta_0$ , we see

$$n_e(T) \leq \frac{1}{V} e^{\epsilon_1\beta_0} (\text{Tr}' e^{-\hat{h}\beta_0}) \sum_{k=1}^{\infty} e^{-k\epsilon_1\beta} = \frac{1}{V} (\text{Tr}' e^{-\hat{h}\beta_0}) \frac{e^{\epsilon_1\beta_0}}{e^{\epsilon_1\beta} - 1}, \quad (5.45)$$

where we used

$$\left(\mathrm{Tr}' e^{-\hat{h}\beta_0}\right) e^{\epsilon_1\beta_0} \geq \left(\mathrm{Tr}' e^{-k\hat{h}\beta_0}\right) e^{k\epsilon_1\beta_0}, \quad \text{for all } k \geq 1. \quad (5.46)$$

So by choosing  $T$  low enough, we can make  $n_e$  less than any preassigned value of  $n$ . Then the particles in excess, whose density is  $n - n_e$ , form condensate in the ground state.

The above analysis is independent of the dimension of the manifold  $M$  and the bound on the Ricci curvature. However, the right hand side of (5.45) is in general divergent as  $V \rightarrow \infty$ . So the bound is useless in the thermodynamic limit.

*Thermodynamic Limit in Terms of the Heat Kernel:* Using the upper bound given in (5.10) we see that

$$n_e \leq \frac{\tilde{C}(d)}{V} \sum_{k=1}^{\infty} e^{-k\beta|\mu|} g(k\beta) \quad (5.47)$$

$$\leq \frac{\tilde{C}(d) D_M^d}{V \beta^{d/2}} \sum_{k=1}^{[D_M^2/\beta]} \frac{e^{-k\beta|\mu|}}{k^{d/2}} + \frac{\tilde{C}(d)}{V} \sum_{k=[D_M^2/\beta]+1}^{\infty} e^{-k\beta|\mu|} \quad (5.48)$$

Here square brackets mean integer part. Now the second term is just a geometric series whose sum is

$$\frac{\tilde{C}(d)}{V} \frac{e^{-([D_M^2/\beta]+1)\beta|\mu|}}{1 - e^{-\beta|\mu|}}. \quad (5.49)$$

Using  $\mu = O(V^{-1})$  we see that derivative of this with respect to volume  $V$  is negative for all values of  $V$ . Therefore, this term goes to zero in the thermodynamic limit  $V, D_M \rightarrow \infty$ .

Our basic assumption regarding the thermodynamic limit will be the following

asymptotic relation between the volume and the diameter of our box  $M$

$$D_M = O(V^{1/d}) \quad \text{as } V \rightarrow \infty. \quad (5.50)$$

Under this assumption, in the thermodynamic limit we get

$$n_e \leq \tilde{C}(d) \frac{A}{\beta^{d/2}} \sum_{k=1}^{\infty} \frac{e^{-k\beta|\mu|}}{k^{d/2}} \leq \tilde{C}(d) \frac{A}{\beta^{d/2}} \sum_{k=1}^{\infty} \frac{1}{k^{d/2}} = \tilde{C}(d) \frac{A}{\beta^{d/2}} \zeta\left(\frac{d}{2}\right). \quad (5.51)$$

Here

$$A = \lim_{V \rightarrow \infty} \frac{D_M^d}{V} > 0. \quad (5.52)$$

For  $d \geq 3$ ,  $n_e$  is clearly finite and vanishes as  $T \rightarrow 0$ . For  $d = 2$ , the above bound is of no use in the thermodynamic limit since it diverges with the Riemann zeta function,  $\zeta(1)$ . In order to deduce the behavior of  $n_e$  at  $d = 2$ , we use the lower bound given in (5.10).

$$n(T) = \frac{1}{V} \sum_{k=1}^{\infty} e^{-k\beta|\mu|} \left( \text{Tr} e^{-k\beta\hat{h}} \right) \quad (5.53)$$

$$\geq \frac{1}{(4\pi\beta)^{d/2}} \sum_{k=1}^{\infty} \frac{e^{-k\beta|\mu|}}{k^{d/2}}. \quad (5.54)$$

By a simple integral test the series is seen to be larger than

$$\int_1^{\infty} dx \frac{e^{-x\beta|\mu|}}{x^{d/2}} = (\beta|\mu|)^{d/2-1} \int_{\beta|\mu|}^{\infty} dy \frac{e^{-y}}{y^{d/2}} = (\beta|\mu|)^{d/2-1} \Gamma\left(1 - \frac{d}{2}, \beta|\mu|\right), \quad (5.55)$$

since  $k$  depending terms in the sum decreases with increasing  $k$ . If it was the case that  $\mu = O(V^{-1})$  then for  $d = 2$  we would have a divergent  $n$

$$\Gamma(0, w) = -\gamma - \ln(w) - \sum_{k=1}^{\infty} (-1)^k \frac{w^k}{k(k!)} \rightarrow \infty \quad \text{as } w \rightarrow 0, \quad (5.56)$$

where  $\gamma$  is the Euler-Mascheroni constant. Diverging  $n$  contradicts with the constant number of particles given in the system. Thus  $\mu \neq O(V^{-1})$  and condensation does not take place in two dimensions.

*Thermodynamic Limit in Terms of Eigenvalues:* Now using the bounds (5.12) and (5.13) on the eigenvalues of the Laplacian we get

$$\sum_{\sigma=1}^{\infty} \frac{1}{V} \frac{1}{e^{\beta\left(\frac{B}{V^{2/d}} \sigma^{2/d} - \mu\right)} - 1} \leq n_e \leq \sum_{\sigma=1}^{\infty} \frac{1}{V} \frac{1}{e^{\beta\left(\frac{C}{D_M^2} \sigma^{2/d} - \mu\right)} - 1}. \quad (5.57)$$

But  $\mu = O(V^{-1})$  and the depletion coefficient can be bound in the  $V, D_M \rightarrow \infty$  limit as

$$\int_0^{\infty} dx \frac{1}{e^{\beta B x^{2/d}} - 1} \leq n_e \leq A \int_0^{\infty} dx \frac{1}{e^{\beta C x^{2/d}} - 1}, \quad (5.58)$$

as a result of bounding the sums with integrals

$$\sum_{y=1}^{\infty} \frac{1}{V} \frac{1}{e^{\beta B (y/V)^{2/d}} - 1} \geq \int_1^{\infty} \frac{dy}{V} \frac{1}{e^{\beta B (y/V)^{2/d}} - 1} \rightarrow \int_0^{\infty} dx \frac{1}{e^{\beta B x^{2/d}} - 1}, \quad (5.59)$$

and,

$$\sum_{y=1}^{\infty} \frac{1}{V} \frac{1}{e^{\beta C (y/D_M^d)^{2/d}} - 1} \leq A \int_0^{\infty} \frac{dy}{V} \frac{1}{e^{\beta C (y/D_M^d)^{2/d}} - 1} = A \int_0^{\infty} dx \frac{1}{e^{\beta C x^{2/d}} - 1}. \quad (5.60)$$

After a change of variable we have

$$\frac{d}{2(\beta B)^{d/2}} \int_0^{\infty} d\eta \frac{\eta^{\frac{d}{2}-1}}{e^{\eta} - 1} \leq n_e \leq \frac{Ad}{2(\beta C)^{d/2}} \int_0^{\infty} d\eta \frac{\eta^{\frac{d}{2}-1}}{e^{\eta} - 1}. \quad (5.61)$$

Note that the numerator of the integrand is in accordance with the Weyl asymptotic

formula for the eigenvalue density of the Laplacian (see *e.g.* [51]). Since

$$\int_0^{\infty} d\eta \frac{\eta^{\frac{d}{2}-1}}{e^\eta - 1} = \Gamma\left(\frac{d}{2}\right) \zeta\left(\frac{d}{2}\right), \quad (5.62)$$

we get

$$\frac{d}{2(\beta B)^{d/2}} \Gamma\left(\frac{d}{2}\right) \zeta\left(\frac{d}{2}\right) \leq n_e \leq \frac{Ad}{2(\beta C)^{d/2}} \Gamma\left(\frac{d}{2}\right) \zeta\left(\frac{d}{2}\right). \quad (5.63)$$

On the other hand in flat space

$$n_e^{flat} = S(d) \frac{1}{\beta^{d/2}} \Gamma\left(\frac{d}{2}\right) \zeta\left(\frac{d}{2}\right), \quad (5.64)$$

which is given by (2.70). So

$$\left(\frac{d}{2S(d)B^{d/2}}\right) n_e^{flat} \leq n_e \leq \left(\frac{Ad}{2S(d)C^{d/2}}\right) n_e^{flat}. \quad (5.65)$$

Thus we see that  $n_e$  is divergent for  $d \leq 2$  and convergent for  $d > 2$ . Moreover, for  $d > 2$ ,  $n_e \rightarrow 0$  as  $T \rightarrow 0$  and we have Bose-Einstein condensation at low temperatures.

In fact, using (2.71) the critical temperature can be bound as

$$\left[\frac{Ad}{2nC^{d/2}} \Gamma\left(\frac{d}{2}\right) \zeta\left(\frac{d}{2}\right)\right]^{-2/d} \leq kT_c \leq \left[\frac{d}{2nB^{d/2}} \Gamma\left(\frac{d}{2}\right) \zeta\left(\frac{d}{2}\right)\right]^{-2/d}. \quad (5.66)$$

### 5.3. Bogoliubov Theory on a Compact Riemannian Manifold

The many-body Hamiltonian with a hard-core repulsive potential in a Riemann manifold which has the same form as (3.13) is given by [15–18],

$$\hat{H}' = \int d\mu_g(\mathbf{x}) \left[ \hat{\psi}^\dagger(\mathbf{x}) \hat{h} \hat{\psi}(\mathbf{x}) + \frac{g}{2} \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \hat{\psi}(\mathbf{x}) \right]. \quad (5.67)$$

It is convenient to include the chemical potential in the Hamiltonian and define the number preserving Hamiltonian

$$\hat{H} = \hat{H}' - \mu \hat{N}. \quad (5.68)$$

We will study this Hamiltonian and the Bose-Einstein condensation by applying the curved space version of the standard Bogoliubov theory [15] to it. In flat space the Bogoliubov approximation consists of three steps. First, one replaces the zero energy (ground state) creation and annihilation operators by their coherent state lower symbols and then one expands the Hamiltonian around the c-number background obtained in the first step, ignoring third and higher order terms in the fluctuation. The resulting Hamiltonian is quadratic in the creation and annihilation operators but not diagonal. The final step is the diagonalization of this Hamiltonian by the Bogoliubov transformation. The justification of the c-number replacement was first given in [19] and more recently (and with less assumptions) in Lieb *et al.* [20] (see also [21, 22]). We see that in the case of a manifold, thanks to the Neumann boundary condition which implies the constancy of the ground state wave-function, the c-number substitution is justified in a way similar to the flat case proposed by Lieb *et al.* [20]. The justification of the c-number substitution on a curved manifold is given in the appendix. On the other hand, in the semiclassical approximation of the Hamiltonian, the Neumann boundary condition and the constancy of the wave-function again play an important role. Finally the Bogoliubov transformation which is a purely algebraic manipulation proceeds in the usual way.

Our starting point will be the expansion of the field operator  $\hat{\psi}(\mathbf{x})$  around the background and putting  $\hat{H}$  in a form of combinations of the particle creation and annihilation operators.

$$\phi_0 := \hat{\phi}_0(\mathbf{x}) = \sqrt{N_0} f_0 = \sqrt{\frac{N_0}{V}} = \sqrt{n_0} \quad (5.69)$$

as

$$\hat{\psi}(\mathbf{x}) = \hat{\phi}_0(\mathbf{x}) + \hat{\eta}(\mathbf{x}) \quad (5.70)$$

with

$$\hat{\eta}(\mathbf{x}) = \sum_{\sigma \neq 0} \hat{a}_\sigma f_\sigma. \quad (5.71)$$

Assuming the quantum fluctuations to be small we can approximate (first order approximation)  $\hat{H}'$  as

$$\begin{aligned} H'_{eff} = \int d\mu_g(\mathbf{x}) \left\{ \phi_0 \hat{h} \hat{\eta}(\mathbf{x}) + \hat{\eta}^\dagger(\mathbf{x}) \hat{h} \hat{\eta}(\mathbf{x}) + \frac{g}{2} [\phi_0^4 + 2\phi_0^3(\hat{\eta}^\dagger(\mathbf{x}) + \hat{\eta}(\mathbf{x})) \right. \\ \left. + \phi_0^2(\hat{\eta}(\mathbf{x})\hat{\eta}(\mathbf{x}) + 4\hat{\eta}^\dagger(\mathbf{x})\hat{\eta}(\mathbf{x}) + \hat{\eta}^\dagger(\mathbf{x})\hat{\eta}^\dagger(\mathbf{x}))] \right\}. \end{aligned} \quad (5.72)$$

Expanding in terms of creation and annihilation operators and using (5.8) and (5.9) we get

$$\hat{H}'_{eff} = \frac{gn_0^2V}{2} + \sum_{\sigma \neq 0} \left[ (\epsilon_\sigma + 2gn_0) \hat{a}_\sigma^\dagger \hat{a}_\sigma + \frac{gn_0}{2} (\hat{a}_\sigma^\dagger \hat{a}_\sigma^\dagger + \hat{a}_\sigma \hat{a}_\sigma) \right]. \quad (5.73)$$

as in the flat case.

Similarly, the number operator is given by

$$\begin{aligned} \hat{N} &= \int d\mu_g(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \\ &= \int d\mu_g(\mathbf{x}) [\phi_0^2 + \phi_0 (\hat{\eta}^\dagger(\mathbf{x}) + \hat{\eta}(\mathbf{x})) + \hat{\eta}^\dagger(\mathbf{x})\hat{\eta}(\mathbf{x})] \\ &= n_0V + \sum_{\sigma \neq 0} \hat{a}_\sigma^\dagger \hat{a}_\sigma. \end{aligned} \quad (5.74)$$

So,

$$\hat{H}'_{eff} - \mu\hat{N} = \frac{gn_0^2V}{2} - \mu n_0V + \sum_{\sigma \neq 0} \left[ (\epsilon_\sigma + 2gn_0 - \mu) \hat{a}_\sigma^\dagger \hat{a}_\sigma + \frac{gn_0}{2} (\hat{a}_\sigma^\dagger \hat{a}_\sigma^\dagger + \hat{a}_\sigma \hat{a}_\sigma) \right]. \quad (5.75)$$

For a fixed  $n_0$ , the thermodynamic pressure

$$\frac{P}{kT} = \frac{1}{V} \ln \mathcal{G} = \frac{1}{V} \ln \left( \text{Tr}' e^{-\beta(\hat{H}'_{eff} - \mu\hat{N})} \right) \quad (5.76)$$

is maximized at the zeroth order in  $\hat{\eta}(\mathbf{x})$  by  $\mu = gn_0$  as in (3.41). Here  $\text{Tr}'$  means that the trace is taken over the states with no quanta in the  $f_0$  mode. With this value of  $\mu$  we get

$$\hat{H}'_{eff} - \mu\hat{N} = -\frac{gn_0^2V}{2} + \sum_{\sigma \neq 0} \left[ (\epsilon_\sigma + gn_0) \hat{a}_\sigma^\dagger \hat{a}_\sigma + \frac{gn_0}{2} (\hat{a}_\sigma^\dagger \hat{a}_\sigma^\dagger + \hat{a}_\sigma \hat{a}_\sigma) \right]. \quad (5.77)$$

Therefore the thermal averages can be calculated using the effective Hamiltonian

$$\hat{H}_{eff} = \sum_{\sigma \neq 0} \left[ (\epsilon_\sigma + gn_0) \hat{a}_\sigma^\dagger \hat{a}_\sigma + \frac{gn_0}{2} (\hat{a}_\sigma^\dagger \hat{a}_\sigma^\dagger + \hat{a}_\sigma \hat{a}_\sigma) \right]. \quad (5.78)$$

which can be diagonalized by the Bogoliubov transformation

$$\hat{a}_\sigma = (\cosh\theta_\sigma) \hat{b}_\sigma + (\sinh\theta_\sigma) \hat{b}_\sigma^\dagger. \quad (5.79)$$

where

$$\lambda_\sigma = \epsilon_\sigma + gn_0 = \omega_\sigma \cosh 2\theta_\sigma, \quad (5.80)$$

$$gn_0 = -\omega_\sigma \sinh 2\theta_\sigma, \quad (5.81)$$

$$\omega_\sigma = \sqrt{(\epsilon_\sigma + gn_0)^2 - (gn_0)^2}. \quad (5.82)$$

The last equation is the curved space analog of the Bogoliubov dispersion relation.

The resulting diagonal Hamiltonian is

$$\begin{aligned}\hat{H}_{eff} &= E_0 + \sum_{\sigma \neq 0} [\lambda_\sigma \cosh 2\theta_\sigma + gn_0 \sinh 2\theta_\sigma] \hat{b}_\sigma^\dagger \hat{b}_\sigma \\ &= E_0 + \sum_{\sigma \neq 0} \omega_\sigma \hat{b}_\sigma^\dagger \hat{b}_\sigma,\end{aligned}\tag{5.83}$$

where  $E_0$  is the ground state energy

$$\begin{aligned}E_0 &= -\frac{1}{2} \sum_{\sigma=1}^{\infty} (\lambda_\sigma - \omega_\sigma) \\ &= -\frac{1}{2} \sum_{\sigma=1}^{\infty} \frac{(gn_0)^2}{\lambda_\sigma + \omega_\sigma} \\ &= -\frac{1}{2} \sum_{\sigma=1}^{\infty} \frac{(gn_0)^2}{2\epsilon_\sigma \left[1 + O\left(\frac{1}{\epsilon_\sigma}\right)\right]} \\ &= -\frac{1}{2} \sum_{\sigma=1}^{\infty} \frac{(gn_0)^2}{2} \frac{1}{\epsilon_\sigma} + O\left(\frac{1}{\epsilon_\sigma^2}\right).\end{aligned}\tag{5.84}$$

Here, we used binomial theorem to get this expansion.

Now using the lower eigenvalue bound given in (5.12), we see that for  $k \geq 2$  and  $d = 3, 2$ ,

$$\sum_{\sigma=1}^{\infty} \frac{1}{\epsilon_\sigma^k}\tag{5.85}$$

is convergent. On the other hand, using (5.13) we see that the  $k = 1$  sum is divergent for  $d = 3, 2$ . This result is non-physical, and must be corrected by a perturbation term in the next order. In the flat case, reforming the coupling constant led us to the renormalized ground state energy

$$E_0 = -\frac{1}{2} \sum_{\sigma=1}^{\infty} \left[ (\epsilon_\sigma + gn_0) - \omega_\sigma - \frac{(gn_0)^2}{2\epsilon_\sigma} \right].\tag{5.86}$$

We will seek now a perturbation term in the next order to make the ground state energy  $E_0$  convergent, without tuning the coupling constant  $g$ .

To understand the ground state energy better we will now express it in terms of the heat kernel. Consider the first two terms before the renormalization. Let's write  $s$  for  $\epsilon_\sigma$  and  $a$  for  $gn_0$ , for simplicity. When we get  $e^{-st}$  the sum over whole set of single-particle states  $\sigma$  gives us  $\text{Tr } e^{\Delta t}$ . Consider the expression

$$s + a - \sqrt{s^2 + 2sa}. \quad (5.88)$$

This function is equal to the shifted version  $s \rightarrow s + a$  of

$$s - \sqrt{s^2 - a^2} \quad (5.89)$$

which is equal to

$$s - \sqrt{s^2 - a^2} = \frac{a^2}{s + \sqrt{s^2 - a^2}}. \quad (5.90)$$

Now we note the following integral representation (see p. 326 line 8 of [54]):

$$\int_0^\infty \frac{xdx}{[x^2 + 2sx + s^2 - a^2]^{3/2}} = \frac{1}{s + \sqrt{s^2 - a^2}}. \quad (5.91)$$

This function is equal to a Laplace transform

$$\begin{aligned} \frac{1}{[x^2 + 2sx + s^2 - a^2]^{3/2}} &= \frac{1}{[(x+s)^2 - a^2]^{3/2}} \\ &= \int_0^\infty dt e^{-(s+x)t} \frac{\sqrt{\pi}}{\Gamma(3/2)} \left(\frac{t}{2a}\right) I_1(at). \end{aligned} \quad (5.92)$$

Here  $I_\nu(t)$  is the modified Bessel function of the first kind of order  $\nu$ , which has an integral representation [55],

$$I_\nu(t) := \sum_{k=0}^{\infty} \frac{1}{k! \Gamma(k + \nu + 1)} \left(\frac{t}{2}\right)^{\nu+2k} = \frac{1}{\pi} \int_0^\pi e^{t \cos \xi} \cos(\nu \xi) d\xi. \quad (5.93)$$

Notice that

$$\frac{dI_0(t)}{dt} = I_1(t). \quad (5.94)$$

Asymptotic expansions of  $I_\nu(x)$  can be written as

$$\begin{cases} I_\nu(t) \sim \frac{t^\nu}{2^\nu \Gamma(\nu+1)} \left( 1 + \frac{t^2}{2(2\nu+2)} + \dots \right), & t \ll 1 \\ I_\nu(t) \sim \frac{e^t}{\sqrt{2\pi t}} \left[ 1 - \frac{1}{2t} \left( \nu^2 - \frac{1}{4} \right) + \dots \right], & t \gg 1. \end{cases} \quad (5.95)$$

Now we simplify the numerical parts of (5.92) and again shift  $s$  to  $s+a$  to finally write

$$\int_0^\infty dt \int_0^\infty x dx e^{-(s+a+x)t} \left( \frac{t}{a} \right) I_1(at) = \int_0^\infty \frac{dt}{at} I_1(at) e^{-at} e^{-st}. \quad (5.96)$$

In the original sums we recognize now  $\sum_\sigma e^{-\epsilon_\sigma t}$  as integral of the heat kernel, which comes from the Laplace transform variable,

$$\sum_{\sigma=1}^\infty \int_0^\infty dt \int_0^\infty x dx e^{-(s+a+x)t} \left( \frac{t}{a} \right) I_1(at) = \int_0^\infty \frac{dt}{at} I_1(at) e^{-at} \text{Tr}' e^{\Delta t}, \quad (5.97)$$

which is equal to (5.84) up to factor  $-a^2/2$ . Let us see the convergence properties. Using (5.18) we see  $\text{Tr}' e^{\Delta t} = O(t^{-3/2})$ , and  $I_1(t) \sim e^t/\sqrt{t}$  from (5.95), we say there is no divergence as  $t \rightarrow \infty$ . However, as  $t \rightarrow 0^+$  which corresponds to the ultraviolet properties, we have  $I_1(t) \sim t/2$ , and we get

$$\frac{1}{at} I_1(at) e^{-at} \text{Tr}' e^{\Delta t} \sim \frac{1}{at} \frac{at}{2} \frac{1}{t^{3/2}} \quad \text{as } t \rightarrow 0^+. \quad (5.98)$$

which diverges. Noticing the binomial expansion of  $e^{-at}$ , we suggest an extra term

$$\frac{1}{2} \text{Tr}' e^{\Delta t} \quad (5.99)$$

to subtract from (5.98). Then we have

$$\left(\frac{1}{at}I_1(at)e^{-at} - \frac{1}{2}\right)\text{Tr}'e^{\Delta t} \sim \frac{at}{2} \frac{1}{t^{3/2}} \quad \text{as } t \rightarrow 0^+. \quad (5.100)$$

which becomes convergent when integrated over  $t$ . The subtracted term, with the overall  $a^2$  term being inserted back again, is indeed

$$\begin{aligned} \int_0^\infty -\frac{a^2}{2} \text{Tr}'e^{\Delta t} dt &= -\frac{a^2}{2} \sum_{\sigma \neq 0} \int_0^\infty dt e^{-\epsilon_\sigma t} \\ &= -\sum_{\sigma \neq 0} \frac{a^2}{2\epsilon_\sigma}. \end{aligned} \quad (5.101)$$

Thus, we arrive at the renormalized ground state energy as in (5.87). Note that the subtraction does not lead to an ultraviolet divergence thanks to  $t^{-3/2}$  behavior of the heat kernel.

The ground state is given as

$$|\Omega\rangle = \mathcal{N} \prod_{\sigma=1}^{\infty} e^{-\frac{1}{2} \tanh \xi_\sigma a_\sigma^{\dagger 2}} |0\rangle \quad (5.102)$$

with the normalization constant

$$\mathcal{N} = \prod_{\sigma=1}^{\infty} \frac{1}{\sqrt{\cosh \xi_\sigma}} = \left[ \prod_{\sigma=1}^{\infty} 1 - \frac{\lambda_\sigma - \omega_\sigma}{\lambda_\sigma + \omega_\sigma} \right]^{1/4}. \quad (5.103)$$

Since  $0 \leq (\lambda_\sigma - \omega_\sigma)(\lambda_\sigma + \omega_\sigma)^{-1} < 1$  the convergence of the product is equivalent to the convergence of the series

$$\sum_{\sigma=1}^{\infty} \frac{\lambda_\sigma - \omega_\sigma}{\lambda_\sigma + \omega_\sigma}. \quad (5.104)$$

But,

$$\sum_{\sigma=1}^{\infty} \frac{\lambda_{\sigma} - \omega_{\sigma}}{\lambda_{\sigma} + \omega_{\sigma}} \leq \sum_{\sigma=1}^{\infty} \frac{\lambda_{\sigma} - \omega_{\sigma}}{\epsilon_{\sigma}} = \sum_{\sigma=1}^{\infty} \frac{\lambda_{\sigma} - \omega_{\sigma} - \frac{(gn_0)^2}{2\epsilon_{\sigma}}}{\epsilon_{\sigma}} + \sum_{\sigma=1}^{\infty} \frac{(gn_0)^2}{2\epsilon_{\sigma}^2}. \quad (5.105)$$

By the eigenvalue estimates given above, the last series is convergent. On the other hand for  $\sigma$  large enough

$$\frac{\lambda_{\sigma} - \omega_{\sigma} - \frac{(gn_0)^2}{2\epsilon_{\sigma}}}{\epsilon_{\sigma}} \leq \lambda_{\sigma} - \omega_{\sigma} - \frac{(gn_0)^2}{2\epsilon_{\sigma}}. \quad (5.106)$$

Combining this with our discussion of the ground state energy we see that the first series is convergent as well. Thus we conclude  $\mathcal{N} < \infty$ , *i.e.*, we have a well-defined ground state.

#### 5.4. Heat Kernel Analysis of the Depletion of the Condensate

The occupation number of excited states

$$n_e = \frac{1}{V} \sum_{\sigma \neq 0} \langle \hat{a}_{\sigma}^{\dagger} \hat{a}_{\sigma} \rangle \quad (5.107)$$

is expressed in terms of quasiparticle states as

$$\begin{aligned} n_e &= \frac{1}{V} \sum_{\sigma \neq 0} \left[ \sinh^2 \theta_{\sigma} + \cosh 2\theta_{\sigma} \langle \hat{b}_{\sigma}^{\dagger} \hat{b}_{\sigma} \rangle + \frac{1}{2} \sinh 2\theta_{\sigma} \langle \hat{b}_{\sigma}^{\dagger} \hat{b}_{\sigma}^{\dagger} + \hat{b}_{\sigma} \hat{b}_{\sigma} \rangle \right] \\ &= \frac{1}{V} \sum_{\sigma \neq 0} \left[ \cosh 2\theta_{\sigma} \left( \frac{1}{2} + \langle \hat{b}_{\sigma}^{\dagger} \hat{b}_{\sigma} \rangle \right) - \frac{1}{2} \right] \\ &= \frac{1}{V} \sum_{\sigma \neq 0} \left[ \frac{1}{2} \cosh 2\theta_{\sigma} \coth \frac{\beta\omega_{\sigma}}{2} - \frac{1}{2} \right] \\ &= \frac{1}{2V} \sum_{\sigma \neq 0} \left[ \frac{\lambda_{\sigma}}{\omega_{\sigma}} \coth \frac{\beta\omega_{\sigma}}{2} - 1 \right], \end{aligned} \quad (5.108)$$

where we used

$$\langle \hat{b}_\sigma^\dagger \hat{b}_\sigma \rangle = \frac{1}{e^{\beta\omega_\sigma} - 1}, \quad (5.109)$$

and

$$\langle \hat{b}_\sigma^\dagger \hat{b}_\sigma^\dagger + \hat{b}_\sigma \hat{b}_\sigma \rangle = 0. \quad (5.110)$$

The zero temperature limit is

$$n_e = \frac{1}{2V} \sum_{\sigma \neq 0} \left[ \frac{\lambda_\sigma}{\sqrt{\lambda_\sigma^2 - (gn_0)^2}} - 1 \right], \quad (5.111)$$

since

$$\coth \frac{\beta\omega_\sigma}{2} \rightarrow 1 \quad \text{as} \quad \beta \rightarrow \infty. \quad (5.112)$$

Now noting the Laplace transform

$$\frac{1}{\sqrt{\lambda_\sigma^2 - (gn_0)^2}} = \int_0^\infty dt e^{-\lambda_\sigma t} I_0(gn_0 t). \quad (5.113)$$

Using integration by parts and (5.95), we get

$$\begin{aligned} \frac{\lambda_\sigma}{\sqrt{\lambda_\sigma^2 - (gn_0)^2}} &= \int_0^\infty dt \left[ -\frac{d}{dt} e^{-\lambda_\sigma t} \right] I_0(gn_0 t) \\ &= 1 + gn_0 \int_0^\infty dt e^{-\lambda_\sigma t} I_1(gn_0 t). \end{aligned} \quad (5.114)$$

Thus

$$\begin{aligned}
n_e &= \frac{gn_0}{2V} \int_0^\infty dt \left[ \sum_{\sigma \neq 0} e^{-\epsilon_\sigma t} \right] e^{-gn_0 t} I_1(gn_0 t) \\
&= \frac{gn_0}{2} \int_0^\infty dt \frac{1}{V} (\text{Tr}' e^{-\hat{h}t}) e^{-gn_0 t} I_1(gn_0 t).
\end{aligned} \tag{5.115}$$

Now, we will inspect the finite volume case and the thermodynamic limit separately.

*Finite Volume:* At finite  $V$ , we can use either (5.21) or the simpler observation

$$\text{Tr}' e^{-\hat{h}t} = \sum_{\sigma \neq 0} e^{-t\epsilon_\sigma} \leq \sum_{\sigma \neq 0} e^{-t\epsilon_1} = \Sigma_e e^{-t\epsilon_1}, \tag{5.116}$$

where  $\Sigma_e$  denotes the total number of excited single-particle states, which is finite under finite volume. Using this upper bound together with the limit, we get

$$e^{-gn_0 t} I_1(gn_0 t) \sim \frac{1}{\sqrt{gn_0 t}} \quad \text{as } t \rightarrow \infty. \tag{5.117}$$

which converges. As for the lower limit of integration, we combine the short time asymptotic of the heat kernel

$$\text{Tr}' e^{-\hat{h}t} \sim -1 + \frac{V}{(4\pi t)^{d/2}} \quad \text{as } t \rightarrow 0 \tag{5.118}$$

with

$$e^{-gn_0 t} I_1(gn_0 t) \sim \frac{gn_0 t}{2} \quad \text{as } t \rightarrow 0, \tag{5.119}$$

to conclude that the integral is convergent for  $d = 3$  and  $d = 2$ .

*Thermodynamic Limit:* Using (5.18) in the limit  $V, D_M \rightarrow \infty$ ,  $D_M^d/V \rightarrow A$  we

get

$$n_e \leq \frac{gn_0}{2} \frac{A}{C^{d/2}} \Gamma\left(\frac{d}{2} + 1\right) \int_0^\infty dt \frac{1}{t^{d/2}} e^{-gn_0 t} I_1(gn_0 t). \quad (5.120)$$

The integral is convergent for  $d = 3$ .

On the other hand

$$n_e \geq \frac{gn_0}{2} \frac{1}{B^{d/2}} \frac{d}{2} \int_0^\infty dt \Gamma\left(\frac{d}{2}, \frac{tB}{V^{2/d}}\right) \frac{1}{t^{d/2}} e^{-gn_0 t} I_1(gn_0 t). \quad (5.121)$$

Again the integral is convergent for  $d = 3$ . Moreover, the integrand is a positive, increasing function of  $V$  and by the monotone convergence theorem the limit  $V \rightarrow \infty$  gives

$$n_e \geq \frac{gn_0}{2} \frac{1}{B^{d/2}} \Gamma\left(\frac{d}{2} + 1\right) \int_0^\infty dt \frac{1}{t^{d/2}} e^{-gn_0 t} I_1(gn_0 t). \quad (5.122)$$

Finally, upon the change of variable  $s = gn_0 t$  we see that the bounds scale as  $(gn_0)^{d/2}$

$$(gn_0)^{d/2} m \gamma_d \leq n_e \leq (gn_0)^{d/2} M \gamma_d, \quad (5.123)$$

where

$$m = \frac{1}{2} \frac{1}{B^{d/2}} \Gamma\left(\frac{d}{2} + 1\right), \quad M = \frac{1}{2} \frac{A}{C^{d/2}} \Gamma\left(\frac{d}{2} + 1\right), \quad (5.124)$$

and

$$\gamma_d = \int_0^\infty \frac{ds}{s^{d/2}} e^{-s} I_1(s). \quad (5.125)$$

Thus we get, as in the flat case (3.71),

$$\frac{n_e}{n_0} = O(g^{d/2} n_0^{(d/2)-1}). \quad (5.126)$$

The smallness of the parameter  $g^{d/2} n_0^{(d/2)-1}$  can now be used as a criterion for the validity of the Gross-Pitaevskii equation (see *e.g.* Pethick and Smith [45]).

### 5.5. Depletion of the Condensate at Finite Temperature

In order to analyze the depletion of the condensate at finite temperatures we expand  $N_e$  given by (5.108) in terms of exponentials

$$N_e(T) = \frac{1}{2} \sum_{\sigma \neq 0} \left[ \frac{\lambda_\sigma}{\omega_\sigma} - 1 + 2 \sum_{k=1}^{\infty} \frac{\lambda_\sigma}{\omega_\sigma} e^{-k\beta\omega_\sigma} \right]. \quad (5.127)$$

Here, we used

$$\begin{aligned} \coth \frac{\beta\omega_\sigma}{2} &= 1 + 2 \frac{e^{-\frac{\beta\omega_\sigma}{2}}}{e^{\frac{\beta\omega_\sigma}{2}} - e^{-\frac{\beta\omega_\sigma}{2}}} \\ &= 1 + 2 \sum_{k=1}^{\infty} e^{-k\beta\omega_\sigma}. \end{aligned} \quad (5.128)$$

Noticing the Laplace transform,

$$\frac{e^{-k\beta\omega_\sigma}}{\omega_\sigma} = \frac{e^{-k\beta\sqrt{\lambda_\sigma^2 - (gn_0)^2}}}{\sqrt{\lambda_\sigma^2 - (gn_0)^2}} = \int_{k\beta}^{\infty} dt e^{-\lambda_\sigma t} I_0(gn_0 \sqrt{t^2 - k^2\beta^2}), \quad (5.129)$$

using integration by parts we find

$$\begin{aligned}
\frac{\lambda_\sigma e^{-k\beta\omega_\sigma}}{\omega_\sigma} &= e^{-\lambda_\sigma k\beta} + gn_0 \int_{k\beta}^{\infty} dt e^{-\lambda_\sigma t} \frac{I_1(gn_0\sqrt{t^2 - k^2\beta^2})}{\sqrt{t^2 - k^2\beta^2}} \\
&= e^{-\lambda_\sigma k\beta} + gn_0 \int_0^{\infty} dt e^{-\lambda_\sigma\sqrt{t^2+k^2\beta^2}} I_1(gn_0t). \tag{5.130}
\end{aligned}$$

Thus, we arrive at

$$n_e(T) = n_e(0) + \tilde{n}_e(T), \tag{5.131}$$

where

$$\begin{aligned}
\tilde{n}_e(T) &= \frac{1}{V} \sum_{\sigma \neq 0} \sum_{k=1}^{\infty} \left[ e^{-\lambda_\sigma k\beta} + gn_0 \int_0^{\infty} dt e^{-\lambda_\sigma\sqrt{t^2+k^2\beta^2}} I_1(gn_0t) \right] \\
&= \sum_{k=1}^{\infty} \left[ \left( \frac{1}{V} \text{Tr}' e^{k\beta\Delta} \right) e^{-k\beta gn_0} + \right. \\
&\quad \left. gn_0 \int_0^{\infty} dt \left( \frac{1}{V} \text{Tr}' e^{\Delta\sqrt{t^2+k^2\beta^2}} \right) e^{-gn_0\sqrt{t^2+k^2\beta^2}} I_1(gn_0t) \right]. \tag{5.132}
\end{aligned}$$

We will now analyze this expression in the thermodynamic limit. Using the heat kernel upper bound given by (5.18) in the limit  $V \rightarrow \infty$  we get

$$\begin{aligned}
\tilde{n}_e(T) &\leq C_1 \sum_{k=1}^{\infty} \left[ \frac{1}{(k\beta)^{3/2}} e^{-k\beta gn_0} + \right. \\
&\quad \left. gn_0 \int_0^{\infty} dt \frac{1}{(t^2 + k^2\beta^2)^{3/4}} e^{-gn_0\sqrt{t^2+k^2\beta^2}} I_1(gn_0t) \right] \tag{5.133}
\end{aligned}$$

for  $d = 3$ . Here

$$C_1 = \frac{A}{C^{3/2}} \Gamma\left(\frac{5}{2}\right). \tag{5.134}$$

We will estimate each term separately. An upper bound for the first expression is

$$\begin{aligned} & C_1 \sum_{k=1}^{\infty} \frac{1}{(k\beta)^{3/2}} - C_1 \sum_{k=1}^{\infty} \frac{1}{(\beta k)^{3/2}} (1 - e^{-k\beta gn_0}) \\ & \leq C_1 \sum_{k=1}^{\infty} \frac{1}{(k\beta)^{3/2}} - C_1 \int_1^{\infty} \frac{dk}{(\beta k)^{3/2}} (1 - e^{-k\beta gn_0}) \end{aligned} \quad (5.135)$$

which is equal to

$$C_1 \sum_{k=1}^{\infty} \frac{1}{(k\beta)^{3/2}} + C_1' \frac{(gn_0)^{1/2}}{\beta}. \quad (5.136)$$

The second part is somewhat more subtle, we first apply the subordination identity for the exponent and find that the second becomes,

$$C_2 gn_0 \int_0^{\infty} dt \sum_{k=1}^{\infty} \frac{1}{(t^2 + k^2 \beta^2)^{3/4}} \int_0^{\infty} \frac{ds}{s^{3/2}} e^{-\frac{1}{4s} - s(gn_0)^2(t^2 + k^2 \beta^2)} I_1(gn_0 t). \quad (5.137)$$

Next we estimate the summation, again the terms of the sum are monotonically decreasing as the summand increases, hence the integral gives an upper bound which we estimate separately;

$$\begin{aligned} & \sum_{k=1}^{\infty} \frac{1}{(t^2 + k^2 \beta^2)^{3/4}} e^{-(gn_0)^2 s k^2 \beta^2} < \int_0^{\infty} \frac{dk}{(t^2 + k^2 \beta^2)^{3/4}} e^{-(gn_0)^2 s k^2 \beta^2} \\ & < \left[ \int_0^{\infty} \frac{dk}{(t^2 + k^2 \beta^2)^{3/2}} \right]^{1/2} \left[ \int_0^{\infty} dk e^{-2s(gn_0)^2 k^2 \beta^2} \right]^{1/2} \\ & = C_3 \frac{1}{\beta^{1/2} t} \frac{1}{s^{1/4} (gn_0)^{1/2} \beta^{1/2}}. \end{aligned} \quad (5.138)$$

Here we used the Cauchy-Schwarz inequality. Note that in the first integral given by (5.138) we scale the variable  $k$  with  $t\beta^{-1}$  and the second integral by  $(\sqrt{s}\beta gn_0)^{-1}$ . We

may place this estimate now to find the upper bound,

$$\frac{C_4(gn_0)^{1/2}}{\beta} \int_0^\infty \frac{dt}{t} \int_0^\infty \frac{ds}{s^{1+3/4}} e^{-\frac{1}{4s} - s(gn_0)^2 t^2} I_1(gn_0 t). \quad (5.139)$$

We recognize the modified bessel function of the second kind, which is given in an integral form by [55],

$$K_\nu(x) = \frac{1}{2} \int_0^\infty \frac{ds}{s^{1-\nu}} e^{-\frac{x}{2}(s+\frac{1}{s})} \quad (5.140)$$

to rewrite the upper bound given by (5.139) as,

$$\frac{C_5(gn_0)^{1/2}}{\beta} \int_0^\infty \frac{dt}{t} (gn_0 t)^{3/4} K_{3/4}(gn_0 t) I_1(gn_0 t). \quad (5.141)$$

Here we used  $K_\nu(x) = K_{-\nu}(x)$ . Note that in the integral  $gn_0$  completely scales out. The integral is of the type given in Prudnikov *et al.* [56] formula 2.16.28.3.

$$\int_0^\infty dx x^{\rho-1} K_\mu(x) I_\nu(x) = \frac{2^{\rho-1} \Gamma(\frac{1}{2}(\rho + \nu + \mu)) \Gamma(\frac{1}{2}(\rho + \nu - \mu)) \Gamma(1 - \rho)}{\Gamma(1 + \frac{1}{2}(-\rho + \nu + \mu)) \Gamma(1 + \frac{1}{2}(-\rho + \nu - \mu))} \quad (5.142)$$

for  $|\mu| - \nu < \rho < 1$ . Hence we find that

$$\tilde{n}_e(T) < C_1 \sum_{k=1}^\infty \frac{1}{(k\beta)^{3/2}} + C_6 \frac{(gn_0)^{1/2}}{\beta}, \quad (5.143)$$

the last piece of which will go to zero as  $g \rightarrow 0^+$  and moreover the full expression will go to zero as  $\beta \rightarrow \infty$ .

Next, we will show that the Bogoliubov approximation at finite temperatures is actually inconsistent, in accordance with the Hohenberg-Mermin-Wagner theorem [32, 57], rigorously established in spin systems or interacting bosons in flat spaces. To see this, we will use lower bounds on the heat kernel defined by (5.18) in the limit

$V \rightarrow \infty$ . We will further estimate sums of monotonically decreasing expressions from below by integrating them from 1 to  $\infty$ . As a result, for  $d = 2$  we see that  $\tilde{n}_e(T)$  is larger than

$$\frac{1}{\beta} \int_1^{\infty} \frac{dk}{k} e^{-(gn_0)k\beta} + gn_0 \int_0^{\infty} dt \int_1^{\infty} \frac{dk}{\sqrt{t^2 + k^2\beta^2}} e^{-gn_0\sqrt{t^2+k^2\beta^2}} I_1(gn_0t). \quad (5.144)$$

up to a constant multiple  $1/B$ . Note that we may shift  $k$  to  $k + 1$  and replace all  $k^2 + 2k + 1$ 's by  $3k^2 + 1$  since  $k^2 + 2k + 1 < 3k^2 + 1$  for  $k \geq 0$ . By this substitution, we get an integral which is smaller than the above integral, since the integrand is a monotonically decreasing function with increasing  $k$ . Then, we scale  $k$  to  $k\sqrt{t^2 + \beta^2}/\sqrt{3}\beta$  and we find that  $\tilde{n}_e(T)$  is larger than

$$\frac{1}{\beta} \int_1^{\infty} \frac{dk}{k} e^{-gn_0k\beta} + \frac{1}{\sqrt{3}} \frac{gn_0}{\beta} \int_0^{\infty} dt \int_0^{\infty} dk \frac{e^{-gn_0\sqrt{t^2+\beta^2}\sqrt{1+k^2}}}{\sqrt{1+k^2}} I_1(gn_0t). \quad (5.145)$$

We notice that

$$\int_0^{\infty} dk \frac{e^{-a\sqrt{1+k^2}}}{\sqrt{1+k^2}} = K_0(a), \quad (5.146)$$

hence the lower bound becomes,

$$\frac{1}{\beta} \int_1^{\infty} \frac{dk}{k} e^{-gn_0k\beta} + \frac{1}{\sqrt{3}} \frac{gn_0}{\beta} \int_0^{\infty} dt K_0(gn_0\sqrt{t^2 + \beta^2}) I_1(gn_0t) < \tilde{n}_e(T). \quad (5.147)$$

Nevertheless, the integral of Bessel functions is ultraviolet divergent (which reflects the infrared behavior of the theory in the heat kernel approach) as a result of the asymptotics of the Bessel functions,

$$K_0(x) \sim \frac{e^{-x}}{\sqrt{x}}, \quad \text{and} \quad I_1(x) \sim \frac{e^x}{\sqrt{x}} \quad \text{as} \quad x \rightarrow \infty. \quad (5.148)$$

This contradiction forces  $n_0 = 0$  to be the only consistent choice. An upper bound for

weakly interacting Bose system at absolute zero temperature given by (5.120) is also convergent for  $d = 2$ , hence the condensed phase takes place. However, for finite temperatures we have a divergent lower bound for the number density of excited particles, which is inconsistent with the given number of particles in the Bose system. Then we say in two dimensions, there is no condensation at finite temperatures.

## 6. CONCLUSION

Expressing the number density of a Bose system in terms of the trace of the heat kernel has great advantages, since there exist many studies about the heat kernel of the Laplace operator in the literature. On a compact Riemannian manifold, we can actually estimate the eigenvalues of the Laplace operator, hence the bounds for the depletion of the condensate for a Bose system follow. Note that these bounds work regardless of the geometry of the manifold.

In this thesis, we defined the behaviour of the trace of the heat. For an ideal Bose system, we derived an estimation for the depletion coefficient of the condensate and moreover we gave bounds for the critical temperature. We observed that for finite volumes, the condensate is formed in three dimensions, but not in two dimensions. Our bounds are actually consistent with the flat space results, *i.e.*, the condensation is formed in three dimensions, but it does not take place in two dimensions in the thermodynamic limit also. We studied the ground state of a dilute Bose system at absolute zero temperature under Bogoliubov approximation using heat kernel methods, and we fixed the ultraviolet divergence of the series rendering the ground state by the same methods. In doing so, noticing Laplace transforms of certain expressions helped fairly enough. Another interesting result is, we observed the condensation takes place in two dimensions for a weakly interacting gas in the finite volume limit. At finite temperatures, we derived an upper bound for the depletion of the condensate in three dimensions. We also displayed the inconsistency of the Bogoliubov approximation in the thermodynamic limit in two dimensions.

It is motivating to see that the heat kernel methods are actually very useful in offering bounds for the depletion of the condensate. It is promising that the same methods can also be applied on Fermi systems yielding consistent results, which may be another study.

## APPENDIX A: JUSTIFICATION OF THE C-NUMBER SUBSTITUTION

Let  $\{|z\rangle : z \in M\}$  be an over-complete set labeled by the points of a manifold  $M$  with measure  $d\mu(z)$ . The lower symbol  $A_L(z)$  of an operator  $A$  is the expectation value

$$A_L(z) = \langle z|A|z\rangle. \quad (\text{A.1})$$

On the other hand, if there exists a function  $A_U(z)$  on  $M$  such that

$$A = \int d\mu(z) A_U(z) |z\rangle\langle z| \quad (\text{A.2})$$

then  $A_U(z)$  is called the upper symbol of  $A$ . Here the equality is in the weak sense.<sup>14</sup>

Let

$$|z\rangle = e^{-\frac{|z|^2}{2} + z\hat{a}_0^\dagger} |0\rangle, \quad z \in \mathbb{C}, \quad (\text{A.3})$$

be the standard coherent states for the annihilation operator  $\hat{a}_0$ . This is an over-complete set relative to the measure

$$d\mu(z) = \frac{dzdz^*}{\pi}. \quad (\text{A.4})$$

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<sup>14</sup>For a vector space  $V$ ,  $a \in V$  and  $b \in V$  are said to be weakly equal when  $\langle v, a - b \rangle = 0$  for all  $v \in V^\dagger$ , where  $V^\dagger$  is the dual vector space with respect to the given inner product.

The following list of the symbols of various combinations of creation and annihilation operators is useful in calculating the lower and upper symbols of the Hamiltonian [58].

$A$	$A_L$	$A_U$
$\hat{a}_0$	$z$	$z$
$\hat{a}_0^\dagger$	$z^*$	$z^*$
$\hat{a}_0\hat{a}_0$	$z^2$	$z^2$
$\hat{a}_0^\dagger\hat{a}_0^\dagger$	$z^{*2}$	$z^{*2}$
$\hat{a}_0^\dagger\hat{a}_0$	$ z ^2$	$ z ^2 - 1$
$\hat{a}_0^{\dagger 2}\hat{a}_0^2$	$ z ^4$	$ z ^4 - 4 z ^2 + 2$

(A.5)

We assume our Hamiltonian includes the chemical potential

$$\hat{H} = \hat{H}' - \mu\hat{N}, \quad (\text{A.6})$$

where  $H'$  is given by (5.67). In the Hamiltonian  $\hat{H}$ , we replace every monomial of the form  $\hat{a}_0^{\dagger n}\hat{a}_0^m$  first by its lower and then by its upper symbol and thus obtain the two Hamiltonians  $\hat{H}_L(z, z^*)$  and  $\hat{H}_U(z, z^*)$ . For a given  $V$ , let  $\mathcal{G}_L(T, \mu)$  and  $\mathcal{G}_U(T, \mu)$  be the corresponding grand canonical partition functions integrated over  $z$ ,

$$\mathcal{G}_{L,U}(T, \mu) = \int \frac{dzdz^*}{\pi} \mathcal{G}_{L,U}(T, \mu, z, z^*), \quad (\text{A.7})$$

where

$$\mathcal{G}_{L,U}(T, \mu, z, z^*) = \text{Tr}' e^{-\beta\hat{H}_{L,U}(z, z^*)}. \quad (\text{A.8})$$

Here  $\text{Tr}'$  means that the trace is taken over the states with no excitations in the  $f_0$  mode. Then we have the following inequalities

$$\mathcal{G}_L(T, \mu) \leq \mathcal{G}(T, \mu) \leq \mathcal{G}_U(T, \mu). \quad (\text{A.9})$$

The first inequality is the Jensen's inequality and the second is the Berezin-Lieb inequality [20, 59–63]. These inequalities are valid on any manifold since geometry does not play any role whatsoever in their derivations.

Comparing  $H_L$  and  $H_U$  we see that

$$\begin{aligned}\delta &= H_U(z, z^*) - H_L(z, z^*) = \mu + \frac{g}{4V}(-4|z|^2 + 2 - 4 \sum_{\sigma \neq 0} \hat{a}_\sigma^\dagger \hat{a}_\sigma) \\ &= \mu + \frac{g}{2V}(2 - 4N_L).\end{aligned}\tag{A.10}$$

In deriving this we used the list of symbols given above and the fact that  $f_0 = V^{-1/2}$ . Thus, we find

$$\begin{aligned}\mathrm{Tr}' e^{-\beta H_U(z, z^*)} &= \mathrm{Tr}' e^{-\beta(H_L(z, z^*) + \mu + \frac{g}{V} - \frac{2g}{V} N_L)} \\ &= e^{-\beta(\mu + \frac{g}{V})} \mathrm{Tr}' e^{-\beta(H_L(z, z^*) - \frac{2g}{V} N_L)},\end{aligned}\tag{A.11}$$

or

$$\mathcal{G}_U(T, \mu) = e^{-\beta(\mu + \frac{g}{V})} \mathcal{G}_L\left(T, \mu + \frac{2g}{V}\right).\tag{A.12}$$

So

$$\begin{aligned}\lim_{V \rightarrow \infty} \frac{1}{V} \ln \mathcal{G}_U(T, \mu) &= \lim_{V \rightarrow \infty} \frac{1}{V} \left[ -\beta \left( \mu + \frac{g}{V} \right) \right] + \frac{1}{V} \ln \mathcal{G}_L\left(T, \mu + \frac{2g}{V}\right) \\ &= \lim_{V \rightarrow \infty} \frac{1}{V} \ln \mathcal{G}_L(T, \mu).\end{aligned}\tag{A.13}$$

Then, from (A.9) we get the equality of the pressures in the thermodynamic limit

$$\frac{1}{V} \ln \mathcal{G}_U(T, \mu) = \frac{1}{V} \ln \mathcal{G}(T, \mu) = \frac{1}{V} \ln \mathcal{G}_L(T, \mu).\tag{A.14}$$

Let  $z_0$  be the value of  $z$  for which  $\mathcal{G}_L(\beta, \mu, z, z^*)$  is maximum. Then the integrals in the above expressions localize around  $z_0$  and the following inequalities hold [20],

$$\frac{1}{V} \ln \mathcal{G}_L(T, \mu, z_0, z_0^*) \leq \frac{1}{V} \ln \mathcal{G}(T, \mu) \leq \frac{1}{V} \ln \mathcal{G}_U(T, \mu, z_0, z_0^*) + O\left(\frac{\ln V}{V}\right). \quad (\text{A.15})$$

Note that the usual choice  $\mu = gn_0$  in the Bogoliubov theory is in accordance with this result. Again using (A.10), in the thermodynamic limit we obtain

$$\frac{1}{V} \ln \mathcal{G}(T, \mu) = \frac{1}{V} \ln \mathcal{G}_L(T, \mu, z_0, z_0^*). \quad (\text{A.16})$$

Here, we have four different thermodynamic pressures which agree in the thermodynamic limit

$$P_L(T, \mu) = P(T, \mu) = P_U(T, \mu) = P_{max}(T, \mu). \quad (\text{A.17})$$

This equivalence of thermodynamic pressures imply that the weakly interacting Bose system has the same statistics when the creation and the annihilation operators are substituted with complex numbers  $z$  and  $z^*$ . By this substitution, we get another Hamiltonian  $\hat{H}_L(z, z^*)$  describing the system which acts on the Fock space of all the modes other than the  $\hat{a}_0$  mode. We notice that the c-number substitution for the zero energy mode does not alter the statistics governing the behaviour of the system. It is interesting to note that macroscopic occupation of the zero mode is not assumed as we did in Section 3.3. Actually, the Bose-Einstein condensation justifies the c-number substitution with the macroscopic occupation of the zero mode, *i.e.*,  $N_0 \gg 1$ . Nevertheless, Ginibre [19] showed that the c-number substitution still gives the right answer even if  $N_0$  is small (but it is a useful calculational tool only if  $N_0$  is macroscopic) [25].

## APPENDIX B: SUBORDINATE IDENTITY FOR THE EXPONENTIAL

We will show how (5.137) is recovered explicitly. We notice the equivalence of integrals

$$\sqrt{\frac{\pi}{a}} = \int_{-\infty}^{\infty} e^{-ax^2} dx = \int_{-\infty}^{\infty} \frac{e^{-ax^2}}{\sqrt{1+x^2}(x+\sqrt{1+x^2})}, \quad (\text{B.1})$$

where  $a$  is a constant. Using the substitution

$$x = \frac{1}{2} \left( y - \frac{1}{y} \right), \quad (\text{B.2})$$

we get

$$\begin{aligned} \int_0^{\infty} \frac{dy}{y^2} e^{-\frac{a}{4} \left( y - \frac{1}{y} \right)^2} &= e^{a/2} \int_0^{\infty} \frac{dy}{y^2} e^{-\frac{a}{4} \left( y^2 + \frac{1}{y^2} \right)} \\ &= \frac{e^x}{2} \int_0^{\infty} \frac{du}{u^{3/2}} e^{-\frac{x}{2} \left( u + \frac{1}{u} \right)} \end{aligned} \quad (\text{B.3})$$

where,  $x = a/2$  and  $u = y^2$ . As a final step, we scale  $u$  to  $2sx$  and obtain

$$\sqrt{\frac{\pi}{2x}} = \frac{e^x}{2\sqrt{2x}} \int_0^{\infty} \frac{ds}{s^{3/2}} e^{-\frac{1}{4s} - sx^2}. \quad (\text{B.4})$$

Here, we see the exponent can be expressed as

$$e^{-x} = \int_0^{\infty} \frac{ds}{s^{3/2}} e^{-\frac{1}{4s} - sx^2}, \quad (\text{B.5})$$

up to a multiplication constant.

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