Evaluation of the particle numbers via the two root mean square radii in a 2-species Bose-Einstein condensate

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The coupled Gross-Pitaevskii equations for two-species BEC have been solved analytically under the Thomas-Fermi approximation (TFA). Based on the analytical solution, two formulae are derived to relate the particle numbers \( N_A \) and \( N_B \) with the root mean square radii of the two kinds of atoms. Only the case that both kinds of atoms have nonzero distribution at the center of an isotropic trap is considered. In this case the TFA has been found to work nicely. Thus, the two formulae are applicable and are useful for the evaluation of \( N_A \) and \( N_B \).

PACS numbers: 03.75.Mn,03.75.Kk

Keywords: Bose-Einstein condensate,2-species BEC, root mean square radius, determination of particle numbers

Since the pioneer theoretical study by Ho and Shenoy\textsuperscript{1} in 1996, the interest in two-species Bose-Einstein condensate (2-BEC) is increasing in recent years. There are many theoretical studies \textsuperscript{1–19}. Experimentally, this system was first achieved by Myatt, et al.\textsuperscript{20} in 1997. Making use of a magnetic trap, an optical trap, or a combined magneto-optical trap, various types of 2-BEC can be created \textsuperscript{21–24} (also refer to the references listed in \textsuperscript{24}). In related experiments most parameters involved in the experiments. Since the root mean square radii are observable, these two formulae are useful for the determination or refinement of the parameters. In details, the followings are performed.

(i) For the condensate with the A- and B-atoms, we have derived two formulae to relate the two root mean square radii \( r_{\text{RMS}}^a \) and \( r_{\text{RMS}}^b \), respectively, to the parameters involved in the experiments. Since the root mean square radii are observable, these two formulae are useful for the determination or refinement of the parameters.

(ii) We have found out the border separating the whole parameter-space into two subspace for miscible and immiscible phases, respectively. The determination of the border provides a base for plotting the phase-diagrams,\textsuperscript{25} and therefore helps to understand intuitively the inherent physics.

(iii) Since we have introduced the Thomas-Fermi approximation (TFA) in the derivation (in which the kinetic energy has been neglected), we have performed a numerical calculation to evaluate the error caused by the TFA. In this way the applicability of the two formulae is clarified.

Let the masses of the A- and B-atoms be \( m_A \) and \( m_B \). These cold atoms are subjected to the isotropic parabolic potentials \( \frac{1}{2} m_s \omega_s^2 r^2 \) (\( S = A \) or \( B \)). We introduce a mass \( m \) and a frequency \( \omega \). \( \hbar \omega \) and \( \lambda \equiv \sqrt{\hbar/(m\omega)} \) are used as units for energy and length in this paper. Then, the intra-species interaction \( V_S = c_S \sum_{i<i'} \delta(r_i - r_{i'}) \), and the inter-species interaction \( V_{AB} = c_{AB} \sum_{i<j} \delta(r_i - r_j) \). Their spin-degrees of freedom are considered as being frozen. The ground state (g.s.) \( \Psi_{\text{gs}} \) is assumed to have the following form

\[
\Psi_{\text{gs}} = \prod_{j=1}^{N_A} \frac{u(r_j)}{\sqrt{4\pi r_j}} \prod_{k=1}^{N_B} \frac{v(r_k)}{\sqrt{4\pi r_k}} \tag{1}
\]

where \( u(r) \) and \( v(r) \) are for the A- and B-atoms, respectively, and they are most advantageous to binding. We further introduce \( \gamma_S \equiv m (\omega^2 / \lambda^2)^2 \) and a set of four parameters \( \alpha_1 \equiv N_A |c_A|/\lambda^2, \beta_1 \equiv N_B |c_{AB}|/\lambda^2, \alpha_2 \equiv N_B |c_{AB}|/\lambda^2, \beta_2 \equiv N_A |c_{AB}|/\lambda^2 \), where \( |c_A| \) is dimensionless and is the value of \( c_A \) in the new units, etc.. This set is called the weighted strengths (W-strengths). Under the TFA, the coupled Gross-Pitaevskii equations (CGP) for \( u \) and \( v \) in the dimensionless form appear as

\[
\left( \frac{\mu^2}{2} + \alpha_1 \frac{u^2}{r^2} + \beta_1 \frac{v^2}{r^2} - \varepsilon_1 \right) u = 0 \tag{2}
\]
\[
\left( \frac{\mu^2}{2} + \alpha_2 \frac{u^2}{r^2} + \beta_2 \frac{v^2}{r^2} - \varepsilon_2 \right) v = 0 \tag{3}
\]

where \( \alpha_1 \) and \( \alpha_2 \) are for the intra-species interaction and they are considered as positive. The chemical potential for the A-atoms (B-atoms) is equal to \( \gamma_A \varepsilon_1 \) (\( \gamma_B \varepsilon_2 \)). The normalization \( \int u^2 dr = 1 \) and \( \int v^2 dr = 1 \) are required. \( u \geq 0 \) and \( v \geq 0 \) are safely assumed.

It turns out that the solutions of eqs.\textsuperscript{21,22} can be divided into two phases. When both kinds of atoms have
nonzero distribution at the center, i.e. \( u/r|_{r=0} > 0 \) and \( v/r|_{r=0} > 0 \) (obviously, it is required that, when \( r \) tends to zero, both \( u \) and \( v \) should tend to zero as fast as \( r \)), and are distributed compactly (i.e., not distributed in disconnected regions), then it is in miscible phase. Otherwise, in immiscible phase. For the miscible states, under the TFA, the analytical expression for \( u/r \) and \( v/r \) have been given previously \[19\]) but in a rather complicated form. In this paper, by introducing the W-strengths defined ahead eq.(2), we obtain a much simpler expression as given in the Appendix. Where the kind of atoms having a narrower distribution is named as the A-atom and described by \( u \), while the other kind by \( v \). The border in the parameter-space that separates the two phases is also given in the Appendix.

With this very simple analytical expression of \( u/r \) and \( v/r \), it is straight forward to obtain the root mean square radii from the definitions \( r^u_{\text{RMS}} = (\int u^2 r^2 dr)^{1/2} \) and \( r^v_{\text{RMS}} = (\int v^2 r^2 dr)^{1/2} \). Thus we have

\[
\begin{align*}
(r^u_{\text{RMS}})^2 &= \frac{3}{4} \left[ \frac{15(\alpha_1 \alpha_2 - \beta_1 \beta_2)}{\alpha_2 - \beta_1} \right]^{2/5} \quad (4) \\
\beta_2 (r^u_{\text{RMS}})^2 + \alpha_2 (r^v_{\text{RMS}})^2 &= 15^{2/3} \left( \frac{3}{7} \alpha_2 + \beta_2 \right)^{5/7} \quad (5)
\end{align*}
\]

Obviously, when all the parameters are known except \( N_A \) and \( N_B \), and when \( r^u_{\text{RMS}} \) and \( r^v_{\text{RMS}} \) have been measured, \( N_A \) and \( N_B \) can be known from eqs. (4). Since the TFA has been adopted, we have to evaluate the deviation caused by TFA. For this aim, we go to the one-species BEC. When \( \hbar \omega_S \) and \( \lambda_S = \sqrt{\hbar / (m_S \omega_S)} \) are used as units, the dimensionless Gross-Pitaevskii equation is

\[
\left( -\frac{d^2}{2dr^2} + \frac{1}{2} r^2 + \frac{\alpha}{r^2} \right) u = \varepsilon u \quad (6)
\]

where \( \alpha = N_S |c_S|^2 / (4\pi) \). Under the TFA, \( u/r = \sqrt{\frac{3}{2\pi}} (1 - \frac{r^2}{r_0^2})^{1/2} \), where \( r_0 = (15\alpha)^{1/5} \). The root mean square radius \( R_{\text{TFA}} = \sqrt{3\sqrt[5]{15\alpha}} \). Let the radius obtained from the exact solution of eq.(6) be denoted as \( R_{\text{exac}} \), and we define \( \alpha' = \frac{1}{r_{\text{exac}}^2} R_{\text{TFA}}^2 \), where \( \alpha'/\alpha \) measures the deviation in \( \alpha \) caused by TFA. For \(^{87}\)Rb, the dimensionless strength \( |c_S| = 0.00249 \sqrt{\omega} \cdot \text{sec} \). When \( \omega = 1000 / \text{sec} \) as an example, \( \alpha = 0.0063 N_S \), where \( N_S \) is assumed to be very large. For a general evaluation, \( \alpha = 10, 100, 1000, \) and \( 10000 \) are adopted. The wave function \( u/r \) obtained under TFA and from exact calculation are plotted in Fig.11 \( R_{\text{TFA}}, R_{\text{exac}}, \) and \( \alpha'/\alpha \) are listed in Table I.

The above results demonstrate that, when the wave functions obtained under TFA and from exact calculation overlap nicely (say, when \( \alpha \geq 1000 \)), \( R_{\text{TFA}} \) is close to \( R_{\text{exac}} \) and \( \alpha' \) is close to \( \alpha \). It turns out that, for 2-BEC and for the case that both \( u/r \) and \( v/r \) are nonzero at \( r = 0 \), the overlap of the wave functions from TFA and beyond TFA overlap nicely (refer to Fig.1a and 1b of \[19\]). Therefore, \( N_A \) and \( N_B \) obtained via eqs. (4) is reliable.

\begin{table}[h]
\centering
\caption{The root mean square radii and \( \alpha'/\alpha \).
\begin{tabular}{cccc}
\hline
\( \alpha \) & \( R_{\text{TFA}} \) & \( R_{\text{exac}} \) & \( \alpha'/\alpha \) \\
\hline
10\(^1\) & 1.783 & 1.883 & 1.311 \\
10\(^2\) & 2.826 & 2.859 & 1.059 \\
10\(^3\) & 4.480 & 4.490 & 1.011 \\
10\(^4\) & 7.100 & 7.103 & 1.002 \\
\hline
\end{tabular}
\end{table}

In conclusion, we have proposed an approach helpful to the determination of the particle numbers, at least in the qualitative aspect. This approach is limited to the case that the numbers of both kinds of atoms are huge and they have nonzero distribution at the center. Incidentally, if the parameters other than \( N_A \) and \( N_B \) are tuned to ensure \( r_{\text{exac}} \), then eqs. (4) together will lead to the equation given as eq.(6) in the preprint \[25\] which can be used to determine the ratio of the two particle numbers.

Acknowledgments

Supported by the National Natural Science Foundation of China under Grants No.11372122, 11274393, 11574404, and 11275279; the Open Project Program of State Key Laboratory of Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences, China; and the National Basic Research Program of China (2013CB933601); and Guangdong Natural Science Foundation (2016A030313313).
Appendix: Analytical solutions of the CGP under TFA for the case related to this paper

Let \( Y_1 = \frac{1}{2}(\alpha_2 - \beta_1)/(\alpha_1\alpha_2 - \beta_1\beta_2) \) and \( Y_2 = \frac{1}{2}(\alpha_1 - \beta_2)/(\alpha_1\alpha_2 - \beta_1\beta_2) \). For the case that both \( u/r \) and \( v/r \) are nonzero at \( r = 0 \) and \( u/r \) has a narrower distribution, \( u \) is distributed in the domain \((0 \leq r \leq \frac{\sqrt{5} \varepsilon}{Y_1})\) and appears as

\[
\frac{u^2}{r^2} = X_1 - Y_1 r^2
\]

where \( X_1 = \frac{(15/2)^{2/3}Y_1^{2/3}}{2} \). \( v \) is distributed in the domain \((0 \leq r \leq \frac{\sqrt{2} \varepsilon}{Y_1})\), when \( r \leq r_a \),

\[
\frac{v^2}{r^2} = X_2 - Y_2 r^2
\]

where \( X_2 = \frac{(\varepsilon - \beta_2 X_1)}{\alpha_2} \). When \( r_a < r \leq \frac{\sqrt{2} \varepsilon}{Y_1} \),

\[
\frac{u^2}{r^2} = 0
\]

\[
\frac{v^2}{r^2} = \frac{1}{\alpha_2}(\varepsilon - r^2/2)
\]

when \( r > \sqrt{2} \varepsilon_2 \), both \( u \) and \( v \) are zero. Thus \( r_a \) and \( \sqrt{2} \varepsilon_2 \) mark the borders for the A-atoms and B-atoms, respectively. Incidentally, when \( X_1 \) and \( X_2 \) are known, \( \varepsilon_1 \) is related to them as \( \varepsilon_1 = \alpha_1 X_1 + \beta_1 X_2 \).

One can check directly that the above \( u \) and \( v \) satisfy the CGP, they are normalized, and they are continuous at the borders (however their derivatives are not).

Obviously, the above solution would be physically meaningful only if the W-strengths are so preset that \( Y_1 > 0 \) and \( \alpha_2 + \beta_2 > 0 \) are ensured. To ensure \( \sqrt{2} \varepsilon_2 > r_a \), \( Y_1 \geq Y_2 \) is required. Besides, to ensure both \( u/r \) and \( v/r \) being \( \geq 0 \) at \( r = 0 \), \( X_2 \geq 0 \) (equivalently, \( 2(\alpha_2 + \beta_2)Y_1^{2/3} \geq 2 \beta_2 Y_1 \)) is required. These requirements imply that the suitable W-strengths will be constrained in a subspace of the whole parameter-space.

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