



Bose–Einstein condensation of an imperfect Bose gas using cluster expansion

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Abstract. Bose–Einstein condensations (BEC) for an ideal Bose gas and an imperfect Bose gas are presented using cluster expansion method by using a new generating function obtained by Ushcats. The saturation density is calculated from the known values of virial coefficients for both ideal and uniform hard-sphere imperfect Bose gas. The values of saturation densities are found for some experimentally observed Bose–Einstein condensates and the fractional shift in the saturation densities are also calculated using this method, which are found to be positive.

Keywords. Cluster expansion; equation of state; Bose–Einstein condensation; radius of convergence.

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1. Introduction

The properties of ideal bosons and Bose–Einstein condensation (BEC) were introduced by Bose [1] and Einstein [2]. With the advancement in the field of atomic trapping systems and laser cooling technique, the first experimental production of BEC in rubidium and sodium [3,4] was observed in 1995. These developments provided the motivation for the theoretical analysis of BEC of ideal and interacting bosons. Quantum mechanically there is an attraction between bosons which can be explained by the symmetric nature of spatial wave functions. Apart from this attractive spatial correlation, if we consider the real collection of bosons like vapours of rubidium or sodium atoms, they may possess statistical mutual interaction which can be attractive or repulsive with separation between particles, like Lennard–Jones potential or hard-core potential. Thus, if we consider pair interaction among bosons, it affects the equation of state, saturation density for condensation and other thermodynamic properties.

The statistical mechanics of interacting systems can be studied using Mayer’s cluster expansion [5]. Due to the attractive spatial correlation and pair interaction of bosons, there is a formation of clusters of particles satisfying the condition $\sum_l l m_l = N$ with m_l clusters of l particles each. When density increases and approaches

saturation density, this clustering produces condensation which is purely quantum mechanical. The macroscopic increase in the population of non-interacting bosons in the lowest energy quantum mechanical state below a particular critical temperature is called BEC [2–7]. The theoretical study of interacting Bose system was done by Bogoliubov [8]. There are a large number of legendary works on the virial series of ideal Bose gas and the phase transition parameters [9–11]. Recently, BEC of ideal bosons and the thermodynamic properties are studied using cluster expansion and also with a new modified generating function for partition function [12,13]. But when considering the case of interacting bosons with any type of potential, the calculation of virial coefficient is very difficult. The quantum mechanical l th cluster integral involves either the wave functions or energy levels of l interacting particles, so that to evaluate it explicitly we would have to solve the general quantum mechanical l body problem. Thus, only for the second virial coefficient, we have a volume-independent formula involving the scattering phase shifts of the two-body system [14]. But using pseudopotential method for hard-sphere interaction, Huang and Yang [14], Huang *et al* [15] and Yang and Lee *et al* [16] calculated the virial coefficients of an imperfect hard-sphere Bose gas. But the effect of imperfections to the BEC was not discussed. In order to get the equation of state, we can use

Mayer’s cluster expansion [11]. But this method has a limitation to explain condensation due to the restrictive condition on the particle number density ρ as

$$\sum_l l\beta_l \rho^l < 1 \tag{1}$$

which is applicable only in the low-density region. An equation of state not limited by condition (1) was introduced by Ushcats [17–19] which was later modified by Bannur [20] using a new generating function. In this paper, we analyse the theory of BEC and its saturation density values for an ideal collection of bosons and also for the case of imperfect bosons with hard-sphere interaction.

2. New generating function for partition function

In the case of real gases, the constituent particles interact by virtue of a two-particle potential U_{ij} . Considering a collection of bosons interacting through some statistical potential, the Hamiltonian can be represented as [5,6,11]

$$\sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i,j,i < j} U_{ij}(|\vec{r}_i - \vec{r}_j|), \tag{2}$$

where p is the momentum, m is the mass of particles, and U_{ij} is the potential that depends on the distance $|\vec{r}_i - \vec{r}_j|$ between the particles. With the above Hamiltonian, the partition function is given by

$$Q_N(V, T) = \sum_{m_l} \left[\prod_{l=1}^N \left(\frac{b_l V}{\lambda^3} \right)^{m_l} \frac{1}{m_l!} \right], \tag{3}$$

where b_l are the cluster integrals and λ is the thermal wavelength. In terms of cluster integrals, the virial coefficients are [5–7]: $B_1 = b_1 = 1$, $B_2 = -b_2$, $B_3 = 4b_2^2 - 2b_3$, $B_4 = -20b_2^3 + 18b_2b_3 - 3b_4$ etc. The virial coefficients are related to the irreducible cluster integrals β_k as

$$B_{k+1} = \frac{-k}{k+1} \beta_k. \tag{4}$$

In terms of the irreducible cluster integrals, the new generating function for partition function is given by [17–20]

$$\begin{aligned} F(y) &= \left(1 - \sum_k k\beta_k y^k \right) e^{N \left[\frac{vy}{\lambda^3} (1 - \sum_k \frac{k}{k+1} \beta_k y^k) + \sum_k \beta_k y^k \right]} \\ &= \sum_n a_n y^n. \end{aligned} \tag{5}$$

In the complex plane y , the N th coefficient of the expansion will give the N particle partition function given by

$$a_N = Q_N = \frac{1}{2\pi i} \oint \frac{F(y) dy}{y^{N+1}}. \tag{6}$$

With the values of irreducible cluster integrals (β_k), the equation of state can be written as [5–7]

$$\frac{PV}{NkT} = 1 - \sum_{k=1}^{\infty} \frac{k}{k+1} \beta_k (\rho \lambda^3)^k, \tag{7}$$

where $\rho = N/V$ is the number density of particles. Using the Ushcats formalism [16–18], the equation of state becomes

$$\frac{PV}{NkT} = \left[\frac{1 - \sum_{k \geq 1} [k/(k+1)] \beta_k (\rho/Z)^k}{Z} \right], \tag{8}$$

where Z is a function of the number density and is taken as one of the roots of the equation

$$Z = 1 + (Z - 1) \sum_{k \geq 1} \frac{k\beta_k \rho^k}{Z^k}. \tag{9}$$

When the root of the equation is 1, the equation of state retains the Mayer’s virial form at the high-temperature low-density region and in the high-density low-temperature region $Z = \rho/\rho_0$, where ρ_0 is the saturation density [17,18]. So, for high-temperature and low-density region, $\rho < \rho_0$

$$\frac{P}{kT} = \rho \left[1 - \sum_{k=1}^{\infty} \frac{k}{k+1} \beta_k (\rho \lambda^3)^k \right] \tag{10}$$

and for high-density region, $\rho > \rho_0$

$$\frac{P}{kT} = (\rho_0 \lambda^3) \left[1 - \sum_{k=1}^{\infty} \frac{k}{k+1} \beta_k (\rho_0 \lambda^3)^k \right], \tag{11}$$

where $\rho_0 \lambda^3$ is the minimum real positive root of the equation

$$\sum_k k\beta_k (\rho_0 \lambda^3)^k = 1 \tag{12}$$

which can be considered as the saturation density for condensation. Thus, we have the virial equation in the high- and low-density regime for a collection of particles which are not restricted by condition (1). The same equation of state and the condensation condition can be found from the generating function given by eq. (5) and by using Mayer’s convergence method, which is based on Cauchy Hadamard theorem, where the coefficient of the series is related to the radius of convergence [5,20]. The application of Mayer’s convergence method

using the generating functions provided by Mayer and Ushcats was used to find the thermodynamic properties of ideal bosons at condensation [12,13].

3. Condensation of ideal bosons using cluster expansion

In order to find the high-density equation of state for the Bose system and to find the BEC, the irreducible cluster coefficients (β_k) up to the order 14 are obtained. Using the free particle propagator theory [21] and the cluster expansion theory, the values of the cluster integral for ideal collection of bosons confined in a large volume is given by

$$b_l = \frac{(l-1)!}{l!h^3} \int_0^\infty 4\pi p^2 e^{-l\beta p^2/2m} dp. \tag{13}$$

Integrating we get

$$b_l = \frac{1}{\lambda^3 l^{5/2}}. \tag{14}$$

In order to make the variables in the equation of state dimensionless, they are scaled by λ^3 . Thus, the temperature dependence of b_l has been combined in variables like pressure and number density. Then for bosons b_l are given by [5–10,21]

$$b_l = \frac{1}{l^{5/2}}. \tag{15}$$

Using the relationship between cluster integrals (b_l) and the virial coefficients (B_k), the values of irreducible cluster integrals are calculated using the equation and the values are shown in table 1.

$$\beta_k = \frac{-(k+1)}{k} B_{k+1}. \tag{16}$$

As the remaining values are so small and negligible, they are not considered here. Using these values, ρ_0 at a particular temperature can be calculated using eq. (11) as

$$\beta_1(\rho_0\lambda^3)^1 + 2\beta_2(\rho_0\lambda^3)^2 + 3\beta_3(\rho_0\lambda^3)^3 + \dots = 1. \tag{17}$$

Substituting the values of β_k , we get

$$\rho_0\lambda^3 = 2.6123757 \tag{18}$$

which is the value of Riemann zeta function $\zeta(3/2)$. This shows that saturation density obtained by this method exactly matches with the quantum statistical calculations using Bose–Einstein distribution functions. Then, the high-density equation of state can be written as

Table 1. Values of irreducible cluster integrals.

β_1	$3.535533905932738 \times 10^{-1}$
β_2	$4.950089729875255 \times 10^{-3}$
β_3	$1.483857712887233 \times 10^{-4}$
β_4	$4.425630118996707 \times 10^{-6}$
β_5	$1.006361644748311 \times 10^{-7}$
β_6	$4.272405418573282 \times 10^{-10}$
β_7	$-1.174926531930948 \times 10^{-10}$
β_8	$-7.936985074019214 \times 10^{-12}$
β_9	$-2.984404389769838 \times 10^{-13}$
β_{10}	$-4.462901839886734 \times 10^{-15}$
β_{11}	$3.051320702281767 \times 10^{-16}$
β_{12}	$3.074464622622820 \times 10^{-17}$
β_{13}	$1.506932077279162 \times 10^{-18}$
β_{14}	$3.889612806544511 \times 10^{-20}$

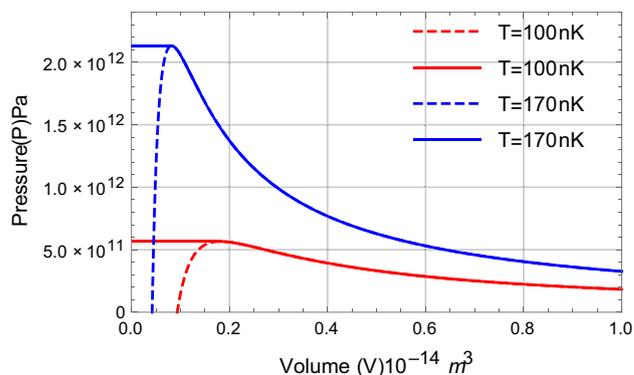


Figure 1. Isotherms for bosons using eqs (8) and (9).

$$\frac{P}{kT} = \rho_0 \left[1 - \left(\frac{1}{2} \beta_1 (\rho_0 \lambda^3)^1 + \frac{2}{3} \beta_2 (\rho_0 \lambda^3)^2 + \dots \right) \right]. \tag{19}$$

The isotherms are plotted using this equation of state. Figure 1 shows isotherms using the new equation of state. The nature of the isotherms in figure 1 clearly exhibits a phase transition by showing the independence of volume on pressure in the high-density region, as indicated by the horizontal part of the isotherm.

4. High-density equation of state and condensation of imperfect bosons

The analysis of imperfect Bose gas for calculating the virial coefficients are done in [14–16] using hard-core interaction between the particles. The quantum mechanical many-body problem in terms of solutions

Table 2. Comparison of saturation density and fractional shift of imperfect Bose gas with experiment.

Material	T_c (nK)	a (nm)	$\rho_0^i \lambda^3$	ρ_0^i / cm^3	ρ_0^i / cm^3 from experiment	$\Delta\rho / \rho_0$
Rb-87	160	$104a_0$	2.933367	2.739815×10^{13}	4.0×10^{13}	0.122874
Na-23	2000	$56.6a_0$	2.921708	1.496843×10^{14}	1.5×10^{14}	0.118411
Sr-84	420	$122.7a_0$	3.153590	1.085177×10^{14}	1.2×10^{14}	0.207174
Ce-133	46	$1200a_0$	3.127140	0.777077×10^{13}	1.3×10^{13}	0.197049

of two-body problem was discussed. Let the Hamiltonian for an imperfect Bose system is given by

$$H = H_0 + H', \quad (20)$$

where H_0 is the kinetic contribution and H' is the pseudopotential or interaction Hamiltonian which can be treated as small perturbation and account up to the hard-sphere contribution of a^2 . In this analysis, the hard-sphere diameter (a) enters into the calculation as a scattering length of the interaction potential [14,15]. The virial equation derived for the imperfect Bose gas in [15] is given by

$$\frac{PV}{NkT} = 1 + \sum_{l=2}^{\infty} B_l \left(\frac{\lambda^3 N}{V} \right)^{l-1}. \quad (21)$$

The virial coefficients B_l can be decomposed to

$$B_l = B_l^0 + B_l', \quad (22)$$

where B_l^0 are independent of scattering length a and are the virial coefficients for ideal bosons. B_l' are the virial coefficients which include the imperfections due to the interaction [15]. Substituting the values of B_l' , the virial coefficients becomes

$$B_2 = \left[\frac{-1}{4\sqrt{2}} \right] + \left[2 \left(\frac{a}{\lambda} \right) - \frac{44\pi^2}{3} \left(\frac{a}{\lambda} \right)^5 \right] \quad (23)$$

$$B_3 = \left[- \left(\frac{2}{9\sqrt{3}} - \frac{1}{9} \right) \right] + \left[-4 \left(\frac{a}{\lambda} \right)^2 \right] \quad (24)$$

$$B_4 = \left[- \left(\frac{3}{32} + \frac{5}{32\sqrt{2}} - \frac{1}{2\sqrt{6}} \right) \right] + \left[\frac{67\sqrt{2}}{6} \left(\frac{a}{\lambda} \right)^2 \right]. \quad (25)$$

Using the pseudopotential Hamiltonian, the first-order and second-order corrections to the partition function are obtained. With the values of cluster integrals and virial coefficients, the ground-state pressure in terms of scattering length (a) can be found [15,16], and is given by

$$P_0 = \frac{2\pi a \hbar^2 \rho^2}{m} \left[1 + \frac{64}{5\sqrt{\pi}} (\rho a^3)^{1/2} + \dots \right]. \quad (26)$$

This equation matches with the ground-state pressure obtained by the method of field quantisation [7]. In order to study BEC using the values of virial coefficients, the irreducible cluster integrals β_k up to the order three, are found using the conversion relation (4). Substituting these values in eq. (11) we can write

$$\begin{aligned} & -2 \left[\frac{-1}{4\sqrt{2}} + 2 \left(\frac{a}{\lambda} \right) - \frac{44\pi^2}{3} \left(\frac{a}{\lambda} \right)^5 \right] (\rho_0^i \lambda^3)^1 \\ & + \frac{-6}{2} \left[- \left(\frac{2}{9\sqrt{3}} - \frac{1}{9} \right) + -4 \left(\frac{a}{\lambda} \right)^2 \right] (\rho_0^i \lambda^3)^2 \\ & + \frac{-12}{3} \left[- \left(\frac{3}{32} + \frac{5}{32\sqrt{2}} - \frac{1}{2\sqrt{6}} \right) \right. \\ & \left. + \frac{67\sqrt{2}}{6} \left(\frac{a}{\lambda} \right)^2 \right] (\rho_0^i \lambda^3)^3 \\ & = 1. \end{aligned} \quad (27)$$

Thus, we can calculate the value of the saturation density (ρ_0^i) for the condensation of an imperfect Bose gas by knowing the values of s -wave scattering length (a) and thermal wavelength (λ). The s -wave scattering lengths for different materials are calculated experimentally [22–28]. With the experimental observation of BEC in different atomic gases, the values of transition temperature and number density are available, so that we can make calculations if we know any of these values. By considering critical temperature (T_c) and a in terms of Bohr radius $a_0 = 0.52917 \text{ \AA}$ for different BEC samples [3,4,28–30], the saturation densities are calculated for the imperfect Bose gases and are shown in table 2. It is interesting to note that, this method provides a new way to find saturation density for samples with both positive and negative scattering lengths. The fractional shift in the saturation density can be found from the equation

$$\frac{\Delta\rho}{\rho_0} = \frac{\rho_0^i - \rho_0}{\rho_0}. \quad (28)$$

The calculated values are shown in table 2. It is seen that the fractional changes in values of ρ_0 are positive for atoms with positive a , and hence the fractional change in T_c will be negative. This observation is correct according to the findings of Fetter and Walecka [31], Girardeau [32] and also by Tayoda [33]. Huang [34] obtained the

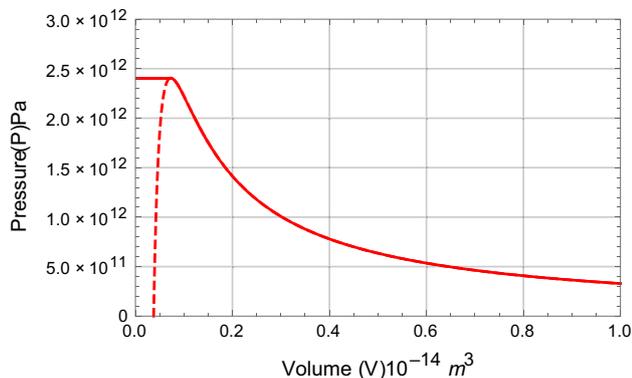


Figure 2. Isotherm for imperfect rubidium-87 gas. Dashed line shows Mayer's relation and solid line is for this work for 170 nK temperature.

fractional change in T_c the same as Tayoda, but with opposite sign. There are works which give negative fractional change in ρ_0 , so that the fractional change in T_c is positive [34–36]. Thus, there is no consensus on how the values of a and hence imperfections depend on fractional shift in ρ_0 and T_c [34].

5. Earlier experiments and correlation with our results

BEC was first obtained in the vapour of rubidium-87 in 1995 [3], and in the case of rubidium, atoms are cooled to a temperature up to 10 nK and the particle number density was $2.5 \times 10^{12}/\text{cm}^3$. The condensate fraction first observed at 170 nK and the value of transition temperature changes according to the variation of number density. Similar experiments were conducted by different research groups and BEC was produced in rubidium-87 and in different materials like alkali metals, alkaline earth metals etc. Examples are sodium-23, lithium-7, cesium-133 and strontium-84 [28–30]. Using experimental details like number density of particles ($2.5 \times 10^{12}/\text{cm}^3$) and the number of particles (2×10^4) in rubidium, we here present the plots of equation of state calculated using the Ushcats method. The graph using Mayer's method are shown in dotted lines (figure 2).

The saturation densities at the onset of BEC are calculated for the above imperfect Bose gases and are compared with the experimental values and are given in table 2, which show a close matching.

6. Discussion and conclusions

The equation of states for an ideal collection of bosons and hard-sphere interacting bosons are found using Mayer's cluster expansion with a new generating function provided by Ushcats. The isotherms are drawn for

both ideal gas and imperfect Bose gas, and the nature of these graphs shows the character of a first-order phase transition. The values of ρ_0 at condensation are also calculated. For ideal bosons, ρ_0 exactly matches with quantum statistical calculations. For imperfect bosons, ρ_0 depends upon a . The values of ρ_0 for different experimentally observed condensates are compared with our calculations and the fractional shift in the values of ρ_0 are calculated. This method provides an excellent way of studying BEC in ideal bosons and imperfect Bose systems with hard-sphere interaction.

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