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Quantum Depletion in Pairs and Thermal Depletion

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ABSTRACT

For ultra-cold atoms, thermal depletion creates the BEC from the normal component, whereas quantum depletion ejects atoms from the BEC via interactions. Strong interactions in the Zero-Momentum State promote coherent quantum state transitions. As a result of quantum fluctuations, the particles will leave the ZMS (k=0) and occupy states above ZMS (k>0). This is quantum depletion. Quasi-particles with k>0 are described by the Hamiltonian using the pairs of creation and annihilation operators which correspond to the excitations of pairs of particles. Using Bogoliubov theory, it can be shown that it's possible for particles to leave the ZMS in pairs and move to states with k>0. If ZMS exists at finite temperature, there will be thermal depletion.

***Keywords*:** Zero Momentum State, Quantum depletion, Thermal depletion, Pair depletion

1. INTRODUCTION

Real-life (physical) or macroscopic systems are made up of thousands of millions of elementary components, which ultimately interact with each other via forces of all kinds. These components have been classified broadly as bosonic (particles with integer spin) and fermionic (particles with half-integral spin) and each is described by a specific statistic from the numerous quantum statistics [1]. Since these components (bosons and fermions) do not exist independently of each other, it follows naturally also that they do not behave independently but instead display an intrinsically many-body behavior, regardless of whether it is interactive or non-interactive. At sufficiently low temperatures, the atomic de Broglie waves of neighboring

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atoms in an assembly start overlapping, giving rise to the quantum statistical effects that discriminate between fermions and bosons (depending on their atomic spin). The Pauli Exclusion Principle prohibits any two fermions from occupying exactly the same quantum state. On the other hand, bosons are not limited in this way, and an arbitrary number of bosons can occupy the same quantum state.

A Bose gas is a quantum system consisting of a large number of particles, e.g., atoms or molecules, obeying the so-called Bose-Einstein statistics. Interactions in quantum mechanics can have several origins, among them are conservative external forces, spin-spin or spin-orbit coupling and matter-light interaction. In general, interaction and quantum statistics are responsible for collective behaviors and underlie original phenomena and fascinating quantum phases, such as superconductivity and superfluidity. Bose gases are very interesting in the field of quantum mechanics because of their behavior at extremely low-temperatures. Theoretical and experimental investigations have shown that bosons at proper temperature and particle density can suddenly populate the collection's ground state in observable large numbers (in the container they are in).

This macroscopic occupation of the ground state is a phase transition and takes place at critical temperature, T_c and/or number density, n_c. This quantum phenomenon where a large number of bosons simultaneously occupy the ground state of a system was given the name 'Bose-Einstein Condensation' (BEC). For homogeneous many-body systems, the condensation occurs into a single momentum component, i.e., a state where the wave vector $\vec{\boldsymbol{k}} = 0$ in the condensate rest frame. This state, i.e., $\vec{\boldsymbol{k}} = 0$, is usually referred to as Zero-Momentum State (ZMS). The BEC was predicted theoretically by Satyendra Nath Bose and Albert Einstein in the early 20th century, and verified experimentally 70 years later in 1995 by the Nobel laureates in Physics namely Cornell, Ketterle and Wieman [2, 3]. The experimental verifications have been realized in different atoms, such as ^{4}He [4], ^{39}K [5], ^{87}Rb [1], ^{7}Li [6], ^{22}Na [7], and also in photons, quasi-particles and molecules [8]. Alkali gases (^{7}Li, ^{22}Na, ^{39}K, and ^{87}Rb) have been proved to be excellent for studying BEC because, experimentally, they can be laser-cooled to temperatures in the μK.

In quantum systems, interesting many-body phenomena becomes apparent from the interplay between quantum fluctuations and interactions. Quantum depletion is an emblematic example of such an effect, and usually occur in simple many-body systems, e.g., a gas of interacting bosons at zero temperature [9]. For ideal bosonic gas (i.e., in the absence of interactions), the ground state consists of all particles occupying the same single-particle ground state. The quantum depletion can be expressed quantitatively by considering a system with total particle density $\rho(0) = n = n_c + \delta n$, which is the sum of condensate density, n_c and non-condensed density δn.

The condensate fraction is $n_c/n = 1 - \delta n/n$. Within Bogoliubov theory, the existence of a finite non-condensed fraction $\delta n/n$ at temperature T = 0 is called 'quantum depletion', and it arises from the quantum fluctuations around the mean-filed approximation to the true condensate [10].

The fraction of the atoms in the quantum depletion state increases with the strength of interparticle interactions and with the density. The fraction is usually 90% in liquid ^{4}He, but in ultracold gases, which are characterized by small densities, has smaller fraction of less than 1% of the total population. However, at nonzero temperature, the thermal fluctuation impacts energy to some condensate state bosons, which in turn are promoted to the single-particle states thereby increasing their population.

2. THEORETICAL DERIVATIONS

(i) Quantum Depletion in Pairs from the Condensed State (ZMS) or Superfluid State

Quantum depletion from the condensed state is a result of strong interactions among the particles in the condensate. Due to inter particle interactions, the particles acquire enough energy so as to shift to the single- particle state above the ZMS ($k = 0$) i.e, the particles shift to single particle state with $k \neq 0$ ($k > 0$). It is quite possible that instead of single particles shifting from ZMS to the states with $k > 0$, pairs of particles may shift to the states with $k > 0$. It should be understood that, in general, in the ZMS, the particles interact in pairs.

Now if N is the total number of particles in the boson assembly, then we can write,

$$\mathrm{N} = \mathrm{N}_0 + \mathrm{N}_1 + \mathrm{N}_2 \tag{1}$$

where the number of particles in the Zero-Momentum State is, N_0. N_1 is the single particle quantum depletion number of particles and N_2 is the number of pairs due quantum depletion.

$\in_2$ $--\circ\longleftrightarrow\circ---\circ\longleftrightarrow\circ--\circ\longleftrightarrow\circ--$ (j)*pairs of particles*

$\in_1$ $---\circ---\circ--\circ---\circ--$ (i)*single particles*

$\in_0$ $\circ-\circ-\circ-\circ-\circ-\circ-\circ-\circ-\circ-\circ$ $ZMS\ (K = 0)$

Figure 1. Diagram showing depletion from ZMS

In terms of creation and annihilation operators, we can write N as,

$$N = N_0 + \sum_{i\neq 0} a_i^+ a_i + \sum_{j\neq 0} a_j^+ a_j^+ a_j a_j \tag{2}$$

Now we can write the expectation value of N when the wave function of the system is say $|n\rangle$, i.e,

$$\langle n|N|n\rangle = \langle n|N_0|n\rangle + \langle n|\sum_{i\neq 0} a_i^+ a_i|n\rangle + \left\langle n\left|\sum_{j\neq 0} a_j^+ a_j^+ a_j a_j\right|n\right\rangle = N_0 + \sum_{i\neq 0} n_i + \left\langle n\left|\sum_{j\neq 0} a_j^+ a_j^+ a_j a_j\right|n\right\rangle \tag{3}$$

Using commutation laws for bosons, one can write,

$$[a_j, a_j^+] = a_j a_j^+ - a_j^+ a_j = 1$$

or

$$a_j^+ a_j = a_j a_j^+ - 1 \tag{4}$$

Substituting from Eq. (4) for $a_j^+ a_j$ in the third term of Eq. (3), we get,

$$\left\langle n\left|\sum_{j\neq 0} a_j^+ a_j^+ a_j a_j\right|n\right\rangle = \left\langle n\left|\sum_{j\neq 0} a_j^+ (a_j a_j^+ - 1) a_j\right|n\right\rangle$$

$$= \left\langle n \right| \sum_{j \neq 0} (a_j^{+} a_j \, a_j^{+} a_j - a_j^{+} a_j) \left| n \right\rangle$$

$$= \left\langle n \right| \sum_{j \neq 0} (n_j \, n_j \; - n_j \,) \left| n \right\rangle$$

$$= \langle n | n \rangle \left[\sum_{j \neq 0} \left(n_j^2 - n_j \,\right) \right] = \sum_{j \neq 0} \left(n_j^2 - n_j \,\right) \tag{5}$$

Substituting Eq. (5) in Eq. (3), we get,

$$N = N_0 + \sum_{i \neq 0} n_i + \sum_{j \neq 0} n_j^2 - \sum_{j \neq 0} n_j \tag{6}$$

If, however, we write that a pair of particles is destroyed from the ZMS and is created in the jth state, then we can write for the pair depletion term as,

$$= \left\langle n \right| \sum_{j \neq 0} a_j^{+} a_j^{+} a_0 a_0 \left| n \right\rangle \tag{7}$$

or

$$= \left\langle n \middle| \sum_{j \neq 0} (a_j^{+} a_j^{+} (n_0)^{\frac{1}{2}} a_0) \middle| n - 1 \right\rangle$$

$$= \left\langle n \middle| \sum_{j \neq 0} (a_j^{+} a_j^{+} (n_0)^{\frac{1}{2}} (n_0 - 1)^{\frac{1}{2}}) \middle| n - 2 \right\rangle$$

$$= (n_0)^{\frac{1}{2}} (n_0 - 1)^{\frac{1}{2}} \left\langle n \right| \sum_{j \neq 0} (a_j^{+} a_j^{+}) \left| n - 2 \right\rangle$$

$$= (n_0)^{\frac{1}{2}} (n_0 - 1)^{\frac{1}{2}} \left\langle n \middle| \sum_{j \neq 0} (a_j^{+} \, (n_j - 1)^{\frac{1}{2}} \middle| n - 1 \right\rangle$$

$$= (n_0)^{\frac{1}{2}} (n_0 - 1)^{\frac{1}{2}} \left\langle n \middle| \sum_{j \neq 0} (n_j - 1)^{\frac{1}{2}} \, (n_j)^{\frac{1}{2}} \middle| n \right\rangle$$

$$= (n_0)^{\frac{1}{2}} (n_0 - 1)^{\frac{1}{2}}) \sum_{j \neq 0} (n_j - 1)^{\frac{1}{2}} \, (n_j)^{\frac{1}{2}} \langle n | n \rangle$$

$$= (n_0)^{\frac{1}{2}} \; (n_0 - 1\,)^{\frac{1}{2}} \left[\sum_{j \neq 0} (n_j)^{\frac{1}{2}} \left(n_j - 1 \right)^{\frac{1}{2}} \right] \tag{8}$$

Since *0* and *j* are arbitrary, Eq. (5) and Eq. (8) are identical.

Now if $\langle n_0 \rangle$ is the average occupation number of the single-particle level with momentum $p = 0$ (same as N_0) which is ZMS, then we can write [11,12]

$$\langle n_0 \rangle \;= \frac{Z}{1 - Z} \tag{9}$$

where Z is the fugacity i.e,

$$Z = \; e^{\beta \mu} = e^{\frac{\mu}{kT}} \; (\mu \; = \; \text{chemical potential}) \tag{10}$$

Depending on the value of Z, a finite fraction of all the particles will occupy the single particle state with the momentum $p = 0$ (ZMS). Variation of μ with temperature T is shown in the fig 4.4 [11, 12].

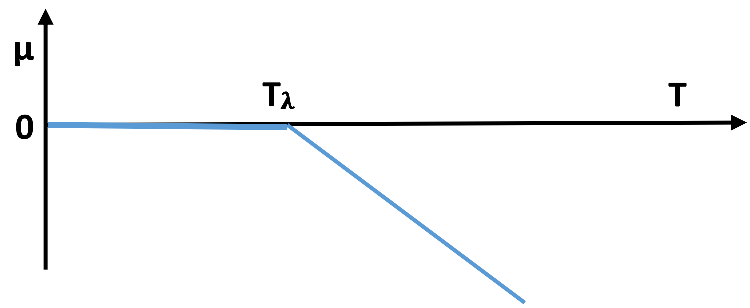

Figure 2. Variation of μ with T in BEC

The chemical potential μ is a function of temperature. Up to the transition temperature (λ-point), μ = 0, and for $T > T_\lambda$, it becomes negative. Thus for bosons we have $0 \leq Z \leq 1$ [11, 12].

(ii) Zero-Momentum State

Zero-Momentum State is also called the condensed state in which all the particles (bosons) are supposed to be, when the temperature $T \to 0$, and the propagation vector or momentum $k \to 0$. Since $k \to 0$, the kinetic energy of the particles in the ZMS is also zero. If N_0 is the occupation number of the ZMS and N is the number of particles, then in the ZMS, $N_0 \leq N$.

Now the general expression for the occupation number of the state for bosons is,

$$n_i = \frac{\omega_1}{e^{\frac{\epsilon_i - \mu}{kT}} - 1} \tag{11}$$

In the condensed state, for bosons, $\mu \to 0$, and Eq. (11) then gives $n_i = N_0 \to \infty$ since $\epsilon_i \to \epsilon_0$ (ZMS) $\to 0$, hence $N_0 \simeq N$ or $\frac{N_0}{N} \simeq 1$ as $T \to T_\lambda$ or $T \leq T_\lambda$. For $T \leq T_\lambda$, the particle number operator, say n_k, can be written as,

$$n_k(\epsilon_k) = N_0[\delta(k)] + \frac{1}{e^{\beta\epsilon_k - 1}} \tag{12}$$

The delta function, $\delta(k)$, at $k = 0$, gives the number of particles in the condensate, and the second term in Eq. (12) applies only for $k \neq 0$ (excited states occupation number). In fact, the particles in the state $k = 0$ are the condensate, which is the ground state of the system. Quasi-particles with $k \neq 0$ are excitations which are described by the effective Hamiltonian of these excitations. The effective Hamiltonian, say H_0, contains combination of operators such as $a_k^+ a_{-k}^+$ which correspond to the excitation of two-particles from the condensate. Since momentum is conserved, the particle momenta that constitute the pair must be k and $-k$ (the pair of particles leaving the condensate will have momenta k for one particle and momenta $-k$ for the second particle). Similarly, the term $a_k a_{-k}$ is the destruction of the two quasi-particles with momenta k and –k when both are returned to the condensate. The term $a_k^+ a_{-k}$ corresponds to the scattering of quasi-particles by the condensate, and there are both direct and exchange processes. The pair creation operator is given by the expression

$$A = \sum_k \frac{v_k}{u_k} a_k^+ a_{-k}^+ \tag{13}$$

where $u_k^2 - v_k^2 = 1$ for bosons in the Bogoliubov canonical transformation for bosons, and u_k and v_k represent the real constants of the transformation. For pair creation for the ZMS (k=0), we can write

$$A(k=0) = \frac{v_0}{u_0} a_0^+ a_{-0}^+ \tag{14}$$

In fact, for k=0, we get a condensate of bound pairs with zero momentum (k,-k=0), and the ZMS can be treated as a state of independent pairs, or a Bose-Einstein-Condensate (BEC) of pairs of particles with opposite momenta. Just as interactions among single particles in the ZMS can lead to depletion from ZMS, similarly interactions among pairs of particles with opposite momenta can lead to depletion of pairs of particles from the condensate (ZMS).

(iii) Thermal Depletion of the Condensate

The depletion of condensate can occur due to particle interactions in the condensate, and or because of the existence of finite temperature in the condensate. At T=0K, all the particles are supposed to condense to the Zero-Momentum-State (ZMS) where N_0 = Total number of particles in the ZMS and N= The total number of particles in the system.

At finite temperature, the total number of particles, N, in the system can be written as [11, 13]

$$N = \sum_{i=0}^{\infty} \sum_{j=1}^{\infty} z^j \, e^{-j\beta\epsilon_i} \tag{15}$$

where

$$\beta = \frac{1}{kT} \; (k = Boltzmann\ constant$$

$$z = fugacity = \; e^{\beta\mu} (\mu = chemical\ potential)$$

$$\epsilon_i = energy\ of\ the\ single\ particle\ i^{th}\ state$$

If the gas is trapped in a three-dimensional harmonic potential trap with frequency ω, we can write,

$$N = \sum_{j=1}^{\infty} z^j \; \left[\sum_{n=}^{\infty} e^{-jn\beta\hbar\omega} \right]^3 \tag{16}$$

Substituting the term, $\quad x = e^{-\beta\hbar\omega} \quad (17)$

in Eq. (16) gives, $$N = \sum_{j=1}^{\infty} z^j \left[\sum_{n=}^{\infty} x^{jn}\right]^3 \quad (18)$$

$$= \sum_{j=1}^{\infty} z^j \left[1 - \frac{1}{x^j}\right]^3 \quad (19)$$

For j=1, we get,

$$N = z\left(1 - \frac{1}{x}\right)^3 \quad (20)$$

For $kT \gg \hbar\omega$, from Eq. (17), we get,

$$x \simeq \left(1 - \frac{\hbar\omega}{kT}\right) \quad (21)$$

Substituting for x from Eq. (21) in Eq. (20) gives,

$$N = z\left(\frac{1}{1-1+\frac{\hbar\omega}{kT}}\right)^3 = z\left(\frac{\hbar\omega}{kT}\right)^3 \quad (22)$$

The number of particles in the ground state (k=0, ZMS) [11, 12] is given by,

$$N_0 = \frac{z}{1-z} \quad (23)$$

Dividing Eq. (23) by Eq. (22), we get,

$$\frac{N_0}{N} = \frac{1}{(1-z)}\left(\frac{\hbar\omega}{kT}\right)^3 \quad (24)$$

The quantity $\frac{N_0}{N}$ is called the condensate fraction η such that $\eta = \frac{N_0}{N}$.
The depletion is,

$$\Delta N = (N - N_0) = N\left(1 - \frac{N_0}{N}\right) \quad (25)$$

or

$$\Delta N = N\left[1 - \frac{1}{(1-z)}\left(\frac{\hbar\omega}{kT}\right)^3\right] \quad (26)$$

Eq. (26) is used to calculate thermal depletion.

Thermal depletion can also be calculated in the following manner. The average occupation of state $|s\rangle$, n_s, may be written as

$$n_s = \frac{r_s}{1-r_s} = \frac{1}{e^{\frac{\epsilon_s-\mu}{kT}}-1} \quad (27)$$

where $r_s = e^{-(\frac{\epsilon_s - \mu}{kT})}$ (28)

For a given value of any single particle state of energy, ϵ_s, (s is the state), the value of n_s depends on the given values of T and μ. For Zero-Momentum-State (ZMS), $\epsilon_0 = 0$, ($\epsilon_s = \epsilon_0 = 0$), for $n_s = n_0 = N_0$ to be positive, for bosons the chemical potential, μ, must be negative, i.e. $\mu < 0$. The chemical potential of liquid Helium at zero temperature is about -7.17K. Thus at least 7.17K is the energy you need to add to the system to evaporate one atom to vacuum (evaporation heat). However, the chemical potential of an ideal gas tends to zero at T=0K [14].

Now the condition $\mu < 0$ assures that the occupation of all states remains regular and finite, it does not prevent the ground state occupation N_0 from becoming macroscopic or exceptionally large, i.e. $N_0 \cong N$ (N is the total number of particles in the assembly) at a finite temperature. This can happen if the following condition is satisfied

$$-\mu \ll \epsilon_1 \ll kT \tag{29}$$

In such a case, from Eq. (27), we get ($\epsilon_s = \epsilon_0 = 0$),

$$N_0 = \frac{1}{e^{\frac{-\mu}{kT}} - 1} = \frac{1}{1 - \frac{\mu}{kT} - 1} = \frac{kT}{-\mu} \tag{30}$$

The occupation number, n_s, of the excited state $|s \neq 0\rangle$ at finite temperature T for the energy state $|s\rangle$, is given as (for $\mu = 0$ in Eq.27)

$$n_s = \frac{kT}{\epsilon_s} \tag{31}$$

The phenomenon according to which macroscopic fraction of bosons collect in the ground state is called Bose-Einstein-Condensation (BEC) and the macroscopically occupied state is called condensate (ZMS). The atoms in the excited states are called thermal cloud or thermal depletion.

Now the total number of particles N can be written as,

$$N = N_0 + \sum_{s \neq 0} n_s \tag{32}$$

or

$$\Delta N = thermal\ depletion = \sum_{s \neq 0} n_s = n_1 + n_2 + \cdots \ldots \ldots$$

$$= N - N_0 = \frac{kT}{\epsilon_1} + \frac{kT}{\epsilon_2} + \cdots \ldots \ldots \tag{33}$$

3. CALCULATIONS AND RESULTS FOR THERMAL DEPLETION

Now for a frequency f=5Hz, $\omega = 2\pi f$=31.42 radians, and for $T = 50nk = 50 \times 10^{-9} K$, $\beta\hbar\omega$=0.00974, Eq. (24) gives the value of η as,

$$\eta = \frac{N_0}{N} = \frac{1}{1-z}\,(0.00974)^3$$

Now 1-z = 0.00001, so that,

$$\eta = \frac{1}{0.00001}\,(0.00974)^3 = \frac{1}{(0.00001)}\,(974)^3 10^{-15} \;=\; 924010424 \times 10^{-10}$$

$$\eta = \; 0.9240 \tag{34}$$

By keeping f = 5Hz, we can vary the temperature T from say 10nK to 100nk and calculate the values of η.

The depletion ΔN is given by

$$\Delta N = (N - N_0) = N\left(1 - \frac{N_0}{N}\right) = N\,(1 - 0.9240)$$
$$= N(0.0760) = N(7.6\%) \tag{35}$$

Eq. (26) shows that the thermal depletion depends on temperature T of the condensate, and the value of ΔN increases as T increases, and this is what has been observed experimentally [9, 15].

Thermal depletion can also be calculated from Eq. (33) where $\in_1 = 0.4834 \times 10^{-16}$ erg and $\in_2 = 0.7251 \times 10^{-16}$ erg [16]. If we assume that the thermal depletion takes place only to the first ($\in_1$) single-particle state, then we get,

$$\Delta N = \frac{kT}{\in_1} \tag{36}$$

If we choose T=1K, the we get,

$$\Delta N = \frac{(1.38\times10^{-16} erg/K)(1K)}{0.4834\times10^{-16}\, erg} = \frac{1.38}{0.4834} \cong 2.85 \tag{37}$$

In fact this is the fraction of particles that account for thermal depletion to the single-particle state ($\in_1$) which is next to ZMS ($\in_0 = 0$).

4. CONCLUSIONS

In conclusion, it should be understood that how the values of the momentum affects the behavior of the assembly arises due to the two-body contact interaction (represented by the scattering length 'a') [17]. Using methods of second quantization, many-body theory, and taking into account two-body scattering properties, quantum depletion of the condensate (ZMS) can be calculated. Quantum depletion in pairs from the condensed state is also achievable. Keeping in mind that pair interaction is also tunable by Feshbach resonance [18].

Depletion of the condensed state takes place not only by the interaction between the particles in the condensed state, but by raising the temperature of the system in the condensed state. Depletion due to change in temperature is called Thermal depletion. General theory of quantum-statistical mechanics have been used to study the problem of Thermal depletion [9, 11, 13]. It is found that the Thermal depletion increases as the temperature of the assembly in the condensed state is increased.

When the temperature of ${}^{4}_{2}He$ gas is reduced in the limit T→0 at ambient pressure, and all the particles condense to the single state k=0, where quantum depletion will take place. When the pressure is increased, the system goes into crystalline state which is inherently restless, and this leads to the fluctuation of atoms from their equilibrium frozen sites, resulting in Zero-Point-Energy (ZPE) that can be calculated using Heisenberg's uncertainty principle. The position fluctuations Δx is roughly 30% of the inter-particle distance [19]. If the ZPE becomes large, depletion could take place from the crystalline state. As of today, I have not come across any experimental measurement showing such a depletion, and no theoretical study seems to have been done so far.

Another problem that could be studied is the depletion from systems with quenched disorder when the assembly is in the super fluid or condensed state. So far, it seems potential depletion has not been studied experimentally or theoretically [10, 20].

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