Waves on an interface between two phase-separated Bose-Einstein condensates

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We examine waves localized near a boundary between two weakly segregated Bose-Einstein condensates. In the case of a wavelength of order of or larger than the thickness of the overlap region the variational method is used. The dispersion laws for the two oscillation branches are found in analytic form. The opposite case of a wavelength much shorter than the healing length in the bulk condensate is also discussed.

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The studies of mixtures of two superfluid Bose liquids ascend to the early work by Khalatnikov [2] who determined the possible sound modes in such a system within a macroscopic (hydrodynamical) approach. Later a microscopic theory was developed: Bassichis [3] considered a neutral mixture of two charged Bose gases with Coulomb interactions, and Nepomnyashchii [4] considered a system composed of bosons of two kinds interacting via short-range potentials. In Ref. [3], most closely related to the case of a two-component degenerate dilute atomic vapor, the two-branch spectrum of elementary excitations and following from it criterion for stability of the ground state were found.

The advances in experiments on Bose–Einstein condensation of trapped alkali atoms gave rise to an interest to this subject. The ground state configuration of a two-component atomic Bose–Einstein condensate (BEC) in the presence of a harmonic confining potential at zero temperature was calculated by Ho and Shenoy [5] in the Thomas–Fermi limit. The collective oscillation frequencies for trapped binary BECs were also determined [5–7]. Interesting numerical results are obtained by Pu and Bigelow [8]. These studies reveal that if the number of trapped atoms of each kind is large enough, the ground state physics can be qualitatively understood from the arguments valid for a case of absence of a trap [9]. In the latter case, the ground state properties are determined by a certain relation between the coupling constants. Namely, if the intercomponent repulsion (we do not consider attractive potentials in the present paper) is small enough, i.e., if \( g_{12} < \sqrt{g_{11}g_{22}} \), where \( g_{ij} = 2\pi\hbar^2\left(m_{i}m_{j}/(m_{i} + m_{j})\right)^{-1}a_{ij} \), \( a_{ij} \) is the corresponding s-wave scattering length of a pair of ultracold atoms when one of them is of the \( j \)th kind, the other is of the \( i \)th kind, \( m_{j} \) is the mass of an atom for the \( j \)th component of the mixed BEC, \( i, j = 1, 2 \), then the two degenerate Bose gases are miscible, i.e. they co-exist in all the volume. In the opposite case, \( g_{12} > \sqrt{g_{11}g_{22}} \), the two components are immiscible and separated in space. In the latter case, a new physics related to the intercomponent boundary arises. The steady-state energetics of such an interface was estimated by Timmermans [9]. Ao and Chiu [10] performed more detailed analysis, in particular, they found that there are two different regimes called, correspondingly, weakly and strongly segregated phase. The former one takes place if \( g_{12} \) exceeds \( \sqrt{g_{11}g_{22}} \) only slightly. In such a case the component interpenetration depth is quite large and proportional to \( \gamma^{-1/2} \), where

\[
\gamma = g_{12}(g_{11}g_{22})^{-1/2} - 1. \tag{1}
\]

The latter limiting case can be achieved provided that \( \gamma \gg 1 \), under such a condition the density profile at the intercomponent boundary has quite a different shape and its thickness is determined by individual healing lengths for the bulk condensates.

There are also experimental works on two-component BECs made by the JILA and NIST group [11,12] and by the MIT group [13]. The JILA and NIST group created binary mixtures of ultracold bosons by populating different magnetic sublevels, \(|F, m_F⟩ \) of \(^{87}\)Rb. It is worth to note that a mixture of the \(|2, 2⟩ \) and \(|1, −1⟩ \) exhibits behaviour of a miscible system [14] (cf. the related theoretical paper [14]), and the mixture of the \(|2, 1⟩ \) and \(|1, −1⟩ \) looks like an example of a weakly segregated system [15].

In the present paper, we consider normal modes for intercomponent boundary oscillations in the weakly segregated phase regime, i.e., for \( 0 < \gamma \ll 1 \), since a study of excited states of an immiscible system was lacking up to now. The Bogoliubov spectrum of a translationally invariant mixed BEC was obtained in Ref. [3], but it revealed only the fact that such a homogeneous system is dynamically unstable against long-wavelength perturbations and, hence, tends to become phase-separated. One can think that dynamics of a phase separated system with an interface between the components 1 and 2 in the long-wavelength regime is adequately described by a concept of a surface tension with the surface tension constant inferred from the ground state properties [9]. However, a rigorous proof of this result was still lacking. In the present paper, we fill this gap and examine also the opposite (short-wavelength) regime.

Let us introduce two macroscopic wave functions for the components \( j = 1, 2 \) as \( \sqrt{n_{j}}Φ_{j}(r,t) \exp(−iμ_{j}t/\hbar) \), where \( μ_{j} = ℏg_{jj}n_{j} \) is the chemical potential of the corresponding component, and \( n_{j} \) is its bulk number density. In the present paper, we consider a case of absence of
any external potential, so the coupled set of the Gross–Pitaevskii equations is reduced to

\[ i\dot{\Phi}_1 = -\frac{\hbar}{2m_1} \nabla^2 \Phi_1 - \frac{\mu_1}{\hbar} \Phi_1 + g_{11} n_1 |\Phi_1|^2 \Phi_1 + g_{12} n_2 |\Phi_2|^2 \Phi_1, \]

\[ i\dot{\Phi}_2 = -\frac{\hbar}{2m_2} \nabla^2 \Phi_2 - \frac{\mu_2}{\hbar} \Phi_2 + g_{22} n_2 |\Phi_2|^2 \Phi_2 + g_{12} n_1 |\Phi_1|^2 \Phi_2. \]

We consider a case of two immiscible BECs. We denote the component occupying a semi-infinite space left to the boundary, i.e., the plane that can be associated with the intercomponent ground state solution for \( \Phi \). We consider a case of two immiscible BECs. We denote the component occupying a semi-infinite space left to the boundary, i.e., the plane that can be associated with the intercomponent ground state solution for \( \Phi \). We consider a case of two immiscible BECs. We denote the component occupying a semi-infinite space left to the boundary, i.e., the plane that can be associated with the intercomponent ground state solution for \( \Phi \). We consider a case of two immiscible BECs. We denote the component occupying a semi-infinite space left to the boundary, i.e., the plane that can be associated with the intercomponent ground state solution for \( \Phi \).

We approximate the latter quantity by the following decomposition in series:

\[ \theta = \sum_{n=0}^{\infty} \theta^{(n)}, \]

where \( \theta^{(n+1)} / \theta^{(n)} = O(\gamma) \). The second unknown function, \( \alpha \), can be treated in a similar way. It is quite easy to find a solution in the lowest order approximation, when we omit the third and fourth terms in the right hand side of Eq. 1 and substitute \( \theta^{(0)} \) instead of \( \theta \) into Eq. 1:

\[ \theta^{(0)} = 1, \quad \alpha^{(0)} = \text{arctan} e^{\nu \gamma z}. \]  

The "slowly varying co-ordinate" \( \sqrt{\gamma} z \) is treated here as a quantity of order of unity. Then we find from Eq. 1 the first order correction to \( \theta \). If we substitute \( \theta = \theta^{(0)} + \theta^{(1)} \) into Eq. 1 and linearize this equation with respect to \( \theta^{(1)} \) we get

\[ \theta^{(1)} - 2\theta^{(2)} = 3 \gamma \cos^2 \alpha^{(0)} \sin^2 \alpha^{(0)}. \]

Then it is important to note that \( \theta^{(1)} \) is of order of \( \gamma^2 \) rather than of \( \gamma^1 \) and, hence, have to be omitted when we find the first order correction which, finally, can be written as

\[ \theta^{(1)} = -\frac{3 \gamma}{2} \frac{e^{2\sqrt{\gamma} z}}{1 + e^{2\sqrt{\gamma} z}}. \]

Note, that only zeroth order approximation for \( \alpha \) is necessary for determination of \( \theta^{(1)} \).

After Eq. 2 has been obtained, we can find the first order correction to \( \alpha \). We approximate the latter quantity by the following formula:

\[ \alpha = \text{arctan} e^{\nu \gamma z + g(\sqrt{\gamma} z)}, \]

where \( g = O(\gamma) \). Substituting this approximation into Eq. 2 where \( \theta^{(0)} + \theta^{(1)} \) stands for \( \theta \), after some tedious calculations we obtain

\[ g = \frac{3 \gamma}{16} \tanh(\sqrt{\gamma} z). \]

Thus the steady state order parameter for the 1st component of the immiscible BEC with the \( O(\gamma^2) \) accuracy reads as

\[ \phi_1(z) = \frac{1}{\sqrt{1 + e^{\zeta z}}} \left[ 1 - \frac{3 \gamma}{2} \frac{e^{2\sqrt{\gamma} z}}{(e^{\sqrt{\gamma} z} + e^{-\sqrt{\gamma} z})^2} \right], \]

where

\[ \zeta = \sqrt{\gamma} z + \frac{3 \gamma}{16} \tanh(\sqrt{\gamma} z). \]

To find \( \phi_2(z) \), one simply have to apply Eq. 7. The analytic approximation given by Eqs. 13, 16 is justified by numerical calculations. The difference between the 0 analytic and numerical solutions behaves as \( O(\gamma^5) \) in a wide range of \( \gamma \) less than 0.1.
To investigate the long-wavelength oscillations, we apply the variational method analogous to that used in Ref. [10] to study the surface oscillations of a dense BEC in a trap. This method implies minimization of the action functional associated with the Lagrangian

\[ \mathcal{L} = \int d^3r \left[ -\frac{i}{2} (\Phi_1^* \dot{\Phi}_1 - \Phi_1 \dot{\Phi}_1^* + \Phi_2^* \dot{\Phi}_2 - \Phi_2 \dot{\Phi}_2^*) + (\nabla \Phi_1)(\nabla \Phi_1^*) + (\nabla \Phi_2)(\nabla \Phi_2^*) + \frac{1}{2} \Phi_1^* \Phi_1 + \frac{1}{2} \Phi_2^* \Phi_2 \right]. \]

(17)

For long-wavelength perturbations, we represent the test functions as

\[ \Phi_j = \left[ \left( \phi_j(z) + \beta_j(t) \cos(kx) \right) h_j(z) \frac{d}{dz} \phi_j(z) \right] \exp[i \xi_j(t) f_j(z) \cos(kx)], \]

(18)

\[ j = 1, 2. \] The quantity \(-\beta_j(t) h_j(z) \cos(kx)\) can be interpreted as a displacement in the \(z\)-direction of an element of a quantum gas that in the stationary case has the density \(\phi_j^2(z)\). The gradient of the phase \(\xi_j(t) f_j(z) \cos(kx)\) multiplied by two gives the velocity of the oscillating quantum gas.

Due to the problem symmetry,

\[ h_1(z) = h_2(-z). \]

(19)

The continuity equation implies that

\[ h_j(z) \frac{d}{dz} \phi_j^2(z) = -2 \frac{d}{dz} \left[ \phi_j^2(z) \frac{d}{dz} f_j(z) \right] + 2k^2 \phi_j^2(z) f_j(z), \]

(20)

\[ j = 1, 2. \] It is easy to see that it follows from Eqs. (18, 20) that

\[ f_1(z) = -f_2(-z). \]

(21)

In the long-wavelength case, when

\[ k \ll \sqrt{\gamma}, \]

(22)

the function \(h_j(z)\) varies on a spatial scale of order of \(k^{-1}\).

From the other hand, since \(h_j(z)\) appears in Eq. (18) only multiplied by \(d\phi_j^2(z)/dz\), one needs to know the exact behaviour of \(h_j(z)\) only for \(|z| \lesssim \gamma^{-1/2}\), provided that \(h_j(z)\) is finite outside this small range of \(z\). It means that, because of Eq. (24), one can choose

\[ h_j(z) = 1. \]

(23)

To find the quantity \(f_j(z)\), we use the technique of tailoring asymptotics. Namely, for large negative \(z\) (let say, for \(z \lesssim -\gamma^{-1/2}\)), where \(\phi_1^2(z) \approx 1\), Eq. (20) is reduced to

\[ \frac{d^2}{dz^2} f_1(z) = k^2 f_1(z), \]

and its solution approaching zero when \(z \to -\infty\) is

\[ f_1(z) = C_1 e^{kz}. \]

In the opposite case, in the range of \(z\) where \(\phi_1(z)\) rapidly decreases, the second term in the right hand side of Eq. (20) is negligible compared to the first one, because of the condition Eq. (22), and, hence,

\[ f_1(z) = C_2 - z/2. \]

The matching condition for these two asymptotics and their first derivatives allows us to determine the constants \(C_1\) and \(C_2\). Thus, in the subsequent calculations we use the following expression

\[ f_1(z) = -\frac{1}{2k} e^{kz} \Theta(-z) - \left( \frac{1}{2k} + \frac{z}{2} \right) \Theta(z), \]

(24)

where \(\Theta(z)\) is the Heaviside’s step function. This expression and its first derivative with respect to \(z\) are continuous everywhere, including the point \(z = 0\). The result of Eq. (24) is also justified by numerical calculations; \(f_2(z)\) is given by Eq. (21).

Then we write the Lagrange equations for the generalized coordinates \(\beta_j(t), \xi_j(t)\). First, two of these equations enable us to exclude the two variables \(\xi_j = \beta_j\). After this has been done, we arrive at the two equations containing \(\beta_1, \beta_2\) and describing two coupled harmonic oscillators.

The normal modes correspond to the two cases,

\[ \beta_1 = \zeta \beta_2, \quad \zeta = \pm 1. \]

For \(k \ll \sqrt{\gamma}\) their eigenfrequencies \(\omega_\zeta\) are given by

\[ \omega_\zeta^2 = 2 \int_{-\infty}^{\infty} dz \left\{ 2(1 + \gamma)(1 - \zeta) P(z) P(-z) + k^2 \left[ \frac{d}{dz} \phi_1(z) \right]^2 \right\} / \left[ \int_{-\infty}^{\infty} dz f_1(z) \frac{d}{dz} \phi_1^2(z) \right], \]

(25)

where \(P(z) = d\phi_1^2(z)/dz\).

If the exact ground state wave function is used in Eq. (25), then \(\omega_0\) is a rigorous upper bound to the oscillation frequency for the normal modes with no nodes along the \(z\)-axis. Expanding the right hand side of Eq. (25) in series in \(\gamma\) as well as in \(k\gamma^{-1/2}\) and retaining the leading terms, we obtain the following expressions for the lowest oscillation frequencies for two weakly segregated BECs in the long wavelength regime:

\[ \omega_{+1}^2 = \sqrt{\gamma} k^3, \]

(26)

\[ \omega_{-1}^2 = \frac{4}{3} \sqrt{\gamma} k. \]

(27)

Now we can clarify the physical meaning of the two branches of the dispersion law Eq. (25). The \(\zeta = +1\) branch corresponds to in-phase oscillations of the two components and represents interface bending. The wave number dependence, \(\omega_{+1} \propto k^{3/2}\) for \(k \to 0\), is specific for this type of surface waves (capillary waves) [17]. Also these interface oscillations are an analog of soft modes [18] in a mixture of miscible BECs with \(\gamma\) being very small by the absolute value. We call these oscillations “in-phase” because for them the \(z\)-projections of the velocities of both the two components have the same sign.
It is necessary to note that the value of $k^{-3} \omega^2_{+1}$ that is, in fact, the ratio of the surface tension constant to the sum of the bulk densities of the 1st and 2nd BEC components is equal to $\sqrt{\gamma}$, i.e., displays the correct dependence on $\gamma$ following from the surface tension energy estimation given by Timmermans [3].

The $\zeta = -1$ branch corresponds to the out-of-phase oscillations and, hence, to a time dependence of the depth of interpenetration of the two components. The dispersion law, $\omega^2_{+1} \propto k$, is analogous to that of surface waves on a boundary between a single component BEC and vacuum [6].

Now it is necessary to explain why in the present problem one cannot choose

$$f_1(z) = e^{kz}, \quad h_1(z) = -2ke^{kz}, \quad (28)$$

as it is done in Ref. [16]. The reason is that if one applies Eq. (28) then for $z \to +\infty$ the difference between the steady-state order parameter $\phi_1(z)$ and the time-dependent order parameter $\Phi_1(x, z, t)$ is much larger (by the exponential factor $e^{kz}$) than $\phi_1(z)$. So, the condition of the relative smallness of the order parameter perturbation breaks down, and the validity of the approach described above cannot be guaranteed. In Ref. [16], the condensate is assumed to fill only half of the space, and Eqs. (28) are used for $z < 0$ only, while the condensate density for $z > 0$ is identically zero, and no such a difficulty occurs.

In our case, the wrong choice of $h_j(z)$ and $f_j(z)$ given by Eq. (28) results in the correct value for $\omega^2_{+1}$ for $k \ll \sqrt{\gamma}$ but substantially, by a factor of order of $\gamma^{-1}$, overestimates the eigenfrequency for the in-phase mode. The latter result is apparently inconsistent with the surface tension estimations given in Ref. [1]. Moreover, use of Eq. (28), instead of Eqs. (23) [24], leads to an erroneous conclusion about non-monotonous behaviour of the dispersion laws for both the in-phase and out-of-phase oscillation when $k$ approaches $\sqrt{\gamma}$. Certainly, the latter is simply an artefact of ineligible choice of the test function.

Another important limiting case is the case of very short wavelengths, $k \gg 1$. Under this condition an elementary excitation is very close to a single particle excitation (in other words, the $v$ coefficient of the Bogoliubov’s transformation [2] is small compared to the $u$ coefficient). Thus, the oscillation frequency is the eigenvalue of the Hamiltonian problem

$$-u_1''(z) + [2\phi_1^2(z) + (1 + \gamma)\phi_1^2(-z) - 1 + k^2] u_1(z) + (1 + \gamma)\phi_1(z)\phi_1(-z)u_1(z) = \omega u_1(z), \quad (29)$$

$$-u_2''(z) + [2\phi_1^2(-z) + (1 + \gamma)\phi_1^2(z) - 1 + k^2] u_2(z) + (1 + \gamma)\phi_1(z)\phi_1(-z)u_1(z) = \omega u_2(z), \quad (30)$$

It is obvious that there are two types of solutions of this set of coupled Schrödinger equations corresponding to the in-phase ($\zeta = +1$) and out-of-phase ($\zeta = -1$) oscillations:

$$u_1(z) = -\zeta u_2(-z). \quad (31)$$

The set of Eqs. (29) [30] was solved taking into account the symmetry condition Eq. (31) by the Hamiltonian diagonalization in the basis of harmonic functions $L^{-1/2}\sin[\pi n(\zeta z + L)/(2L)], \quad m$ is a positive integer number, and $L$ is chosen to be much larger than $\gamma^{-1/2}$. The spectrum of the in-phase oscillations consists of the single discrete value equal to $k^2 + 0.32\gamma$ and the two branches of the continuous spectrum with the dispersion laws $k^2 + 1 + Q^2, \quad Q > 0$, and $k^2 + \gamma + q^2, \quad q > 0$. One branch corresponds to the incidence to the intercomponent boundary of sound waves from both the left and right sides, and $Q$ is the absolute value of the $z$-component of the wave vector of the incident wave. No atoms of one component are injected into the bulk of the condensate composed of atoms of another kind. In contrast, the second branch corresponds to injection of atoms of the 1st kind into the bulk of the condensate of atoms of the 2nd kind, and vice versa; $q$ is the $z$-projection of the momentum of an injected atom.

![FIG. 1. Numerical solutions of Eqs. (29) [30] the in-phase (solid line) and out-of-phase (dashed line) oscillations; $\gamma = 0.01$; $z$-coordinate is dimensionless, the eigenfunctions are plotted in arbitrary units.](image-url)
The eigenfunctions $u_\sigma(z)$ corresponding to the discrete
eigenfrequencies are shown in Fig. 1. Note, that the out-
of-phase oscillation is much localized than the in-phase one.

To summarize, we performed an analysis of dispersion of
dilute atomic BEC. For very small wavenumbers $k$ we recover usual capillary and surface waves, with frequency
proportional to $k^3$ and $k$, respectively. For large
wavenumbers, each of the two types of oscillations (the in-phase and out-of-phase modes) has only one particular
mode well localized in $z$-direction near the boundary. 
Other surface modes are associated to simultaneous emis-
sion of either sound into the bulk condensate or to free particles of one kind to the BEC composed of atoms of
another kind. The latter fact must make (due to the effect of quantum depletion) the depth of overlapping of the two weakly segregated ultracold bosonic clouds even larger than the simple mean-field theory predicts. This may be a very important cause of difficulties in an experimental determination of the parameter $\gamma$ [2].

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