Momentum dependent higher partial wave interactions in Bose-Einstein condensate

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1 Introduction

For a very dilute Bose-Einstein condensate which is the case in most of the experiments, the interatomic interaction is sufficiently weak, the mean field Gross-Pitaevskii theory is a logical tool to study such a system [1]. The physics of the cold atom scattering is dominated by the two-body contact interaction which is well described by the s-wave scattering length. If we confine ourselves to the case of low momentum (k) and the small values of scattering length (a) such that ka << 1, the momentum dependence of the scattering amplitude of two interacting atoms can be neglected [2, 3]. However the value of the parameter ka increases with the increase in a, even for small momentum (k). Recent experiments [4, 5, 6] have explored the possibilities of increasing the scattering length by exploiting magnetic Feshbach resonance. In an experiment performed at JILA [4] it was possible to confine $10^4$ atoms of $^{85}$Rb in a cylindrically symmetric trap at 100 nK. Around the Feshbach resonance at a magnetic field B $\sim$ 155 Gauss, the scattering length was varied from negative to very high positive values $\sim$ 10000 a$_0$ by varying the magnetic field. In this case the value of the parameter ka becomes greater than 1 at and above $a = 3000 a_0$. In this regime of ka > 1, the momentum dependence of scattering amplitude becomes important. The first order theory of Beliaev [2] gives the momentum dependence of scattering amplitude by applying field-theoretic diagrammatic treatment to the zerotemperature homogeneous dilute interacting Bose gas [2, 7]. The Beliaev

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theory was generalized to give the temperature dependence of the excitation spectrum of Bose gas [5, 9]. In the regime $ka << 1$, the Beliaev’s first order theory reduces to Bogoliubov spectrum [10] for contact potential. The work of Lee, Huang, Yang (LHY) [11, 12] on the low temperature properties of dilute hard sphere gas considering the perturbation theory gives the first correction to the Bogoliubov mean field theory for dilute gases for relatively stronger interaction. The energy correction obtained from Beliaev’s second order theory [2] coincides with the LHY result assuming momentum independent scattering length. Brueckner and Sadwa also determined the quantum depletion and correction to the ground state energy of a homogeneous dilute Bose gas [13]. To study the ground state properties of a dilute Bose gas with strong interactions momentum dependent scattering amplitudes along with the contribution from LHY correction term is important. For strongly interacting system ($ka >> 1$), the higher order partial waves likely to give significant contribution to the scattering amplitudes. For $ka > 1$, only the even higher partial waves (e.g. d-wave, g-wave etc.) will contribute to the atomic interactions in the Bose gases. It has been mentioned by Beliaev [2] that the d-wave contribution to energy spectrum can be $\sim 10\%$. Here we will show that d-wave contribution to the column density can be double of this value $\sim 20\%$ at the centre of the trap for large values of scattering length.

In this letter we present the ground state energy functional of trapped atomic Bose condensate including the effect of momentum dependent scattering amplitude (with full generality) and also including the LHY correction term. Higher partial wave interactions have been incorporated in the energy functional. From the ground state energy functional the time-independent equation has been derived to give the condensate density. We have considered $10^4$ $^{85}$Rb atoms which are cooled to a temperature of 100 $nK$ with the scattering length varying from 3000 $a_0$ to 8700 $a_0$. The corresponding range of variation of $ka$ is 1.15 to 3.33 and the values of peak gas-parameter $x_{pk} \sim 10^{-2}$ ($x_{pk}=n(0)a^3$, where $n(0)$ is the peak density of Bose gas and $a$ is the s-wave scattering length of interatomic interaction) [see Table 1]. It is found that for $ka > 1$, the contribution of the momentum dependent scattering (considering s, d and g waves) to the column density becomes important and the nature of column density differs significantly from that obtained for k-independent scattering (contact interaction with LHY correction). The contribution from the g-wave interaction to the column density is negligible (less than 1%) for $ka= 3.33$. As in the vicinity of Feshbach resonance the two and three body loss rates play a crucial role [14, 15, 16, 17], their effect have also been included phenomenologically in the time-independent equations of the condensate. The patterns of the column densities as observed experimentally agree well with our results considering momentum dependent
scattering amplitude at B=157.2 Gauss (a \approx 3000a_0).

2 Theory

Quantum scattering theory can be formulated in terms of partial waves. The wave function for relative motion is written as $\psi = e^{ikz} + f(\theta)e^{ikr}/r$, where $f(\theta)$ is the scattering amplitude and $k$ is the wave vector of the scattered wave. The first term gives an incoming plane wave travelling along z axis and the second term represents a radially outgoing scattered wave \[18\]. Using partial wave expansion the scattering amplitude for identical bosons can be expressed as

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \exp(i\delta_l) \sin \delta_l P_l(\cos \theta)$$

Here, $l= 0, 1, 2, \ldots$ denotes the contribution of s, p, d, \ldots partial waves to the total scattering amplitude, $\delta_l$ are the phase shifts associated with each partial wave, and $P_l(\cos \theta)$ are Legendre polynomials. For identical bosons only even $l$ partial waves can contribute to the scattering amplitude. According to Beliaev’s first order theory \[2\] the excitation spectrum of a dilute Bose gas can be given by the dispersion relation

$$\epsilon_k^{(1)} = \sqrt{\epsilon_k^0 + 2n_0 \{ f_s(k/2, k/2) - n_0 f(0, 0) \frac{\hbar^2}{m} \}^2 - (n_0 f(k, 0) \frac{\hbar^2}{m})^2}$$

where $\epsilon_k^0 = \hbar^2 k^2/(2m)$ is the kinetic energy and $m$ is the atomic mass. Here only the forward scattering of atoms are considered. The two distinct scattering amplitudes (considering s-wave) are $f(0, 0) = 4\pi a$ and $f(k, 0) = 4\pi \sin(ka)/k$. The symmetrized amplitude $f^d(k/2, k/2)$ for higher partial wave (l=2) is added with $f^s(k/2, k/2)$ (for l=0) to give the following dispersion relation

$$\epsilon_k^{(1)} = \sqrt{\epsilon_k^0 + 2n_0 \{ (f_s(k/2, k/2) + f^d(k/2, k/2)) - n_0 f(0, 0) \frac{\hbar^2}{m} \}^2 - (n_0 f(k, 0) \frac{\hbar^2}{m})^2}$$

The values of symmetrized scattering amplitudes considering s and d waves are $f^s(k/2, k/2) = 4\pi (\sin(ka) - i2\sin^2(ka/2))/k$ and $f^d(k/2, k/2) = -40\pi (\cos\delta_2 \sin\delta_2 + i\sin^2\delta_2)$; where $\delta_2 = \tan^{-1}\{(3k^2a^2\cos^2\frac{ka}{2} - (3 - k^2a^2)\sin^2\frac{ka}{2})/(3 - k^2a^2)\cos\frac{ka}{2} + 3ka\sin\frac{ka}{2}\}$.

The LHY correction term for the ground state energy of a dilute Bose gas \[11, 12\] is

$$E[n] = \frac{2\pi \hbar^2 an}{m} \frac{128}{15} \left( \frac{na^3}{\pi} \right)^{1/2}$$
This term can also be obtained from second order Beliaev’s theory \[2\]. The ground state energy functional can be given as

\[
E[\psi] = \int d\vec{r} \left[ -\frac{\hbar^2}{2m} \psi^* \nabla^2 \psi + V_{tr}(\vec{r}) |\psi|^2 + \frac{1}{2} \{ g_1 |\psi|^2 + \frac{(g_1^2 - g_2^2)}{2\epsilon_k^0} |\psi|^6 + \frac{256 \hbar^2}{15 m} \sqrt{\pi a_s/2} |\psi|^5 \} \right]
\]

where \( g_1 = \frac{\hbar^2}{m} \{ 2(f^s(k/2, k/2) + f^d(k/2, k/2)) - f(0, 0) \} \) and \( g_2 = \frac{\hbar^2}{m} f(k, 0) \); \( V_{tr} \) is the trapping potential. In \( g_1 \) and \( g_2 \) the imaginary part of the scattering amplitudes has not been taken into account.

By performing a functional variation with respect to \( \psi^* \) the Euler-Lagrange equation \([19, 20]\) takes the following form

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{tr} + g_1 |\psi|^2 + \frac{3}{4} \frac{g_1^2 - g_2^2}{\epsilon_k^0} |\psi|^4 + \frac{128 \hbar^2}{3 m} \sqrt{\pi a_s/2} |\psi|^3 - \frac{i\hbar}{2} (K_2 |\psi|^2 + K_3 |\psi|^4) \right] \psi = \mu \psi \quad (6)
\]

where \( \mu \) is the chemical potential which accounts for the conservation of number of particles. In Eq. (6) the two body and three body losses are introduced phenomenologically to give

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{tr} + g_1 |\psi|^2 + \frac{3}{4} \frac{g_1^2 - g_2^2}{\epsilon_k^0} |\psi|^4 + \frac{128 \hbar^2}{3 m} \sqrt{\pi a_s/2} |\psi|^3 - \frac{i\hbar}{2} (K_2 |\psi|^2 + K_3 |\psi|^4) \right] \psi = \mu \psi
\]

where \( K_2 \) and \( K_3 \) are the two body and three body recombination loss rate coefficients, respectively.

At small momenta \( (ka < 1) \), neglecting the d-wave scattering and setting \( f^s(k/2, k/2) = f(k, 0) = f(0, 0) \) Eq. (6) reduces to

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{tr} + g_1 |\psi|^2 + \frac{128 \hbar^2}{3 m} \sqrt{\pi a_s/2} |\psi|^3 \right] \psi = \mu \psi \quad (8)
\]

where \( g_1 = 4\pi \hbar^2 a/m \). The Eq. (8) is known as modified Gross-Pitaevskii equation for the atomic condensate \([19]\).

The trapping potential for the cylindrical trap with two angular frequencies \( \omega_\perp \) and \( \omega_z \) is given as

\[
V_{tr}(\vec{r}) = \frac{1}{2} m (\omega_\perp^2 r_\perp^2 + \omega_z^2 z^2)
\]

The column density which is an accessible experimental quantity is defined as \( n_c(z) = \int d\vec{r}_\perp |\psi(r_\perp, z)|^2 \). A measure of the extension of the condensate is the half width of the column density \( R_{1/2} \), defined as the z-value when \( n_c(z = R_{1/2}) = \frac{1}{2} n_c(z = 0) \).
Table 1: Results for the ground-state properties of $10^4 \ ^{85}\text{Rb}$ atoms trapped in a cylindrically symmetric trap with $\omega_\perp = 17.5 \text{ Hz}$ and $\omega_z = 6.8 \text{ Hz}$. Chemical potentials are in the units of $\hbar \omega_\perp$; half widths are in the units of $\mu \text{m}$. Results are given for $k$-dependent $s$-wave scattering [$s(k)$], $k$-dependent $(s+d)$-wave scattering [$s+d(k)$] and $k$-independent $s$-wave scattering [$s$].

| $a \ (a_0)$ | $ka$ | $\mu$ | $x_{pk}$ | half width |
|-------------|------|-------|----------|------------|
| 3000        | 1.15 | s(k)  | 12.47    | 3.89(-3)   | 21.01      |
|             |      | s+d(k)| 12.59    | 3.84(-3)   | 21.09      |
|             |      | s     | 14.48    | 3.19(-3)   | 22.42      |
| 5000        | 1.92 | s(k)  | 12.74    | 1.49(-2)   | 22.52      |
|             |      | s+d(k)| 13.79    | 1.37(-2)   | 23.09      |
|             |      | s     | 18.77    | 9.72(-3)   | 25.88      |
| 7000        | 2.68 | s(k)  | 11.51    | 3.61(-2)   | 23.72      |
|             |      | s+d(k)| 15.15    | 2.97(-2)   | 25.15      |
|             |      | s     | 22.56    | 1.96(-2)   | 28.62      |
| 8700        | 3.33 | s(k)  | 11.16    | 5.89(-2)   | 25.05      |
|             |      | [s+d](k)| 17.79   | 4.45(-2)   | 27.32      |
|             |      | s     | 25.57    | 3.08(-2)   | 30.58      |

3 Results and discussion

Our aim here is to emphasize the significance of the momentum ($k$)-dependent scattering amplitudes (both for $s$-wave and higher partial wave scattering) to determine the ground state of the system for large scattering lengths even at small values of momentum. In order to do so we have considered a condensate of $10^4 \ ^{85}\text{Rb}$ atoms confined in a cylindrical trap with radial (axial) frequency $\omega_\perp = 17.5 \text{ Hz}$ ($\omega_z = 6.8 \text{ Hz}$) with large gas parameter values ($\sim 10^{-2}$) as achieved in the experiment of Cornish et al. [4]. We have made an attempt to explain some experimental results in light of the $k$-dependent scattering phenomena. In Table I we list the values of the chemical potential ($\mu$), peak gas-parameter ($x_{pk}$) and also the half widths of the column density distributions (to be demonstrated in Fig. 1) along with the values of the parameter $ka$ considering $k$-independent $s$-wave and also $k$-dependent $s$- and $(s+d)$-wave scattering. For the range of $a$ considered here the parameter $ka$ is greater than 1 and assumes the maximum value of 3.33 for $a = 8700 \ a_0$. As expected
the differences between k-dependent s and (s+d) results increases with the increase in \(ka\) and are of the order of 59\% for \(\mu\), 24\% for \(x_{pk}\) and 9\% for the half width at \(a = 8700a_0\). The differences between these results (considering momentum-dependent scattering) and those for k-independent s-wave scattering are also enhanced at large values of \(ka\). Note that for the k-dependent s-wave scattering \(\mu\) decreases with the increase in \(a\) after 5000 \(a_0\). This effect of the negative contribution to the chemical potential is nullified due to the inclusion of d-wave in the k-dependent scattering amplitude.

The column densities considering k-dependent s- and (s+d)-wave [obtained by solving Eq. (6)] and k-independent s-wave [obtained by solving Eq. (8)] atom-atom scattering are presented in Fig. 1(a), (b) and (c) for \(a = 3000a_0\), 7000 \(a_0\) and 8700 \(a_0\) respectively. The dotted and solid lines correspond to the k-dependent s-wave and (s+d)-wave scattering results; circles are the k-independent s-wave results; the red dashed lines give the column densities with (s+d)-wave scattering considering two-body \((K_2)\) and three-body \((K_3)\) losses [obtained by solving Eq. (7)]. The values of \(K_2\) and \(K_3\) are taken from the Fig. 2 in Ref. [15] where two- and three- body loss rates of \(^{85}\)Rb atoms are shown as a function of magnetic field near Feshbach resonance. Column densities considering k-dependent s- and (s+d)-wave scattering almost coincides at \(a = 3000a_0\) (\(ka = 1.15\)), whereas for larger values of \(ka\), the (s+d)-wave scattering lowers the central column density with an expansion in the density distribution leading to a larger half width (as shown in Table 1) than the column density corresponding to k-dependent s-wave scattering.

At \(a = 8700a_0\) the deviation is 20.6\% at \(z=0\), which can be experimentally detected where the accuracy of measurement is higher [21]. The column density considering k-independent s-wave scattering is consistently lowered in the centre than the k-dependent results and the half width of the atomic cloud condensate is larger.

In Fig. 2 we have compared our results for \(a = 3000a_0\) with that obtained in the experiment [4] for B= 157.2 Gauss. In the conditions of this experiment the scattering length corresponding to B=157.2 Gauss is \(\sim 3000a_0\) (as obtained by manual interpolation from Fig. 1 of Ref. [4]). We have solved Eqs. (6) and (7) by taking \(a = 3000a_0\). In Fig. 2 the circles are the plots of the experimental data obtained by the interpolation of the condensate column density curve taken from Fig. 3(d) in Ref. [4]. The solid line indicates column densities for k-dependent (s+d)-wave scattering considering two and three body losses [obtained by solving Eq. (7)] and the dotted line gives the same without considering any losses [obtained by solving Eq. (6)]. The theoretical results are fitted with the experimental data at the second point from the \(z=0\) axis (at \(z=4.03 \, \mu m\)) and the deviation between experimental and theoretical results at \(z=0\) is about 10\%. By comparison we find that
our theoretical results are in good agreement with the experimental data up to $z = 27 \mu m$, but the long tail obtained in the experiment beyond $27 \mu m$ could not be reproduced. As the half width of the of the column density for k-independent s-wave interaction is larger than that for the k-dependent interaction [see Table 1 and Fig. 1(a)], it is obvious that the column density corresponding to the k-independent scattering will deviate outwardly from the experimental data. We have repeated the calculation with $a = 3100a_0$ and $2900a_0$ (as the error in the interpolation of the curve in Fig. 1 of Ref. [4] is within $90a_0$) and found the results are almost coincident with those for $3000a_0$. Increases in the half widths obtained from our theoretical column densities due to the increase in $a$ from 3000 $a_0$ to 8700 $a_0$ are 29.5% and 36.4% for k-dependent (s+d)-wave and k-independent s-wave scattering [see Table 1]. In the experiment $a = 3000a_0$ and 8700 $a_0$ correspond to $B = 157.2$ Gauss and 156.4 Gauss [obtained by manual interpolation of Fig.1 in Ref. [4]]. The increase in the half width of the column density is $\sim 15\%$ due to the change in $B$ from 157.2 G to 156.4 G. Smaller increase in the half widths due to increase in $a$ in the case of k-dependent results than the k-independent results indicates that k-independent results are closer to the experiment. In this study we have not considered the effect of coherent loss process and also the finite temperature corrections which may affect the column density for the large values $a$.

To summarize, we have shown that the inclusion of the momentum dependent scattering amplitudes due to s-wave and higher partial waves are important to determine the ground state properties of the condensate when $ka > 1$ and $x_{pk} \sim 10^{-2}$. Experimentally detectable significant quantitative differences are found between the results considering momentum independent and momentum dependent scattering. Theoretical column densities for $^{85}\text{Rb}$ atom considering (s+d)-wave scattering are found to exhibit good agreement with the experimental results for $a = 3000a_0$.

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Figure captions

Fig. 1 Column densities of $10^4$ $^{85}$Rb atoms at $a = 3000 \ a_0$ (a), $a = 7000 \ a_0$ (b) and $a = 8700 \ a_0$ (c) as a function of axial distance for a cylindrical trap with $\omega_{\perp}/2\pi = 17.5$ Hz and $\omega_z/2\pi = 6.8$ Hz. The vertical axis is multiplied by $2 \times a_{\perp}^2/\hbar/(m\omega_{\perp})$. The dotted and solid lines represent the densities with k-dependent s-wave and (s+d)-wave scattering; circles are the k-independent s-wave results; the red dashed lines give the column densities considering two-body ($K_2$) and three-body ($K_3$) losses.

Fig. 2 Column densities of $10^4$ $^{85}$Rb atoms at $a = 3000 \ a_0$ (corresponding to B=157.2 gauss in Ref. [4]) as a function of axial distance for a cylindrical trap with $\omega_{\perp}/2\pi = 17.5$ Hz and $\omega_z/2\pi = 6.8$ Hz. The solid line gives the result for k-dependent (s+d)-wave scattering considering two and three body losses and the dotted line gives the column density without considering any losses. Circles are the plots of the experimental condensate column density taken from Fig. 3(d) in Ref. [4].
column density

z (µm)