Beats and expansion of two-component Bose–Einstein condensates in the Thomas–Fermi limit

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Abstract
A unique feature of multi-component Bose–Einstein condensates (BECs) is the possibility of beating frequencies in collective oscillations. We analytically determine this beating frequency for the two-component BEC in one-dimension. We also show that the Thomas–Fermi approximation, where the quantum pressure is neglected, describes well the expansion of the two-component condensate released from an harmonic trap.

Keywords: Bose–Einstein condensates, two-component, Thomas–Fermi

(Some figures may appear in colour only in the online journal)

1. Introduction
Two-component Bose–Einstein condensates (BECs) now form a rich area of theoretical and experimental investigation. Two-component BECs have been realized with two different hyperfine spin states of $^{87}$Rb [1–7], different atomic species [8–11], and different isotopes of the same atomic species [12]. They have been shown to exhibit miscible and immiscible behaviour [2, 7, 12], modulation instabilities [13, 14], dark–bright solitons [15, 16], and vortices [17, 18]. A unique feature of multi-component BECs, is the possibility of beating frequencies; this has been seen in numerical investigations [19] and for the special case of dark–dark solitons, even experimentally observed [20].

This exhibition of a large range of interesting behaviour is the result of the numerous tunable parameters: atom number, mass, interaction strength, trapping frequency, and trap ellipticity for each species or component. In fact the vast parameter space means that it is difficult to fully investigate with computer simulations alone, and analytical solutions are needed. To make the equations tractable, the Thomas–Fermi (TF) approximation is used: in this approximation the kinetic term is either completely or partially ignored. Equations of motion (EOM) for two-components BECs have been developed using the TF approximation [19, 21]. In this work, we will show that such analytical equations can capture the beating frequencies of two-component BECs, which have previously been seen in numerical simulations but only qualitatively described. We will also confirm that these EOM are valid for the case of an expanding two-component BEC released from a trap.

In section 2 we present the coupled Gross–Pitaevskii equation (GPE) and its hydrodynamical form, and discuss the validity of the TF approximation. In section 3 we consider the small oscillation regime to analytically calculate the beating frequencies of two-component BECs. In section 4 we consider the large amplitude regime to analytically determine the dynamics of the expansion of the two-component BEC released from a trap. In both sections 3 and 4 we will confirm the correctness of our analytical predictions with numerical results.

2. The hydrodynamical equations in the TF limit
In the limit of near-zero temperatures, the mean-field of the two-component BEC is well-described by the coupled GPE [22]. We consider the extreme asymmetrical potential $V = m(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2)/2$, where $\omega_x, \omega_y, \omega_z \gg \omega_t$. Numerous experiments with BECs in such extremely
asymmetrical traps have been performed [23–25]. For convenience we will assume that the mass, \( m \), number of atoms, \( N \), and trapping frequencies, \( \omega \), of the two components are identical, so that the variable parameter is the interaction matrix, 
\[
g = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}.
\]
An effective one-dimensional (1D) GPE describes this system
\[
\frac{d^2 \tilde{\psi}_{\ell,x}}{d t^2} = \left( -\frac{\partial^2}{2 \partial x^2} + \tilde{\alpha}(t) \frac{x^2}{2} + \tilde{g}_l \left[ \tilde{\psi}_{\ell,x} \right]^2 + \tilde{g}_h \left[ \tilde{\psi}_{\ell,x} \right]^2 \right)
\times \tilde{\psi}_{\ell,x},
\]
where \( \ell \neq \ell' \) subscripts (\( \ell = 1, 2 \)) mark the components. The tilde indicates that we have used the typical rescaling of variables to get a dimensionless GPE [26, 27]: \( \tilde{\psi} = \frac{\psi}{\rho \alpha} \), \( \tilde{\alpha} = \frac{\alpha(t)}{\rho \alpha} \), \( \tilde{g}_l = \frac{g_{\ell\ell}}{\rho \alpha} \), \( \tilde{g}_h = \frac{g_{hl}}{\rho \alpha} \), \( \tilde{\omega} = \frac{\omega}{\rho \alpha} \), \( \tilde{L} = \frac{L}{\sqrt{m \rho}} \), is the harmonic oscillator length scale and \( \rho \alpha \) the condensate density. As energy along the \( x \)-axis is much larger than along the \( y \)-axis, we make the approximation that there is no excitations in the \( y \), \( z \)-direction. This leads to \( \tilde{g} = \frac{g_{l}(0)\rho(0)}{2m_0(0)} \) [27–30]. With this understanding, we will drop the use of the tilde and co-ordinate subscript.

When there are a lot of particles and the mean-field energy is large compared to the kinetic energy, the TF approximation, where the kinetic term of the GPE is ignored, has been shown to provide a good estimate of the ground state of the time-independent single-component GPE [31]. The validity of the TF approximation in the two-component case, is further restricted to the regime \( g_{12} \ll |g_{11}|, |g_{22}| \) [32]. The groundstate in the TF limit is given by \( \rho_{\ell,ll}^g = \rho_{\ell,l}^g H \left( \rho_{\ell,l}^g \right) H \left( \rho_{\ell,l}^g \right) + \rho_{\ell,l}^g H \left( -\rho_{\ell,l}^g \right) H \left( \rho_{\ell,l}^g \right) \),
\[
\rho_{\ell,l}^g = \frac{g_{\ell l}(\mu_l - V_l) - g_{l h}(\mu_l - V_l)}{|g_l|},
\]
where \( \rho_{\ell,l}^g = \frac{g_{l l}^g}{g_{l h}} \)
\[
\rho_{\ell,l}^g = \frac{g_{l l}^g}{g_{l h}} \frac{\mu_l - V_l}{|g_l|}.
\]

H is the Heaviside step function, and \( \mu_l \) is the chemical potential of component \( \ell \). The superscripts \( o \) and \( s \), indicate regions where the components overlap and are singular, respectively. Figure 1 compares groundstates under the TF approximation with groundstates numerically calculated from the full two-component GPE in a 1D harmonic trap: the TF approximation of the groundstate of the time-independent coupled GPE worsens as \( g_{12}^2 / |g_{11}|, g_{22}^2 \rightarrow 1 \). The TF approximation can also yield asymmetrical groundstate solutions [33], which we will not consider in this work.

By writing the complex order parameter in terms of a density and a phase, \( \psi(x,t) = \rho_l(x,t) e^{i\phi_l(x,t)/\beta} \), the GPE can be reformulated into a set of coupled hydrodynamical equations. In this formulation the kinetic component is split into a phase gradient dependent component \( (m v_l^2 / 2) \) and a density gradient dependent component, known as the quantum pressure \( (\hbar^2 / 2m) \partial^2 \phi_l^2 / \partial x^2 \); the velocity is defined as \( v_l = \frac{1}{m} \frac{\partial \phi_l}{\partial t} \). As \( v_l \) gives the velocity of the condensate flow, we will refer to \( m v_l^2 / 2 \) as the current energy. When the number of particles is large the density profile becomes smooth, and the quantum pressure term can be neglected [34]. In this TF limit, the hydrodynamical equations for the two-component BEC are
\[
-\frac{\partial \rho_l}{\partial t} = \frac{\partial (\rho_l v_l)}{\partial x},
\]
\[
-m_l \frac{\partial v_l}{\partial t} = \partial \left( V_l + g_{ll} \rho_l + g_{lh} \rho_l + \frac{1}{2} m_l v_l^2 \right).
\]

This hydrodynamical formulation of the GPE will prove useful in the analyses of the following sections.

3. Beat frequency

Investigations into collective oscillations were among the first experiments conducted following the realization of BECs. These excitations can be introduced with modulations in the natural frequency of the trapping potential [35–40] or the s-wave scattering length [41, 42]. Investigations into two-component oscillations have been studied both analytically [19, 21, 43] and numerically [19, 44–46]. In particular, beating frequencies were seen in the numerical simulations of [19]. The presence of these beating frequencies were only qualitatively described in this work. In this section we will analytically quantify this beating frequency for the 1D case.

Small amplitude oscillations can be analysed by linearizing the hydrodynamical (equations (5) and (6)) around their equilibrium values: \( \rho_l = \rho_l^{\infty} + \delta \rho_l \), and \( v_l = \delta v_l \). We further make the restriction that the two components of the BEC completely overlap (we will also show how the results degrade as we move away from this regime). This assumption is most valid for miscible systems [19]. The linearize hydrodynamical equations are
\[
\frac{\partial^2 \delta \rho_l}{\partial t^2} = \frac{1}{m} \frac{d}{dx} \left[ \rho_l^{\infty} \frac{d}{dx} \left( g_{ll} \delta \rho_l + g_{lh} \delta \rho_l \right) \right].
\]
An analytical solution to equation (7) is given by the ansatz \( \delta \rho_l(x, t) = \alpha_{l0}(t) - \alpha_{l1}(t) x^2 \), where the time dependence of \( \alpha_{l0}(t) \) are determined by the conditions \( \int dx \delta \rho_l = 0 \) [19]. One then immediately recognizes equation (7) as an equation for coupled oscillators,
\[
\frac{d^2}{dt^2} \left( \alpha_{l1} \right) = \begin{pmatrix} \kappa_{l1} & \kappa_{l2} \\ \kappa_{l2} & \kappa_{l2} \end{pmatrix} \frac{d}{dt} \begin{pmatrix} \alpha_{l1} \\ \alpha_{l2} \end{pmatrix},
\]
where \( \kappa_{l1} = 3\alpha_0^2 \left( g_{l l} - g_{l h}^2 \right) / |g_l| \). The solution to equation (8) takes the form \( \alpha_l = \Lambda_l e^{i\Omega_l t} \). Substitution of this solution into equation (8) and solving the resulting eigen value equations gives the normal mode frequencies \( \Omega_+ = \sqrt{3 \gamma_0} \) and \( \Omega_- = \sqrt{3 \gamma} \), where \( \gamma = \sqrt{\left( g_{ll} - g_{lh}^2 \right) / \left( 2 g_{ll} \right) \left( \left( g_{ll} - g_{lh}^2 \right) / \left( g_{ll} \right) \right) / |g_l|} \). Note
that as we are assuming positive interaction strengths, in the TF limit where $g_{12} \gg g_{11}, g_{22}$, $\gamma$ is upper bounded by 1. Analogous to the classical problem of two coupled oscillators, the difference in the normal mode frequencies give the beating frequency

$$f_b = \frac{\Omega^+ - \Omega^-}{2} = \frac{\sqrt{3}}{2}(1 - \gamma)\omega.$$  \hspace{1cm} (9)

In figure 2 we compare equation (10) with the results of numerical simulations. In our simulation, the BEC is initially in the groundstate of a trapping potential with frequency $\omega(0) = 1$. We excite the collective oscillation by perturbing the trapping potential, $\omega(t > 0) = 1.1$. Figure 2(a) compares the analytical and numerically beating frequencies as a function of $\gamma$. It shows that equation (10) corresponds well with the numerical results when it is in its region of applicability i.e. when the two components overlap and their density distribution are approximately quadratic (e.g. Figure 1(a)). However as $\gamma$ approaches zero, these assumptions are violated (e.g. Figure 1(b)), and equation (10) is no longer applicable. Figure 2(b) plots the mean-squared displacement $<x^2> \equiv \int \rho_1(x,t)x^2dx$ for $\gamma = 6/7$, showing the typical beating characteristic of the two-component BEC.

The energy of the system is composed of an interaction and kinetic component. The interaction energy is given by $E^\text{int}_t = \int (\frac{g_{11}}{2}\rho_1^2 + \frac{g_{12}}{2}\rho_1\rho_2)dx$. The kinetic energy, $E^\text{kin}_t = E^\phi_t + E^Q_t$, is composed of the current energy $E^\phi_t = \frac{1}{2}m_j<v_t^2>$ and the quantum pressure $E^Q_t = \int \frac{1}{2m} |\partial_x\sqrt{\rho}|^2dx$. The TF approximation assumes that $E^Q_t = 0$. Figures 2(c) and (d) plots $E^Q_t$ and $E^\phi_t$ respectively. It is interesting to point out that the quantum pressure here plays the dominate role in the kinetic energy, drastically violating the TF assumption that $E^Q_t = 0$. In spite of this crude approximation, the fact that equation (10) can accurately predict the beat frequency, speaks of the usefulness of the TF approximation.

4. Expansion of released BECs

The method used in the previous section is only valid for small amplitude oscillations. Following the method of [38], [19] developed EOM for two-component BECs which do not
linearize the hydrodynamical equations. In this section we will confirm that these EOM are valid even in the infinite amplitude case of the expanding cloud of BEC released from its trapping potential in 1D. We also relax the assumption that the components need to be completely overlapping.

Following the method of [19, 38] we present here the EOM in 1D. The 1D hydrodynamical equations (equations (5) and (6)) admit a class of analytical solution with the same form as equation (2) but with the ansatz

\[ \rho_n^\alpha(t, x) = \alpha_n^\alpha(t) x^2, \]

\[ v_n^\alpha(t, x) = \beta_n^\alpha(t) x, \]

where \( n = \alpha, s \) indicates whether one is in the overlap or singular region. Substitution of equations (11) and (12) into the hydrodynamical equations yield the following constraints

\[ -\alpha_n^\alpha = 3\alpha_n^\beta \beta_n^\alpha, \]

\[ -\beta_n^\alpha = (\beta_n^\alpha)^2 + \omega(t)^2 - \frac{2g_{II}}{m} \alpha_n^\alpha \]

These equations are further simplified by introducing dimensional parameter \( \lambda_n^d \), defined by \( \alpha_n^\alpha = \frac{g_{II}}{2g_{g I}} \lambda_n^d \) and \( \alpha_n^{\lambda} = \frac{1}{2g_{g I}} \lambda_n^d \). With this substitution, equation (13) reduces to \( \dot{\beta}_n^\alpha = \dot{\lambda}_n^\alpha \lambda_n^\alpha \) and equations (14) and (15) become

\[ \dot{\lambda}_n^d = \frac{g_{II}(g_{II} - g_{g I})}{|g|} + \frac{g_{II}(g_{II} - g_{g I})\lambda_n^d}{|g|} = \omega(t)^2 \lambda_n^d, \]

\[ \dot{\lambda}_n^s = (\lambda_n^s)^2 - \omega(t)^2 \lambda_n^d. \]

Equations (16) and (17) represent the EOM of the two-component BEC in the TF limit in 1D. For completeness a derivation for the general 3D case, in the notation used in this paper, can be found in appendix A. Equations (16) and (17) form six coupled second-order differential equations for the overlap and singular regions respectively. The last terms of equations (16) and (17) represent the effects of the confining potential, whereas the other term arises from the particle–
particle interactions. In the overlap region the dynamics of the system is dependent on the intra- and inter-component interaction strengths. In the singular region the dynamics of the system are independent of the interaction strengths, as is the case for single component dynamics in the large particle number limit [37]. The solutions of equations (16) and (17) determine $\alpha_t^{1,0}(t)$.

$\alpha_t^{1,0}(t)$ are determined by boundary conditions. We consider the case when $g_{11} < g_{22}$, such that component 1 will never form a singular region; in the TF limit, component 2 will form singular regions surrounding component 1 (note the situation is simply reversed for $g_{11} > g_{22}$). Application of the conditions of normalization and continuity at the overlap-singular boundary yield (see appendix B)

\[
\alpha_{1,0}^t(t) = \left( \frac{3}{2} \sqrt{\alpha_t^1(t)} \right)^{2/3}, \quad (18)
\]

\[
\alpha_{2,0}^t(t) = \left( \frac{3 - 12(\alpha_t^1(t) + \alpha_t^2(t))}{8\alpha_t^1(t)} \right)^{2/3}, \quad (19)
\]

\[
\alpha_{2,0}^t(t) = \alpha_{1,0}^t(t) + \left( \frac{3}{2\alpha_t^1(t)} \right)^{2/3} \left[ \alpha_t^2(t) + \alpha_t^2(t) \right]. \quad (20)
\]

The overlap-singular boundary occurs at $R_t(t) = \sqrt{\alpha_{1,0}^t(t)/\alpha_{2,0}^t(t)} = \left[ \frac{3}{2\alpha_t^1(t)} \right]^{2/3}$. The location where the density vanishes (which gives the condensate width) is given by $R_t(0) = \sqrt{\alpha_{1,0}^t(0)/\alpha_{2,0}^t(0)}$.

The confining potential in the $x$-direction is switched off in our model by setting $\omega(t > 0) = 0$ in equations (16) and (17). We then solve these EOM to predict the dynamics of the released gas.

Figure 3 compares the evolution of the released gas as predicted by the EOM with computer simulations of the full model. The top plots show the mean-square displacement for $g_{12}^2/g_{11}g_{22} = 5 \times 10^{-3}$ and 0.5. The bottom plots of figure 3 show the normalized population distribution at $t = 0$ and 10. Figure 3 shows that the EOM is a good approximation of the expansion of the two-component released gas, being more accurate as one approaches the TF regime, $g_{12} \ll |g_{11}|, |g_{22}|$.

One can also use the EOM to calculate the release energy of the BEC. Using the solutions of the EOM, figure 4 plots the kinetic energy and interaction energy of the released BEC in the TF limit, and compares it to the simulated kinetic and interaction energies.

Figure 4 shows that as the BEC expands the interaction energy is converted to kinetic energy. The EOM provides a good approximation of the release energy of the BEC.

5. Conclusion and outlook

We have derived an analytical formulation for the beating frequencies seen in two-component BECs. We have also
confirmed that the large oscillation amplitude EOM for two-component BECs are valid even in the infinite oscillation amplitude case of the freely expanding condensate. The formulation and analysis in this work contributes to a better understandings of the large multivariate parameter space that characterizes two-component BEC systems. It would be interesting in further work to extend the analysis of the beating frequencies to 3D. This extension however is non-trivial, as the extra dimensions introduce other modes of oscillations, such as the quadrupole and scissors modes. Nevertheless, our work should provide a framework upon which a generalization can be achieved.

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Appendix A. Generalization of the EOM to 3D

In this appendix we generalize the EOM two-component BECs to 3D. Here we provide the general case were the mass and number of atoms of each of the components may differ, and the trapping frequencies in the three spatial directions are free to vary. Note that this derivation is independent of parameter rescaling.

In the TF limit, the 3D hydrodynamical equations for the two-component BEC are

\[ -\frac{\partial \rho_1^a}{\partial t} = \nabla \cdot (\mathbf{v}_1 \rho_1), \]  
\[ -m_1 \frac{\partial \mathbf{v}_1}{\partial t} = \nabla \left( \rho_1 \mathbf{v}_1 + g_{11} \rho_1 + g_{12} \rho_2 + \frac{1}{2} m_1 \nabla^2 \mathbf{v}_1 \right). \]  

A solution to the 3D hydrodynamical equations has the same form as equation (2) but with the ansatz

\begin{equation}
\psi_i^n(t, \mathbf{r}) = \alpha_i^n(t) + \beta_i^n(t) \mathbf{x}^2 - \alpha_i^n(t) \mathbf{y}^2 - \alpha_i^n(t) \mathbf{z}^2, \tag{A.3}
\end{equation}

\begin{equation}
\mathbf{v}_i^n(t, \mathbf{r}) = \frac{1}{2} \nabla \left[ \beta_i^n(t) \mathbf{x}^2 + \beta_i^n(t) \mathbf{y}^2 + \beta_i^n(t) \mathbf{z}^2 \right]. \tag{A.4}
\end{equation}

where \( n = \alpha, \sigma \) indicates whether one is in the overlap or singular region. Substitution of equations (A.3) and (A.4) into the hydrodynamical equations yield the following constraints

\[ -\dot{\alpha}_i^n = 2m_\alpha \rho_1^n \beta_i^n + m_\alpha \sum_\beta \rho_\beta^n, \tag{A.5}\]

\[ -\dot{\beta}_i^n = \left( \beta_i^n \right)^2 + \alpha_i^n - \frac{2g_{11}}{m_1} \alpha_i^n - \frac{2g_{12}}{m_1} \beta_i^n, \tag{A.6}\]

\[ -\dot{\gamma}_i^n = \left( \gamma_i^n \right)^2 + \alpha_i^n - \frac{2g_{11}}{m_1} \alpha_i^n, \tag{A.7}\]

where \( i, j = x, y, z \). These equations are further simplified by introducing adimensional parameter \( \lambda_i^n \), defined by

\[ \alpha_i^n = \frac{m_\alpha \rho_1^n (\mathbf{0}_{0} - \mathbf{g}_{0,0})}{g_{11} \mathbf{x}^2 \prod \lambda_i^n} \text{ and } \beta_i^n = \frac{m_\alpha \rho_1^n (\mathbf{0}_{0} - \mathbf{g}_{0,0})}{g_{12} \mathbf{x}^2 \prod \lambda_i^n}. \]

With this substitution, equation (A.5) reduces to \( \dot{\lambda}_i^n = \dot{\lambda}_i^n / \lambda_i^n \) and equation (A.6) and equation (A.7) become

\[ \dot{\alpha}_i^n = \frac{g_{11} (\mathbf{g}_{0,0} - \mathbf{g}_{0,0}) \alpha_i^n (0)^2}{\mathbf{g} \cdot \prod \lambda_i^n} \]  
\[ + \frac{g_{11} (\mathbf{g}_{0,0} - \mathbf{g}_{0,0}) m_\alpha \alpha_i^n (0)^2 \lambda_i^n}{\mathbf{g} \cdot \prod \lambda_i^n} - \omega(t)^2 \lambda_i^n, \]  
\[ \dot{\lambda}_i^n = \frac{\alpha_i^n (0)^2}{\mathbf{g} \cdot \lambda_i^n \prod \lambda_i^n} - \omega(t)^2 \lambda_i^n. \]  

Equations (A.9) and (A.10) represent the EOM of the two-component BEC in the TF limit. Their solutions determine \( \alpha_i^n (t), \beta_i^n (t) \) are determined by conditions of continuity at the overlap-singular boundary \( \rho_1^n (\mathbf{R}) = \rho_2^n (\mathbf{R}) \) (where \( \mathbf{R} \) locates the boundary), and normalization, \( N_i = \int \rho_i^n (\mathbf{r}) d\mathbf{r} \).

Appendix B. Overlap-singular boundary conditions for 1D

Applying the normalization condition (\( \int |\psi_i|^2 d\mathbf{r} = 1 \)) to component 1

\[ \int_{-R(t)}^{R(t)} \alpha_{1,0}^n (t) - \alpha_{1,0}^n (t) x^2 d\mathbf{x} = 1, \]  
we solve for \( \alpha_{1,0}^n (t) \)

\[ \alpha_{1,0}^n (t) = \left[ \frac{3}{2} \sqrt[3]{\alpha_{1,0}^n (t)} \right]^{2/3}. \]
Similarly for component 2
\[
\int_0^{R_2(t)} \alpha_{2,0}^2(t) - \alpha_2^2(t) x^2 dx \\
+ \int_{R_1(t)}^{R_2(t)} \alpha_{2,0}^2(t) - \alpha_2^2(t) x^2 dx = 1/2,
\]
we get
\[
\alpha_{2,0}^2(t) = \left\{ \frac{3 - 12 \sqrt{\alpha_1^2(t)} \left[ \alpha_2^2(t) + \alpha_3^2(t) \right]}{8\alpha_1^2(t)} \right\}^{2/3}.
\]

Finally we apply the continuity condition \( \rho_1^0(R_1, t) = \rho_2^0(R_1, t) \), to get,
\[
\alpha_{2,0}^2(t) = \alpha_{2,0}^2(t) + \left[ \frac{3}{2\alpha_1^2(t)} \right]^{2/3} \left[ \alpha_2^2(t) + \alpha_3^2(t) \right].
\]

Note that the overlap-singular boundary (where \( \rho_1^0 = 0 \)) occurs at \( R_1(t) = \sqrt{\alpha_{1,0}^2(t)/\alpha_1^0(t)} = \left[ \frac{3}{2\alpha_1^0(t)} \right]^{1/3} \). Similarly, \( R_2(t) = \sqrt{\alpha_{2,0}^2(t)/\alpha_2^0(t)} \).

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