

INTERACTING BOSE GAS AND QUANTUM DEPLETION

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ABSTRACT

Quantum depletion is a consequence of strong interaction between particles (bosons) in the condensed state, also known as Zero Momentum State (ZMS). It occurs at $T = 0$ K. Due to quantum depletion, the particles leave the ZMS and go to states above ZMS. This is different from thermal depletion which occurs at a finite temperature. The scattering between particles could be as a consequence of singlet interaction 1S_0 or the triplet interaction 1P_0 . The interspecies scattering length for such interactions have been obtained in the past and we have used those values in the calculations for quantum depletion for a system of particles, both homogeneous and heterogeneous. We have used the singlet and triplet scattering length for Sodium Rubidium system. The results show that quantum depletion increases with increase in the scattering length for both singlet and triplet interaction.

Key words; *Quantum Depletion, Singlet scattering length, Triplet scattering length.*

1. INTRODUCTION

The properties of an interacting Bose gas can be studied within the framework of quantum field theory. The model Hamiltonian can be diagonalized using Bogoliubov canonical transformation to get the energy dispersion relation which is used to study all the physical properties of the Bose gas. If the assembly is dilute, then most of the particles can occupy the Zero Momentum State (ZMS) in the limit that the temperature tends to be zero, and only two body collisions with small momentum transfers play an important role, and such collisions are characterized by a single parameter a_s the s-wave scattering length.

If, however, the assembly is a high density system, then more than two body collisions or multiple scattering can take place, and such collisions are taken into account using the T-matrix formalism of the quantum field theory. Collisions can be characterized by the singlet (s-wave) scattering length a_s , and also triplet scattering length (co-efficient length) a_t . The interaction removes

particles from the Zero Momentum condensate resulting in a finite probability of finding the particle with arbitrarily large momentum. This process by which the particles leave the ZMS due to interaction among the particles in the ZMS is called quantum depletion, or in general depletion.

A number of experiments have been done to observe BEC in dilute gases of Rubidium [1–4], Sodium [5, 6], Lithium [7], and mixtures of any two Bose gases. The scattering lengths of homogeneous [8–10] and heterogeneous^{11–20} gases have also been observed experimentally. Since interactions in BEC or ZMS lead to depletion, the concerned theory for the depletion coefficient, η , must be related to the scattering length, a .

This has to be done by writing the interaction Hamiltonian using the theory of second quantization, and the many-body theory has been used to correlate depletion with the scattering length. Knowing the experimental values of the scattering length a , the values of η have been calculated for different types of bosons assemblies.

2. THEORETICAL EQUATIONS

For a weakly interacting quantum liquid, or a weakly (interacting) non-ideal gas, i.e., an assembly in which the role of interactions between the particles is relatively small, the scattering amplitude of the particles will be small compared to the average wavelength $= \frac{h}{p}$, and the

magnitude of λ for a degenerate gas is of the same order of magnitude as the average distance between the particles. Because of the smallness of momentum of the colliding particles, to a first approximation, only s-wave scattering will be of importance. If the amplitude of the s-wave scattering is denoted by a , the amplitude of the p-wave scattering is of the order $a \left(\frac{a}{\lambda}\right)^2$. This is understood by considering the range of forces. If the range of forces is characterized by r_0 , then according to quantum mechanics, for $\lambda \gg r_0$, the scattering amplitudes for different angular momenta l will be of

the order of $r_0 \left(\frac{r_0}{\lambda}\right)^{2l}$, and for the p-wave scattering $l = 1$, and hence the result. The s-wave scattering contributes the terms of order $\frac{a}{\lambda}$ and higher to the total energy, whereas the p-wave scattering contributes the terms of order $\left(\frac{a}{\lambda}\right)^3$ and higher to the energy. Up to the term of the first order, the scattering can be regarded as anisotropic.

Now if we assume that the interaction between the particles of a Bose gas is repulsive, then the scattering length (amplitude) is positive, and at low temperatures, the Bose gas cannot stay dilute and this is true even for infinitesimal attractive forces. We now calculate the energy of the ground state and the energy spectrum for dilute Bose gas at $T = 0 K$. The model Hamiltonian will consist of a kinetic energy term H_1 and a potential energy (interaction energy) H_2 such that,

$$H = H_1 + H_2 \quad (1)$$

Such that,

$$H_1 = \sum_k \hbar\omega_k a_k^\dagger a_k \quad (2)$$

$$H_2 = \frac{g}{2V} \sum_{k_1, k_2, k_3, k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \delta_{k_1+k_2, k_3+k_4} \quad (3)$$

a_k is the annihilation and a_k^\dagger is the creation operator, where g is the pseudo-potential (interaction potential between a pair of particles) which has been brought out in front of the summation sign, since the interaction between a pair of particles is identical, and the scattering length, a , does not depend on the angle in the s-wave scattering. The constant matrix element (of g) g can be determined by requiring that H correctly reproduce the two body scattering properties in a vacuum. In this case the Fourier transform gives $\frac{mg}{\hbar^2}$ such that,

$$\frac{mg}{\hbar^2} = 4\pi a \quad (4)$$

Or

$$g = \frac{4\pi a \hbar^2}{m} \quad (5)$$

Where $4\pi a$ is the scattering coefficient for a hard sphere of radius a . Eq. (5) shows that the parameter of g has now been related to observable quantity, such as the

scattering length, a . To understand the special role of ZMS ($T \rightarrow 0$ and $k \rightarrow 0$), we can replace the operators a_0 and a_0^\dagger (operators for ZMS) by C numbers, i.e., a_0, a_0^\dagger .

The term of the interaction Hamiltonian H_2 can be classified according to the number of times a_0 and a_0^\dagger appears in H_2 , and we retain only the terms of order N_0^2 and N_0 such that,

$$H_2 = H_{inter} \approx \frac{g}{2V} \left[a_0^\dagger a_0^\dagger a_0 a_0 + \sum_R' \left\{ 2(a_k^\dagger a_k a_0^\dagger a_0 + a_{-k}^\dagger a_{-k} a_0^\dagger a_0) + a_k^\dagger a_{-k}^\dagger a_0 a_0 + a_0^\dagger a_0^\dagger a_k a_k \right\} \right] \quad (6)$$

Where the prime on the summation means that the terms $k = 0$ are omitted from the summation. Eq. (6) gives the truncated Hamiltonian in which the excitations of particles out of the condensate are neglected. This will be a good approximation as long as $N - N_0 \ll N$. Substituting for a_0 and a_0^\dagger into eq. (6), we get,

$$H_{inter} = \frac{g}{2V} \left[N_0^2 + 2N_0 \sum_R' (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + N_0 \sum_R' (a_k^\dagger a_{-k}^\dagger + a_k a_{-k}) \right] \quad (7)$$

And the number operator N becomes,

$$N = N_0 + \frac{1}{2} \sum_R' (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) \quad (8)$$

where N_0 is the number of particles in the ZMS ($k = 0$) and the second terms refer to the particles in the states above $k = 0$. Substituting for N_0 from eq. (8) in eq. (7), and then substituting in eq. (1) for the Hamiltonian of the interacting bosons we get,

$$H = \frac{1}{2} V g n^2 + \frac{1}{2} \sum_R' \left[(\epsilon_k^0 + n g) (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + n g (a_k^\dagger a_{-k}^\dagger + a_k a_{-k}) \right] \quad (9)$$

Where the particle number density $n = \frac{N}{V}$. In obtaining eq. (9), terms like $(\sum_R' a_k^\dagger a_k)^2$ have been neglected on the assumption that $N - N_0 \ll N$. Now since eq. (9) is in a quadratic form in the operators, it can be diagonalized with a canonical transformation to get the energy spectrum or the dispersion relation for the energy. Now the diagonalization of H can be carried out with a canonical transformation by defining a new set of creation and annihilation operators and this transformation is called Bogoliubov transformation²¹. This is written as,

$$a_k = u_k \alpha_k - v_k \alpha_{-k}^+; a_k^+ = u_k \alpha_k^+ - v_k \alpha_{-k} \quad (10)$$

where the coefficient of transformation u_k and v_k are assumed to be real and spherically symmetric. The transformation is said to be canonical if the new and the old operators obey the same commutation laws such that,

$$\begin{aligned} [\alpha_k \alpha_k^+] &= \delta_{kk'} \text{ and } [\alpha_k \alpha_{k'}^+] = [\alpha_k^+ \alpha_{k'}^+] \\ &= 0 \end{aligned} \quad (11)$$

From eq. (10) we can obtain the values of α_k in terms of a_k , and substitute the values of α_k in eq. (11), and for the transformations to be canonical, when the new and the old operator obey the same commutation laws, it will be seen that the u_k and v_k must satisfy the condition,

$$u_k^2 - v_k^2 = 1 \quad (12)$$

For all and each value of k , substituting for the a_k from eq. (10) in eq. (9) gives,

$$\begin{aligned} H &= \frac{1}{2} V g n^2 + \frac{1}{2} \sum_R \left[(\epsilon_k^0 + n g) v_k^2 + n g u_k v_k \right] + \frac{1}{2} \sum_R \left\{ (\epsilon_k^0 + n g) (u_k^2 - v_k^2) - 2 u_k v_k n g \right\} (a_k a_k^+ - a_{-k} a_{-k}^+) \\ &\quad + \frac{1}{2} \sum_R \left\{ (n g (u_k^2 + v_k^2) - 2 u_k v_k (\epsilon_k^0 + n g)) (a_k^+ a_{-k}^+ - a_k a_{-k}) \right\} \end{aligned} \quad (13)$$

The last term in eq.(13) is non-diagonal, and to diagonalize H , this term has to be put equal to zero. Doing this will lead to the condition on the parameters u_k and v_k . Hence we get, since the operators $(a_k^+ a_{-k}^+ - a_k a_{-k})$ are not zero, its coefficient is zero, i.e. substituting for u_k and v_k from eq. (12) in eq. (11) gives,

$$n g (\cos^2 \theta_k + \sin^2 \theta_k) = (\epsilon_k^0 + n g) (2 \cosh^2 \theta_k \sinh^2 \theta_k)$$

Or

$$\frac{\cos^2 \theta_k + \sin^2 \theta_k}{2 \cosh^2 \theta_k \sinh^2 \theta_k} = \frac{\epsilon_k^0 + n g}{n g} = \frac{1}{2} \left[\frac{\cosh \theta_k}{\sinh \theta_k} + \frac{\sinh \theta_k}{\cosh \theta_k} \right] = \tanh 2\theta_k$$

$$n g (u_k^2 + v_k^2) - 2 u_k v_k (\epsilon_k^0 + n g) = 0$$

$$n g (u_k^2 + v_k^2) = 2 u_k v_k (\epsilon_k^0 + n g) \quad (14)$$

Now eqn. (12) will be satisfied if we write the parameters u_k and v_k as,

$$u_k = \cosh \theta_k \text{ and } v_k = \sinh \theta_k$$

Combining eqn. (13) and (14) we get,

$$\tanh 2\theta_k = \frac{n g}{\epsilon_k^0 + n g} \quad (15)$$

In eq. (15), the left hand side lies in between -1 and 1, and hence this equation can be solved for all values of k only if the potential g is positive which means that the potential must be repulsive. Now,

$$(\cosh x)^2 - (\sinh x)^2 = 1 \quad (16)$$

Between eq. (14) and (16), we can write,

$$u_k^2 - 1 = v_k^2 = \frac{1}{2} [-1] \quad (17)$$

$$\text{If we write } E_k = \left\{ (\epsilon_k^0 + n g)^2 - n g^2 \right\}^{\frac{1}{2}} \quad (18)$$

Then we get,

$$v_k^2 = \frac{1}{2} \left[\frac{\epsilon_k^0 + n g}{E_k} - 1 \right] \quad (19)$$

Using eq. (12), (14) and (15) in eq. (13), we get

$$H = \frac{1}{2} V g n^2 + \frac{1}{2} \sum_R (\epsilon_k^0 + n g - E_k) \quad (20)$$

Here the operator $a_k^+ a_k$ can have eigen values $0, 1, 2, \dots$, and consequently the ground state $|0\rangle$ of the Hamiltonian H in eq. (20) is determined by the condition,

$$a_k |0\rangle = 0, \text{ for all } k \neq 0 \quad (21)$$

And the state $|0\rangle$ may be interpreted as quasi-particle vacuum. It should be understood that the state $|0\rangle$ is a complicated combination of unperturbed eigen states. We can now write,

$$\left\langle 0 \left| \frac{1}{2} V g n^2 \right| 0 \right\rangle = \frac{1}{2} V g n^2 \langle 0 | 0 \rangle = \frac{1}{2} V g n^2$$

$$\text{since } \langle 0 | 0 \rangle = 1$$

$$\left\langle 0 \left| \frac{1}{2} \sum_R (E_k - \epsilon_k^0 - n g) \right| 0 \right\rangle = \frac{1}{2} \sum_R (E_k - \epsilon_k^0 - n g) \langle 0 | 0 \rangle = \frac{1}{2} \sum_R (E_k - \epsilon_k^0 - n g)$$

$$\left\langle 0 \left| \frac{1}{2} \sum_R E_k (\alpha_k^+ \alpha_k - \alpha_{-k}^+ \alpha_{-k}) \right| 0 \right\rangle = 0$$

$$\text{Since } \langle 0 | \alpha_k^+ \alpha_k | 0 \rangle = 0$$

Since neither α_k nor α_k^+ annihilates the ground state energy, E is now given by,

$$E = \langle 0 | H | 0 \rangle = \frac{1}{2} V g n^2 + \frac{1}{2} \sum_R (E_k - \epsilon_k^0 - n g) \quad (22)$$

After diagonalization of Hamiltonian H given by eq. (9) using Bogoliubov transformation, we get an assembly of quasi-particles that do not interact and are bosons. All excited state correspond to various numbers of non-interacting bosons, each with an excitation energy E_k .

Now the distribution function in the ground state $|0\rangle$ is given by,

$$n_k = \langle 0 | \alpha_k^+ \alpha_k | 0 \rangle = \mathcal{V}_k^2 \langle 0 | \alpha_k^+ \alpha_k | 0 \rangle = \mathcal{V}_k^2 \quad (23)$$

Now the interaction removes particles from the Zero Momentum State (ZMS), and consequently there is a finite probability of finding a particle with an arbitrarily high momentum. Thus the depletion $\eta = \frac{N - N_0}{N}$ which can be written as

$$\begin{aligned} \eta &= \frac{N - N_0}{N} = \frac{1}{N} \sum_R n_k = \frac{1}{N} \sum_R \mathcal{V}_k^2 = \frac{1}{N} V \int \frac{d^3 k}{(2\pi)^3} \mathcal{V}_k^2 = \frac{1}{(N/V)(2\pi)^3} \int d^3 k \mathcal{V}_k^2 \\ &= \frac{1}{2n(2\pi)^3} \int \left(\frac{\epsilon_k^0 + n g}{\{(\epsilon_k^0 + n g)^2 - n g^2\}^{\frac{1}{2}}} - 1 \right) d^3 k \quad (24) \end{aligned}$$

The value of η is calculated by making the following assumptions;

$$y^2 = \frac{\epsilon_k^0}{n g} = \frac{1}{n g} \left(\frac{p_0^2}{2M} \right) = \frac{1}{2M n g} (\hbar^2 k^2), g = \frac{4\pi \hbar^3 a}{M} \text{ and } d^3 k = 4\pi k^2 dk$$

$$y^2 = \frac{\hbar^2}{2M n g} k^2$$

or

$$k^2 = \frac{2M n g}{\hbar^2} y^2$$

or

$$k = \left(\frac{2M n g}{\hbar^2} \right)^{\frac{1}{2}} y \quad (25)$$

Differentiating both sides of eqn. (25) we get,

$$2k \cdot dk = \frac{2M n g}{\hbar^2} y \cdot dr$$

$$\text{Or } dk = \frac{M n g}{\hbar^2} \cdot \frac{1}{k} y \cdot dy \quad (26)$$

Substituting for the values of y and k in eqn. (26) we get,

$$dk = \frac{M n g}{\hbar^2} \cdot \frac{1}{\left(\frac{2M n g}{\hbar^2} \right)^{\frac{1}{2}} y} y \cdot dy = \frac{(M n g)^{\frac{1}{2}}}{\hbar \sqrt{2}} dy$$

now $d^3 k$ can be written as,

$$d^3 k = 4\pi k^2 dk = 4\pi \frac{2M n g}{\hbar^2} y^2 \cdot \frac{(M n g)^{\frac{1}{2}}}{\hbar \sqrt{2}} dy = 4\pi \sqrt{2} \frac{(M n g)^{\frac{1}{2}}}{\hbar^4} y^2 dy \quad (28)$$

Also

$$\epsilon_k^0 + n g = n g y^2 + n g = n g (y^2 + 1)$$

and

$$(\epsilon_k^0 + n g)^2 - (n g)^2 = n^2 g^2 (y^4 + 2y^2)$$

And substituting in Eqn. (24) we get,

$$\eta = 4 \left(\frac{2n a^3}{\pi} \right)^{\frac{1}{2}} \int_0^\infty y^2 dy \left[\frac{y^2 + 1}{(y^4 + 2y^2)^{\frac{1}{2}}} - 1 \right] = 4 \left(\frac{2n a^3}{\pi} \right)^{\frac{1}{2}} \left(\frac{\sqrt{2}}{3} \right) = \frac{8}{3} \left(\frac{n a^3}{\pi} \right)^{\frac{1}{2}} \quad (29)$$

Eqn. (29) gives η in terms of a , and it is this equation that will be used to do the required calculations and to draw the variation of η against a .

3. RESULTS AND DISCUSSIONS

Figure 1 and 2 below show the variation of quantum depletion with singlet scattering length and variation of quantum depletion with triplet scattering length, respectively.

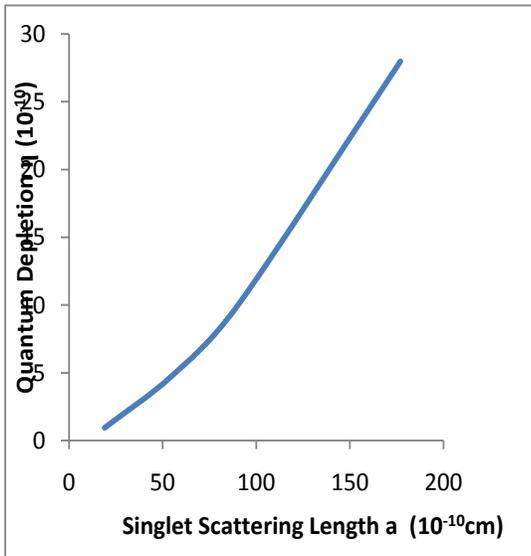


Figure 1: Variation of quantum depletion with singlet scattering length

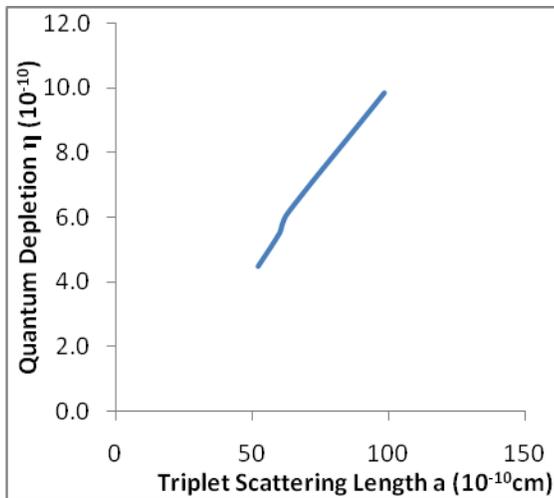


Figure 2: Variation of quantum depletion with triplet scattering length

Figure 1 and 2 above show that for both singlet and triplet scattering lengths, the quantum depletion increases as the scattering length increases. Large scattering length means stronger interaction, and stronger interaction leads to increase in quantum depletion. This is the result of our calculation. As the temperatures decrease, the scattering length decreases. This leads to decrease in fractional depletion. Smaller scattering length means weak interactions and since the fractional depletion decreases as the scattering length decreases, this also means that weak interaction means reduction in depletion. The interaction is large when the

interaction refers to the singlet scattering length compared to triplet scattering length, which means singlet scattering length corresponds to stronger interaction. Such results have been obtained by others [11,12].

4. CONCLUSIONS

We have obtained an equation between the scattering length and quantum depletion. We can also obtain the equation relating scattering length and inter-particle potential $V(r)$. The results show that quantum depletion increases with increase in the scattering length for both singlet and triplet interaction.

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