Critical Properties of Interacting Trapped Boson at BEC

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Undergraduate Honors Thesis

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Contents

1	Abs	tract	4
2	Ack	nowledgement	5
3	History of Bose Einstein Condensate		
	3.1	Bose and Einstein Proposal	6
	3.2	Superfluidity of ⁴ He	7
	3.3	Adventure of Hydrogen	7
	3.4	Rubidium in Dilute Gas	8
4	Exp	eriment Achievements of BEC in Diluted Gas	9
	4.1	Cornell and Wieman Experiment	9
		4.1.1 Laser Cooling	9
		4.1.2 Evaporation	10
		4.1.3 Magnetic Trapping	10
	4.2	Precision Measurement on a Bose gas with tuneable interactions	11
5	Fun	damental Theories of Bose-Einstein Condensation	12
	5.1	Distribution Functions	12
		5.1.1 extreme cases	13
	5.2	Total Number of Particles	13
	5.3	Critical Temperature	14
	5.4	Conditions for BEC	14
6	Furt	ther Theoretical Analysis with Personal Extension	16
	6.1	Non-Interacting Bosons	16

Appendix A Mathematica Files						
	6.4	T-matrix Approximation	22			
	6.3	Hartree-Fock Approximation	19			
	6.2	Local Density Approximation	17			

List of Figures

3.1	Photograph of Satyendra Nath Bose and Albert Einstein	6
3.2	Three atomic clouds at different temperature around BEC transition	8
4.1	Modern Magneto-Optical Trap(MOT) illustration	10
4.2	Illustration of magnetic trapping coupled by evaporation	11
6.1	particle density vs. chemical potential	17
6.2	plot of chemical potential vs radius of the trap at BEC	18
6.3	Local density of spherical harmonic trap vs. radius	18
6.4	total numbers of particles vs. $\frac{\epsilon_F}{k_B T}$	21

1 Abstract

Bose-Einstein condensation, as an extraordinary phase of bosons, has been a well established prediction since early 1920s. However, the experimental discovery of BEC in diluted Boson gas was only achieved by laser cooling until 1995. In the span of nearly a century, both theoretical and experimental physics have studied numerous critical properties of many body boson systems at low temperature. In extension of previous theoretical analysis BEC in different conditions, this thesis attempted several approximations for understanding the properties BEC in diluted gas. The system conditions of local density approximation, Hartree-Fock approximation and tmatrix approximation are all taken account as the change of chemical potential for the system. The modified chemical potentials can further be used to deliver different results of particle density and particle numbers from the Bose-Einstein Distribution for ideal gas. Finally, the parameters of all conditions are compared with the Shi-Griffins approximation to test that it is not consistent at temperature higher than critical temperature.

2 Acknowledgement

This thesis would not be possible without the enlightment of Dr. Theja N. DeSilva and the encouragement of Andrew Snyder.

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3 History of Bose Einstein Condensate

3.1 Bose and Einstein Proposal

The history of Bose Einstein Condensate can be dated back to 1924 when a young scholar Satyendra Nath Bose from India sent his proposal of black-body photon statistics to Albert Einstein for publication. After viewing S.N Bose's proposal, Einstein took another perspective on the matter wave from the de Broglie wavelength of particles. Einstein applied and extended the Bose's prediction of photon onto particles with masses. From that, the theory of Bose-Einstein statistics are conveyed. Later, particles with integer spins are classified as Boson. Interestingly, Einstein's paper came one year before the Schrdinger's quantum mechanics. So, in some senses, the Schrdinger wave equation gained insight from the work of BEC, since both have crossover in the field of quantum statistics.[4]



(a) Satyendra Nath Bose (b) Albert Einstein

Figure 3.1: Photograph of Satyendra Nath Bose and Albert Einstein

3.2 Superfluidity of ⁴He

The superfluidity of ⁴He is the monumental manifestation of BEC. Fizz London and Laszlo Tisza classified the superfluid ⁴He has involved BEC transition in mid-1930s. Even though the liquid helium is very different to Einstein's prediction on uniform ideal gas, the transition temperature estimated by Einstein's equation is very close to the measured ⁴He transition temperature at around 2.17K. Inspired by the conclusion of London, physicists such as Nikolay.N Bogoliubov, Oliver Penrose, Lars Onsager and Richard.P Feynman continued on and contribute series of comprehensive theories to deeply explain the properties of BEC with the factor of interaction and transition phase.

Unfortunately, due to the strong interaction between helium atoms explained by the theories, the fraction of particles to have zero momentum in order to reach BEC is very low, even at absolute zero. With this discovery in hand, BEC scientists are eager to find a better boson that doesn't condensate into solid and liquid at extremely low temperature and possesses low interaction.[2]

3.3 Adventure of Hydrogen

The upcoming candidate boson proposed is the spin-aligned hydrogen atom. This type of weekly acting boson is structural stable and will not recombine to hydrogen molecule. Early experimental attempted to force spin-aligned hydrogen atom by a strong magnetic gradient onto a cryogenically cooled surface. However, due to the interaction with the surface, it is very difficult to reach a desired low temperature at certain particle density.

To limit the contact with the containing surface, the Massachusetts Institute of Technology group led by Greytak and Kleppner invented trapping atoms with purely magnetic field. However, the laser cooling technique is not applicable to hydrogen. The BEC was finally achieved by a combination of magnetic trapping and evaporation in 1998 after two decade of arduous work.

3.4 Rubidium in Dilute Gas

It was only until in 1995, when Eric Cornell and Carl Wieman cooled dilute rubidium gas to around 1.7×10^{-7} nK and reached BEC by advanced laser cooling, magnetic trapping and evaporation techniques. The predicted theory on uniformed diluted gas with weak interaction was finally proved to be valid in lab environment. With the development of technology, so far atoms such as ¹H, ⁷Li, ²³Na, ³⁹K, ⁴¹K, ⁵²Cr, ⁸⁵Rb, ⁸⁷Rb, ¹³³Cs, ¹⁷⁰Yb have recorded to undergo BEC transition. [1]



Figure 3.2: Three atomic clouds at different temperature around BEC transition

4 Experiment Achievements of BEC in Diluted Gas

This chapter focuses on experiment techniques to achieve Bose-Einstein Condensation in laboratory environment. The techniques of magnetic trapping, laser cooling and evaporation are introduced by the example of Cornell and Wieman experiment. With the protocol of cooling dilute gas, a set of new experiments can be conducted on measuring the parameters be tuning interactions.

4.1 Cornell and Wieman Experiment

In 1995, Eric Cornell and Carl Wieman were able to produce BEC in rubidium by mainly using Magneto-Optical Trap (MOT) device, shown in 4.1. By their uttermost effort the dilute rubidium gas is cooled down to around 170 nK. With the protocol of laser cooling to BEC established by Cornell and Wieman, tons of related experiments can be conducted. Later in 2001, Cornell, Wieman and Wolfgang Ketterle received Nobel Prize in Physics. The general techniques of their protocol are described in the following subsections.

4.1.1 Laser Cooling

The laser cooling technique was originally developed by Steven Chu, Claude Cohen-Tannoudji, William D. Phillips. This phenomenal science invention was awarded The Nobel Prize in Physics 1997. This technique utilized the Doppler effect on particles. When frequency of laser is tuned to be close to the frequency of incoming particles, the light frequency becomes larger. The photon would hit the particle with higher energy to slow the particle down. On the other hand, when the particle is bouncing away from the laser, the light frequency it received becomes



Figure 4.1: Modern Magneto-Optical Trap(MOT) illustration

smaller. The particle moving away the laser would be slowed down by another laser shooting at the opposite position. With this fundamental concept, optical molasses can be built by use six beams shooting in three perpendicular coordinates, shown in figure 4.1. However, Doppler limit forbids boson gas to reach any temperature lower than a few hundred mK. To break this barrier predicted by Doppler limit, the Magneto-Optical Trap (MOT) is developed in addition of magnetic trapping and evaporation techniques in the following subsections.

4.1.2 Evaporation

After applying laser cooling technique to the atomic gas, a further step of evaporation is needed to cool the temperature even lower. Since most particles with low energy are trapped at the center of the optical molasses, the particles with higher energy level would move freely outside the center. If apply a vacuum to the chamber, the particles with higher energy that optical molasses failed to cooled can be removed. By reducing the number of particles with high energy, the average energy of total particles remain would be lowered dramatically and undergone temperature drop.

4.1.3 Magnetic Trapping

Attempt to cool polarized hydrogen to reach BEC failed in the 1980s due to the hydrogen is in physical contact with surrounding materials. To solve this problem, the MIT hydrogen group improved this situation by inventing magnetic trapping on atoms. The magnetic trap applied to the dilute gas would hold the atoms in vacuum without contact with the surrounding. The strength of magnetic field could only be capable of holding low energy particles in a trapped. Moreover, the magnetic trapping would allow particles with high energy escape by turning down the magnetic field and applying evaporation shown in figure 4.1.3. The decrease in number of particles with high kinetic energy would lower the average energy of remaining particles in the system which indicates a lower average energy.



Figure 4.2: Illustration of magnetic trapping coupled by evaporation [5]

4.2 Precision Measurement on a Bose gas with tuneable interactions

With the protocol of cooling dilute boson gas in mind, one of the most interesting experiment is to measure boson gas with tunable interactions. The scattering length of the atoms can be modified by an uniform external magnetic field in the vicinity of a Feshbach scattering resonance. To measure the thermal atomic number and condensate atom number, a time of flight(TOF) can be used. The TOF method is to turn off the trap holding all atoms for a small amount of time, usually several ns, and measure the free expansion of atoms to estimate their kinetic energy.[7]

5 Fundamental Theories of Bose-Einstein Condensation

5.1 Distribution Functions

In a many-body particle system, it is very important to predict the energy distribution on single particles. Depending on the classifications of particles, three distribution functions are used to predict the relationship between the energy of the particle , the number of particles N, the temperature T and the chemical potential ϵ_i . For general particles that cannot be distinguished, the **Maxwell Boltzmann Distribution** predicts

$$N_{indistinguishable} = \frac{1}{e^{\frac{\epsilon_i - \mu}{k_B T}}}$$
(5.1)

For Fermions, the Fermi-Dirac Distribution predicts

$$N_{fermion} = \frac{1}{e^{\frac{\epsilon_i - \mu}{k_B T}} + 1}$$
(5.2)

Finally, for bosons, the **Bose-Einstein Distribution** predicts

$$N_{boson} = \frac{1}{e^{\frac{\epsilon_i - \mu}{k_B T}} - 1}$$
(5.3)

5.1.1 extreme cases

When energy of the particle equals to chemical potential, $\epsilon_i = \mu$

$$N_{indistinguishable} = \frac{1}{e^0} = 1 \tag{5.4}$$

$$N_{fermion} = \frac{1}{e^0 + 1} = \frac{1}{2} \tag{5.5}$$

$$N_{boson} = \frac{1}{e^0 - 1} = \frac{1}{0} \approx \infty$$
 (5.6)

With a very simple calculate, a extreme situation is predicted by Bose-Einstein Distribution. At this stage when particle energy and chemical energy are exacted the same, the number of the particle goes to infinity. We call this phase of particles the Bose-Einstein Condensation (BEC). During the transition of BEC, the chemical potential goes from negative to zero. Particles at higher energy level condense to the lowest energy level. The wave functions of each particles overlap with each other.

5.2 Total Number of Particles

With the Bose-Einstein Distribution in mind, certain particle occupation of energy state ϵ_k can be predicted. If we take a further approach to sum over all energy state, the total number of particles N can be calculated by (5.7).[6]

$$N = \sum_{k} f_{boson}(\epsilon_k) = \int D(\epsilon) f_{boson}(\epsilon) d\epsilon$$
(5.7)

Of course, if consider the density of state is uniform, the total number of particles can be calculated simply by taking integral over all space

$$N = \int_{allspace} f_{boson}(\epsilon) d\mathbf{r}$$
(5.8)

5.3 Critical Temperature

The critical temperature of atomic gas is related to the average particle density n, the mass of particle m and the Boltzmann constant k_B

$$T_c = C \frac{\hbar^2 n^{2/3}}{mk_B}$$
(5.9)

Generally, the critical temperature is considered to be very low for BEC to take place. The temperature is included, for most of the time, in the constant β described as

$$\beta = \frac{1}{k_B T} \tag{5.10}$$

5.4 Conditions for BEC

One and the most important requirement for BEC to achieve is extreme low temperature. Since we are looking at the quantum property of boson, the de Broglie wavelength would be equivalent to the atomic size of particles when wave functions of every particles overlaps.

$$\lambda = \frac{h}{mv} \tag{5.11}$$

The average kinetic energy $\langle E_k \rangle$ of a many-body system at temperature T, is given by (5.12)

$$\frac{1}{2}m < v >^2 = < E_k > = \frac{3}{2}k_BT \tag{5.12}$$

If we plug in the thermal statistics expression (5.12) into (5.11), an average deBroglie wavelength is given by (5.13)

$$<\lambda>=rac{h}{\sqrt{3mk_BT}}$$

$$(5.13)$$

or the temperature can be estimated by (5.14)

$$T = \frac{h}{\sqrt{3mk_B < \lambda >}} \tag{5.14}$$

In case we want the deBroglie wavelength to be around 10nm, by (5.14) the temperature required for the particle is 0.002K, which is an extreme temperature that has to be achieved.

6 Further Theoretical Analysis with Personal Extension

6.1 Non-Interacting Bosons

The original proposal on BEC is only applied to non-interacting ideal gas. For ideal gas, the chemical potential μ starts from negative and goes to zero when BEC is achieved. The Hamiltonian of many body non-interacting bosons is shown as in (6.2). Where n_p is the number of occupation of a particular momentum level p. Creation and anilition operator as a_p and a_p^{\dagger} can be used to represent the number of particles .Even non-interacting bosons neglect the interaction between real particles, this approach is still very reliable for further calculation.[?]

$$n_p = \sum_p a_p^{\dagger} a_p \tag{6.1}$$

$$\hat{H} = \sum_{p} n_{p} \frac{p^{2}}{2m} - \mu \sum_{p} a_{p}^{\dagger} a_{p}$$
(6.2)

As Bose-Einstein Distribution predicted for the non-interacting bosons in (6.5), the probability of particle is depend on momentum state p.

$$p = mv = \hbar k \tag{6.3}$$

$$\epsilon_k = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2)$$
(6.4)

$$f_{boson} = \frac{1}{e^{(\frac{\hbar^2 k^2}{2m} - \mu)/k_B T} - 1}$$
(6.5)

By taking a integral of (6.5) over all momentum space $d\mathbf{k} = d^3k = \frac{k^2dk}{4\pi}$, the density of particles can be given below in a form of polylog function $g(\mathbf{x})$

$$n = \int \frac{1}{e^{(\frac{\hbar^2 k^2}{2m} - \mu)/k_B T} - 1} d\mathbf{k} = \int \frac{k^2}{4\pi (e^{(\frac{\hbar^2 k^2}{2m} - \mu)/k_B T} - 1)} dk = \frac{g_{3/2}(e^{\mu/k_B T})}{\lambda^3}$$
(6.6)

where,
$$g_{3/2}(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^{3/2}}$$
 (6.7)

$$\lambda = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{\frac{1}{2}} \tag{6.8}$$

The particle number n with respect to chemical potential μ given by (6.6) is plotted in figure 6.1. For the simplicity of calculation β , m and \hbar are all fixed to 1. By the figure, as the chemical potential goes from negative to zero during the transition of BEC, the particle density dramatically increases.



Figure 6.1: particle density vs. chemical potential

6.2 Local Density Approximation

Sometimes, in a spherical harmonic trap, the chemical potential of particles are distributed proportional to radius square, as shown in (6.9). A plot of the chemical potential vs. radius r at BEC condition when the center of the trap $\mu 0 = 0$ is shown below in figure 6.2. Also, fixing $\mu_0 = 0$, $\omega = 1$ and m = 1.

$$\mu(r) = \mu_0 - \frac{1}{2}m\omega^2 r^2 \tag{6.9}$$



Figure 6.2: plot of chemical potential vs radius of the trap at BEC

By plugging the new local density approximation chemical potential (6.9) into (6.6), a new density distribution with variable of r and μ_0 is obtained as (6.10).

$$n_l(\mu_0, r) = \frac{g_{3/2}(e^{(\mu_0 - \frac{1}{2}m\omega^2 r^2)/k_B T})}{\lambda^3}$$
(6.10)

To fully understand the physics logic hiding behind this new density equation, different values of μ_0 are selected to plot against the radius of the trap, shown in figure 6.2. Chemical potential $\mu_0 = 0$ is chosen for the BEC phase with three other small negative values of μ_0 . Comparing to the non-BEC cases, the enormous amount of particles are condensed into the center of the trap during BEC.



Figure 6.3: Local density of spherical harmonic trap vs. radius

By knowing the density of particles for local density approximation, the total number of particles can be further calculated by taking a integral over all space. If the trapped is assumed to be spherical harmonic, then $d\mathbf{r} = dr^3 = 4\pi dr$.

$$N = \int \frac{g_{3/2}(e^{(\mu - \frac{1}{2}m\omega^2 r^2)/(k_B T)})}{\lambda^3} d\mathbf{r}$$
(6.11)

If the trapped is assumed to be spherical harmonic by changing of variable from r to μ

$$r^{2} = (\mu_{0} - \mu) \frac{2}{m\omega^{2}}$$
(6.12)

$$rdr = \frac{d\mu}{-m\omega^2} \tag{6.13}$$

$$N = \frac{4\sqrt{2}\pi}{(m\omega^2)^{3/2}} \int_{-\infty}^{\mu_0} n(\mu)(\mu_0 - \mu)^{1/2} d\mu$$
(6.14)

6.3 Hartree-Fock Approximation

The Hartree-Fock Approximation focused on the position of particles due to the position of particles in momentum space. The creation and annihilation operators are used to simplify this approximation.

The Hamiltonian of the quantized field for spinless bosons is given by (6.15) [3]

$$\hat{H} = \sum_{p} \frac{p^2}{2m} a_p^{\dagger} a_p - \mu \sum_{p} a_p^{\dagger} a_p + \frac{2\pi a \hbar^2}{mV} \left[\sum_{p} a_p^{\dagger} a_p^{\dagger} a_p a_p + \sum_{p_1, p_2} * (a_{p_1}^{\dagger} a_{p_2}^{\dagger} a_{p_2} a_{p_1} + a_{p_2}^{\dagger} a_{p_1}^{\dagger} a_{p_2} a_{p_1})\right]$$
(6.15)

Here, we are using a Hartree-Fock approximation to assume that only two momentum states p_1 and p_2 exist besides ground state p=0 at extreme low temperature when BEC formed. The interaction between this two energy states makes the BEC boson gas imperfect since not all particles in this system is in the ground state.

Since both cases of Hartree-Fock could happen within this quantum system, creation and annihilation operators have to be include two parts of them.

$$a_{p_1}^{\dagger}a_{p_2}^{\dagger}a_{p_2}a_{p_1} + a_{p_2}^{\dagger}a_{p_1}^{\dagger}a_{p_2}a_{p_1}$$

$$(6.16)$$

$$Hartree \qquad Fock \tag{6.17}$$

However, the properties of creation and annihilation shows that, when $i \neq j$

$$[a_i, a_j] = [a_i^{\dagger}, a_j^{\dagger}] = 0$$
(6.18)

Which means that

$$a_1 a_2 = a_2 a_1 \tag{6.19}$$

$$a_{1}^{\dagger}a_{2}^{\dagger} = a_{2}^{\dagger}a_{1}^{\dagger} \tag{6.20}$$

In such manner, both Hartree and Fock term will end up with the same value

$$\sum_{p_1,p_2} {}^*(a_{p_1}^{\dagger}a_{p_2}^{\dagger}a_{p_2}a_{p_1}) = \sum_{p_1,p_2} {}^*(a_{p_2}^{\dagger}a_{p_1}^{\dagger}a_{p_2}a_{p_1}) = \sum_{p_1,p_2} {}^*(n_{p_1}n_{p_2})$$
(6.21)

$$N = n_{p_1} + n_{p_2} \tag{6.22}$$

$$\sum_{p_1, p_2} {}^*(n_{p_1} n_{p_2}) = \sum_{p_1} n_{p_1} (N - n_{p_1}) = N^2 - \sum_p n_p^2$$
(6.23)

For cases of $p_1 = p_2 = p$, the sum can be evaluated as

$$\sum_{p} a_{p}^{\dagger} a_{p}^{\dagger} a_{p} a_{p} = \sum_{p} a_{p}^{\dagger} (a_{p} a_{p}^{\dagger} - 1) a_{p} = \sum_{p} (n_{p}^{2} - n_{p}) = \sum_{p} n_{p}^{2} - N$$
(6.24)

Finally, by combining everything inside the bracket of interaction, the energy eigenvalues of the system $\{n_p\}$ can be written as

$$E\{n_p\} = \sum_p n_p \frac{p^2}{2m} + \frac{2\pi a\hbar^2}{mV} [2N^2 - N - \sum_p n_p^2] \simeq \sum_p n_p \frac{p^2}{2m} + \frac{2\pi a\hbar^2}{mV} (2N^2 - n_0^2)$$
(6.25)

With the assumption of Hartree-Fock Approximation, the chemical potential of the trapped bosons changes due to the imperfection. With most of the boson laying in the lowest energies states at BEC, their is still a small amount of particles would have limited momentum p_1 and p_2 . Also, from the HF Approximation, it is shown that this chemical potential is correlated with the particle density. So the redefined chemical potential is given as,

$$2N^2 - n_0^2 = N^2 + (N^2 - n_0^2) \simeq N^2 + 2N(N - n_0) = N^2 + 2N\sum_{p \neq 0} a_p^{\dagger} a_p$$
(6.26)



Figure 6.4: total numbers of particles vs. $\frac{\epsilon_F}{k_BT}$

$$\mu(n) = \mu - 2nU = \mu_0 - \frac{1}{2}m\omega^2 r^2 - 2nU$$
(6.27)

where
$$U = \frac{4\pi\hbar^2 a}{m}$$
 (6.28)

The modified Hartree-Fock in (6.27) can be plugged into the distribution for non-interacting ideal gas again to calculate the particle density.

$$n(\beta) = \int \frac{1}{e^{\beta(\epsilon_i - \mu(n))} - 1} d\mathbf{k} = \frac{g_{3/2}(e^{\beta(\mu_0 - \frac{1}{2}m\omega^2 r^2 - 2nU)})}{\lambda^3}$$
(6.29)

The total numbers of particle can be given as

$$N = \frac{4\sqrt{2}\pi}{(m\omega^2)^{3/2}} \int_{-\infty}^{\mu_0} n(\beta)(\mu_0 - \mu)^{1/2} d\mu$$
(6.30)

The ratio of total numbers of particles of Hartree-Fock gas over non-interacting gas can be plotted vs. $\frac{\epsilon_F}{k_BT}$

6.4 T-matrix Approximation

The Hartree-Fock Approximation only assumes low order collection, for higher order collection the T-matrix approximation can be more suitable.Following Shi and Griffin's paper [6] on the Tmatrix approximation on high order collection of interactions, the relations of particle density and particle number can be given as below The modified chemical potential with respect to T-matrix is given as,

$$\Gamma_0 = \frac{U}{1 + \alpha U} \tag{6.31}$$

$$\Delta \equiv \mu - 2n\Gamma_0 \tag{6.32}$$

$$\mu = \Delta + \frac{2nU}{1+\alpha U} \tag{6.33}$$

Here, Shi and Griffin introduced a variable α for temperature higher and lower than critical temperature

$$\alpha = \begin{cases} \int \frac{dk}{(2\pi)^3} \left[\left(\frac{1}{2E_k} + \frac{\Delta^2}{E_k^3} \right) \coth \frac{\beta E_k}{2} - \frac{1}{2\epsilon_k} \right], & T < T_c. \\ \int \frac{dk}{(2\pi)^3} \left(\frac{1}{2E_k} \coth \frac{\beta E_k}{2} - \frac{1}{2\epsilon_k} \right), & T > T_c. \end{cases}$$
(6.34)

By using a this variable α , density of non-condensate atoms for temperature below and above is given as

$$n = \begin{cases} \int \frac{dk}{(2\pi)^3} \left(\frac{\epsilon_k - \Delta}{2E_k} \coth \frac{\beta E_k}{2} - \frac{1}{2}\right), & T < T_c. \\ \int \frac{dk}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_k - \Delta)} - 1}, & T > T_c. \end{cases}$$
(6.35)

Following the same methodology of calculating the density of particles

$$n = \int \frac{1}{e^{\beta(\epsilon_i - \Delta)} - 1} d\mathbf{k} = \frac{g_{3/2}(e^{\beta\Delta})}{\lambda^3}$$
(6.36)

As Shown in the graph above, the Shi and Griffin assumption on the density of particles at high energy is not a smooth transition. Although this approach is commonly used in the field, it doesn't explain the kink happened in the bell curve. The T-matrix approximation for the temperature lower than critical temperature is valid to explain the density of particle, however this approximation have limitation to explain the phase transition at temperature higher than critical.



A Mathematica Files

This thesis highly relied on Mathematica 8 for solving equations and plotting figures of illustrations. By using software, several equations can be solved as ease. All Mathematica files are listed in this appendix. In[1]:= Clear["Global`*"]

Non-Interacting Bosons

Integrate over k space of Bose-Einstein distribution

$$\ln[2] = \operatorname{Integrate}\left[\frac{k^{2}}{4\pi\left(\operatorname{Exp}\left[\left(\hbar^{2}\frac{k^{2}}{2\pi}-\mu\right)\star\beta\right]-1\right)}, \left\{k, -\operatorname{Infinity}, \operatorname{Infinity}\right\}\right]$$

$$\operatorname{Out}[2] = \operatorname{ConditionalExpression}\left[\frac{\operatorname{PolyLog}\left[\frac{3}{2}, e^{\beta\mu}\right]}{2\sqrt{2\pi}\left(\frac{\beta\hbar^{2}}{m}\right)^{3/2}}, \operatorname{Re}\left[\frac{\beta\hbar^{2}}{m}\right] > 0\right]$$

$$\ln[3] = \beta = 1$$

$$\operatorname{Out}[3] = 1$$

$$\ln[4] = \hbar = 1$$

$$\operatorname{Out}[4] = 1$$

$$\ln[6] = \pi = 1$$

$$\operatorname{Out}[5] = 1$$

$$\ln[6] = \lambda = \left(\frac{\left(2\pi\hbar^{2}\beta\right)}{(m)}\right)^{0.5}$$

$$\operatorname{Out}[6] = 2.50663$$

particle density function with respect to μ

$$\ln[7]:= n[\mu_] := \frac{\operatorname{PolyLog}\left[\frac{3}{2}, \frac{e^{\mu}}{\beta}\right]}{\lambda^{3}}$$

In[8]:=

Plot particle density vs. chemical potential

$$Dut[9] = Plot \left[\frac{PolyLog \left[\frac{3}{2}, \frac{e^{\mu}}{\beta} \right]}{\lambda^{3}}, \{\mu, -4, 0\}, PlotRange \rightarrow All, AxesLabel \rightarrow \{"\mu", "n"\} \right]$$

$$Out[9] = 0$$

$$0.15$$

$$0.16$$

$$0.16$$

$$0.05$$

$$0.05$$

$$0.05$$

$$0.05$$

In[80]:= Clear["Global`*"]

Chemical Potential μ vs. Trap Radius r

$$\ln[81]:= \mu[\mathbf{r}, \mu \mathbf{0}] = \mu \mathbf{0} - \frac{1}{2} \mathbf{m} \omega^2 \mathbf{r}^2$$

$$Out[81]= \mu \mathbf{0} - \frac{1}{2} \mathbf{m} \mathbf{r}^2 \omega^2$$

set μ 0=0, assuming BEC at the center of the trap

set m, ω , β , \hbar to one for calculation simplicity

 $\ln[82]:= \mathbf{m} = \mathbf{1}$ Out[82]= 1 $\ln[83]:= \boldsymbol{\omega} = \mathbf{1}$ Out[83]= 1 $\ln[84]:= \boldsymbol{\beta} = \mathbf{1}$ Out[84]= 1 $\ln[85]:= \boldsymbol{\tilde{h}} = \mathbf{1}$ Out[85]= 1 $\ln[86]:= \boldsymbol{\lambda} = \left(\frac{(2\pi \, \tilde{h}^2 \, \boldsymbol{\beta})}{(\mathbf{m} \, \mathbf{i})}\right)^{0.5}$ Out[86]:= 2.50663 $PolyLog\left[\frac{3}{2}, \frac{E}{2}\right]$

$$\ln[98]:= n[r_, \mu0_] := \frac{\operatorname{PolyLog}\left[\frac{3}{2}, \frac{\operatorname{Exp}\left[\mu0-\frac{1}{2}m\omega^{2}r^{2}\right]}{\beta}\right]}{\lambda^{3}}$$

 $ln[88]:= Plot[\mu[r, 0], \{r, -14, 14\}, AxesLabel \rightarrow \{"Trap Radius r", "Chemical Potential \mu"\}]$



set μ 0=0, assuming BEC at the center of the trap

In[122]:= Needs["PlotLegends`"]



when BEC is not forming

$$\begin{split} & \ln[132]:= \ b = Plot[\{n[r, 0], n[r, -0.1], n[r, -0.5], n[r, -1]\}, \\ & \{r, -5, 5\}, \ PlotStyle \rightarrow \{Thick, \ Dotted, \ Dashed, \ Thin\}, \ PlotRange \rightarrow \ All, \\ & AxesLabel \rightarrow \{"r", "n"\}, \ PlotLegend \rightarrow \{"\mu_0=0", \ "\mu_0=-0.1", \ "\mu_0=-0.5", \ "\mu_0=-1"\}] \end{split}$$



Hartree-Fock Approximation

```
In[146]:= (*--integral----*)
         1 / Gamma[3 / 2.] Integrate[x^(1 / 2) / (Exp[x - \alpha] - 1), {x, 0, Infinity}]
Out[146]= 1. PolyLog \begin{bmatrix} 3 \\ -2 \end{bmatrix}, e^{\alpha}
\ln[147] = \text{NIdenF}[\beta_{,\mu_{}}] := 1 / (2 \operatorname{Pi} \beta)^{(3/2)} \operatorname{PolyLog}\left[\frac{3}{2}, e^{\beta \mu}\right]
In[148]:= NIdenF[1, -1.]
Out[148]= 0.0272033
In[149]:= (*----Ideal gas---*)
\ln[150] = \text{NCI}[\beta_{-}] := \text{NIntegrate}\left[1 / (2 \operatorname{Pi} \beta)^{(3/2)} \operatorname{PolyLog}\left[\frac{3}{2}, e^{\beta \mu}\right] (0 - \mu)^{(0.5)}, \{\mu, -\text{Infinity}, 0\}\right]
In[151]:= NCI[1]
Out[151]= 0.0676395
In[152]:= (*---HF-P-Y-Y----*)
ln[153] = HFden[\beta_, \mu_, U_] := FixedPointList
            1 / (2 \operatorname{Pi} \beta)^{(3/2)} \operatorname{PolyLog} \left[ \frac{3}{2}, e^{\beta (\mu - 2 \pm 0)} \right] \&, 0, \operatorname{SameTest} \rightarrow (\operatorname{Abs} [\pm 1 - \pm 2] < 1^{*} - 6 \&) \right]
In[154]:= HFden[0.1, -1, 1]
Out[154]= {0, 3.28559, 1.1563, 2.09741, 1.58334, 1.83697, 1.70498, 1.77185, 1.7375,
           1.75502, 1.74605, 1.75063, 1.74829, 1.74949, 1.74888, 1.74919, 1.74903,
           1.74911, 1.74907, 1.74909, 1.74908, 1.74908, 1.74908, 1.74908, 1.74908}
\ln[155] = \text{HFdenF}[\beta_{\mu}, \mu_{\mu}, U_{\mu}] := \text{FindRoot}\left[n = 1 / (2 \text{Pi}\beta)^{(3/2)} \text{PolyLog}\left[\frac{3}{2}, e^{\beta(\mu-2 n U)}\right], \{n, 0.5\}\right]
In[156]:= HFdenF[0.1, -1, 1]
Out[156]= \{n \rightarrow 1.74908\}
In[157]:= den[β_, U_] :=
           Table [Re@n /. HFdenF[\beta, \mu, U], {\mu, -200, 2U / (2. Pi\beta) ^ (3 / 2) PolyLog [\frac{3}{2}, 1], 0.05}]
\ln[158]:= \mu \text{value}[\beta_{, U_{}}] := \text{Table}\left[\mu, \left\{\mu, -200, 2U/(2. \text{Pi}\beta)^{(3/2)} \text{PolyLog}\left[\frac{3}{2}, 1\right], 0.05\right\}\right]
\ln[159]:= data[\beta, U] := Transpose[\{\mu value[\beta, U], den[\beta, U]\}]
In[160]:= data[0.1, 1];
In[161]:= FunDen[$, U] := Interpolation[data[$, U]]
In[162]:= FunDen[0.1, 1][-10]
In[163]:= FunDenF[$, U_] := FunctionInterpolation
            Re@n /. HFdenF[\beta, \mu, U], {\mu, -200, 2U / (2. Pi\beta) ^ (3 / 2) PolyLog[\frac{3 \cdot}{2}, 1]}]
```

```
 \begin{bmatrix} \ln[164] = \text{NCHF}[\beta_{-}, U_{-}] := \text{NIntegrate}[\text{FunDen}[\beta, U][\mu] \left( 2 \text{ U} / (2 \text{ Pi} \beta)^{(3/2)} \text{ PolyLog}[\frac{3}{2}, 1] - \mu \right)^{(0.5)}, \\ \left\{ \mu, -200, 2 \text{ U} / (2 \text{ Pi} \beta)^{(3/2)} \text{ PolyLog}[\frac{3}{2}, 1] \right\} \end{bmatrix} 
 \begin{bmatrix} \ln[165] = \text{NCHF}[0.1, 1] \\ \text{Out[165] = 154.608} \\ \\ \ln[166] = \text{NCHFF}[\beta_{-}, U_{-}] := \\ \text{NIntegrate}[\text{FunDenF}[\beta, U][\mu] \left( 2 \text{ U} / (2 \text{ Pi} \beta)^{(3/2)} \text{ PolyLog}[\frac{3}{2}, 1] - \mu \right)^{(0.5)}, \\ \left\{ \mu, -200, 2 \text{ U} / (2 \text{ Pi} \beta)^{(3/2)} \text{ PolyLog}[\frac{3}{2}, 1] \right\} \end{bmatrix} 
 Out[167] = 154.608 \\ \\ \ln[170] = \text{HFP} = \text{Plot}[\{\text{NCHFF}[1/T, 0.5] / \text{NCI}[1/T], \text{NCHFF}[1/T, 1] / \text{NCI}[1/T], \\ \end{bmatrix}
```

```
\begin{aligned} & \text{NCHFF[1/T, 3] / NCI[1/T], NCHFF[1/T, 5] / NCI[1/T]}, \{\text{T, 0.5, 3}, \text{Frame} \rightarrow \text{True}, \\ & \text{FrameLabel} \rightarrow \{\{\text{"N/N_0", ""}\}, \{\text{"k}_{\text{B}}\text{T}/\epsilon_{\text{F}}\text{", ""}\}\}, \text{PlotRange} \rightarrow \{\{0.5, 3\}, \{0.8, 5.5\}\}, \\ & \text{PlotStyle} \rightarrow \{\text{Directive[Thick], Directive[Dashed, Thick], Directive[Dotted, Thin],} \\ & \text{Directive[Dashed, Thick]}\}, \text{PlotLegend} \rightarrow \{\text{"U=0.5", "U=1", "U=3", "U=5"}\} \end{aligned}
```



T-matrix Approximation

```
(*--integral----*)
1 / Gamma[3 / 2.] Integrate[x^(1 / 2) / (Exp[x - \alpha] - 1), {x, 0, Infinity}]
1. PolyLog \left[\frac{3}{2}, e^{\alpha}\right]
NIdenF[\beta_{-}, \mu_{-}] := 1 / (2 Pi \beta) ^ (3 / 2) PolyLog\left[\frac{3}{2}, e^{\beta \mu}\right]
NIdenF[1, -1.]
0.0272033
(*----Ideal gas---*)
\operatorname{NCI}[\beta_{-}] := \operatorname{NIntegrate}\left[1 / (2\operatorname{Pi}\beta)^{(3/2)} \operatorname{PolyLog}\left[\frac{3}{2}, e^{\beta \mu}\right] (0 - \mu)^{(0.5)}, \{\mu, -\operatorname{Infinity}, 0\}\right]
NCI[1]
0.0676395
(*----T matrix approach-----*)
alpha[\beta_{,\beta}d_{]} := \beta / Sqrt[Pi] (1 / (2 Pi \beta)^{(3 / 2)})
   NIntegrate[(1 / (x - \beta d) Coth[(x - \beta d) / 2] - 1 / x) Sqrt[x], \{x, 0, Infinity\}]
alpha[1, -0.1]
0.1678
Plot[alpha[1, x], {x, -10, 0}]
-10
                -8
                                -6
                                                -4
                                                               -2
                                                                            -0.1
                                                                            -0.2
                                                                            -0.3
findmu[\betad_, \beta_, U_] :=
   \left(\beta d + 2 U / (1 + alpha[\beta, \beta d] U) (\beta / (2 Pi \beta)^{(3/2)}) PolyLog[\frac{3}{2}, e^{\beta d}]\right) / \beta
findmu[-20, 0.1, 1]
-200.
```



```
INTDENTM[$\beta_$, U_] := Interpolation[dataTM[$, U]]
```

INTDENTM[1, 1][0.]

0.165869

(*----comparison of density from three theories---*)

```
(*--ideal gas--*)
```

 $\begin{aligned} & \text{IdealDen = Plot[NIdenF[1, \eta], \{\eta, -4, 0\}, Frame \rightarrow \text{True, FrameLabel} \rightarrow \{\{"n", ""\}, \{"\eta", ""\}\}, \\ & \text{PlotRange} \rightarrow \{\{-4, 0\}, \{0., 0.17\}\}, \text{PlotStyle} \rightarrow \text{Directive[Brown, Thick]} \end{aligned}$



```
IdealDenPR =
```

```
\begin{aligned} & \texttt{Plot[NIdenF[1, 0 - 1 r^2], \{r, -2, 2\}, Frame \rightarrow \texttt{True, FrameLabel} \rightarrow \{\{\texttt{"n", ""}\}, \{\texttt{"r", ""}\}\}, \\ & \texttt{PlotRange} \rightarrow \{\{-2, 2\}, \{0., 0.17\}\}, \texttt{LabelStyle} \rightarrow \texttt{Directive[Black, Bold, Large],} \\ & \texttt{PlotStyle} \rightarrow \texttt{Directive[Brown, Thick], ImageSize} \rightarrow 500] \end{aligned}
```



(*---T matrix---*)

TMden1 =

Plot[INTDENTM[1, 1][η], { η , -4, 0}, Frame → True, FrameLabel → {{"n", ""}, {" η ", ""}}, PlotRange → {{-4, 0}, {0., 0.17}}, PlotStyle → Directive[Red, Thick]]



```
TMden1PR = Plot[INTDENTM[1, 1][0 - r^2],
    {r, -2, 2}, Frame → True, FrameLabel → {{"n", ""}, {"r", ""}},
    PlotRange → {{-2, 2}, {0., 0.17}}, PlotStyle → Directive[Red, Thick]]
```



TMden2 =

 $\begin{aligned} &\texttt{Plot[INTDENTM[1, 2][\eta], \{\eta, -4, 0\}, Frame \rightarrow True, FrameLabel \rightarrow \{\{"n", ""\}, \{"\eta", ""\}\}, \\ &\texttt{PlotRange} \rightarrow \{\{-4, 0\}, \{0., 0.17\}\}, \texttt{PlotStyle} \rightarrow \texttt{Directive[Red, Thick]]} \end{aligned}$



TMden2PR = Plot[INTDENTM[1, 2][0 - r^2],
 {r, -2, 2}, Frame → True, FrameLabel → {{"n", ""}, {"r", ""}},
 PlotRange → {{-2, 2}, {0., 0.17}}, PlotStyle → Directive[Red, Thin]]



```
UNden1 =
     Plot[Pnumber[\eta, 1], \{\eta, -8, -2.5\}, Frame \rightarrow True, FrameLabel \rightarrow \{\{"n", ""\}, \{"\eta", ""\}\}, \{n_{1}, n_{2}, n_{3}, n_{4}, n_{5}, n_{5
           PlotRange \rightarrow \{\{-8, -2.3\}, \{0., 0.17\}\}, PlotStyle \rightarrow Directive[Blue, Thick]\}
 UNden1PR = Plot[Pnumber[-2.6-r^2, 1],
            \label{eq:rescaled} \texttt{\{r, -Sqrt[8.], Sqrt[8.]\}, Frame \rightarrow True, FrameLabel \rightarrow \{\{\texttt{"n", ""}\}, \{\texttt{"}\eta\texttt{", ""}\}\}, \texttt{}
           PlotRange → {{-Sqrt[8.], Sqrt[8.]}, {0., 0.17}}, PlotStyle → Directive[Blue, Thick]]
             0.15
             0.10
   ц
             0.05
             0.00
                                                       -2
                                                                                                                                                                                                                2
                                                                                             ^{-1}
                                                                                                                                    0
                                                                                                                                                                          1
                                                                                                                                    η
  (*--HFT---*)
HFTden1 = Plot \left[ FunDenF[1, 1][\eta], \left\{ \eta, -8, 2 \times 1 / (2Pi1)^{(3/2)} PolyLog \left[ \frac{3}{2}, 1 \right] \right\},
            \texttt{Frame} \rightarrow \texttt{True}, \texttt{FrameLabel} \rightarrow \{\{\texttt{"n", ""}\}, \{\texttt{"}\eta\texttt{", ""}\}\},\
           \operatorname{PlotRange} \rightarrow \left\{ \left\{ -8, 2 \times 1 / (2 \operatorname{Pi1})^{(3/2)} \operatorname{PolyLog}\left[\frac{3}{2}, 1\right] \right\}, \left\{ 0., 0.17 \right\} \right\},
           PlotStyle \rightarrow Directive[Black, Thick]
             0.15
             0.10
```

q

0.05

0.00 L

-6

-4

η

-2

 $\begin{aligned} & \texttt{HFTden1PR} = \texttt{Plot}\Big[\texttt{FunDenF[1, 1]} \Big[2 \times 1 / (2 \texttt{Pi1})^{(3/2)} \texttt{PolyLog} \Big[\frac{3}{2}, 1 \Big] - \texttt{r}^2 \Big], \\ & \{\texttt{r, -Sqrt[8.], Sqrt[8.]}\}, \texttt{Frame} \rightarrow \texttt{True, FrameLabel} \rightarrow \{\{\texttt{"n", ""}\}, \{\texttt{"r", ""}\}\}, \\ & \texttt{PlotRange} \rightarrow \{\{\texttt{-Sqrt[8.], Sqrt[8.]}\}, \{\texttt{0., 0.17}\}\}, \texttt{PlotStyle} \rightarrow \texttt{Directive[Black, Thick]} \Big] \end{aligned}$



SGvsHF = Show[IdealDenPR, HFTden1PR, TMden1PR]



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