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LETTER TO THE EDITOR

Excitations and phase segregation in a two-component Bose–Einstein condensate with an arbitrary interaction

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Abstract
Bogoliubov–de Gennes equations and the excitation spectrum of a two-component Bose–Einstein condensate (BEC) are derived with an arbitrary interaction between bosons, including long-range and short-range forces. Spectra of optical and acoustic plasmons (APs) are obtained. For the Coulomb interaction the AP has a quadratic long-wavelength dispersion in contrast with the linear dispersion in the normal-state two-component plasma. The nonconverting BEC mixture segregates into two phases for some two-body interactions. Gross–Pitaevskii equations are solved for the phase-segregated BEC. A possibility of boundary–surface and other localized excitations is studied.

Neutral and charged (Coulomb) Bose gases became recently of particular interest motivated by the observations of a Bose–Einstein condensate (BEC) in an alkali vapour [1–5] and by the bipolaron theory of high-temperature superconductors [6], respectively. Their theoretical understanding is based on the Bogoliubov [7] displacement transformation, separating a large matrix element of the condensate field operator, $\phi(\boldsymbol{r}, t)$, from the total $\psi(\boldsymbol{r}, t)$ and treating the rest $\tilde{\psi}(\boldsymbol{r}, t) = \psi(\boldsymbol{r}, t) - \phi(\boldsymbol{r}, t)$ as a small fluctuation. The resulting (Gross–Pitaevskii (GP)) equation for the condensate wavefunction $\phi(\boldsymbol{r}, t)$ provides the mean-field description of the ground state and of the excitation spectrum [8–10]. Beyond the mean-field approach the Bogoliubov–de Gennes- (BdG-) type equations were derived [11], describing eigenstates of the 'supra'condensate bosons.

In this letter we extend the Bogoliubov theory to the two-component nonconverting condensate by deriving the GP and BdG equations and excitation spectrum with arbitrary two-body interactions, and solving GP equations for a phase-segregated BEC. Our motivation originates in the recent experimental [5] and theoretical [9, 10] studies of BEC of ^{87}Rb atoms in two different hyperfine states, and also in an observation [12] that the condensation temperature of a two-component charged Bose gas quantitatively describes the superconducting critical temperature of many cuprates. Differently from [9, 10], we consider nonconverting components (such as different elements), and arbitrary (rather than short-ranged) two-body interactions.

The Hamiltonian of the two-component (1 and 2) mixture of bosons in an external field with the vector, $A(\boldsymbol{r}, t)$, and scalar, $U_j(\boldsymbol{r}, t)$, potentials is given by

$$H = \sum_{j=1,2} \int \mathrm{d}\boldsymbol{r}\, \psi_j^\dagger(\boldsymbol{r}) \left[-\frac{(\nabla - \mathrm{i}q_j \boldsymbol{A}(\boldsymbol{r}, \boldsymbol{t}))^2}{2m_j} + U_j(\boldsymbol{r}, t) - \mu_j \right] \psi_j(\boldsymbol{r}) + \frac{1}{2} \sum_{j,j'} \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{r}'\, V_{jj'}(\boldsymbol{r} - \boldsymbol{r}') \psi_j^\dagger(\boldsymbol{r}) \psi_j(\boldsymbol{r}) \psi_{j'}^\dagger(\boldsymbol{r}') \psi_{j'}(\boldsymbol{r}'), \qquad (1)$$

where m_j and q_j are the mass and the effective charge (if any) of the boson j ($\hbar = 1$). If the two-body interactions $V_{jj'}(\boldsymbol{r})$ are weak, the occupation numbers of one-particle states are not very different from those in the ideal Bose gas. In particular the lowest-energy state remains to be macroscopically occupied and the corresponding component of the field operator $\psi(\boldsymbol{r})$ has an anomalously large matrix element between the ground states of the system containing $(N + 1)$ and N bosons. Hence, it is convenient to consider a grand canonical ensemble, introducing the chemical potentials μ_j to deal with the anomalous averages $\phi(\boldsymbol{r})$ rather than with the off-diagonal matrix elements. Using the Bogoliubov displacement transformation in the equation of motion for the field operators $\psi(\boldsymbol{r}, t) = \phi(\boldsymbol{r}, t) + \tilde{\psi}(\boldsymbol{r}, t)$ and collecting c-number terms of ϕ and terms linear in the *supracondensate* boson operators $\tilde{\psi}$, one obtains a set of the GP and BdG-type equations [9–11]. The macroscopic condensate wavefunctions (i.e. the order parameters) obey two coupled GP equations

$$\mathrm{i}\frac{\partial}{\partial t}\phi_j(\boldsymbol{r}, t) = \hat{h}_j \phi_j(\boldsymbol{r}, t) + \sum_{j'} \int \mathrm{d}\boldsymbol{r}'\, V_{jj'}(\boldsymbol{r} - \boldsymbol{r}') |\phi_{j'}(\boldsymbol{r}', t)|^2 \phi_j(\boldsymbol{r}, t) \qquad (2)$$

with the single-particle Hamiltonian $\hat{h}_j = -(\nabla - \mathrm{i}q_j \boldsymbol{A}(\boldsymbol{r}, t))^2/2m_j + U_j(\boldsymbol{r}, t) - \mu_j$. The supracondensate wavefunctions satisfy four BdG equations

$$\sum_{j'} \int \mathrm{d}\boldsymbol{r}'\, V_{jj'}(\boldsymbol{r} - \boldsymbol{r}') [|\phi_{j'}(\boldsymbol{r}', t)|^2 u_j(\boldsymbol{r}, t) + \phi_j^*(\boldsymbol{r}', t) \phi_{j'}(\boldsymbol{r}, t) u_{j'}(\boldsymbol{r}', t) + \phi_j(\boldsymbol{r}', t) \phi_{j'}(\boldsymbol{r}, t) v_{j'}(\boldsymbol{r}', t)] = \mathrm{i}\frac{\partial}{\partial t} u_j(\boldsymbol{r}, t) - \hat{h}_j u_j(\boldsymbol{r}, t), \qquad (3)$$

and

$$\sum_{j'} \int \mathrm{d}\boldsymbol{r}'\, V_{jj'}(\boldsymbol{r} - \boldsymbol{r}') [|\phi_{j'}(\boldsymbol{r}', t)|^2 v_j(\boldsymbol{r}, t) + \phi_j(\boldsymbol{r}', t) \phi_{j'}^*(\boldsymbol{r}, t) v_{j'}(\boldsymbol{r}', t) + \phi_j^*(\boldsymbol{r}', t) \phi_{j'}^*(\boldsymbol{r}, t) u_{j'}(\boldsymbol{r}', t)] = -\mathrm{i}\frac{\partial}{\partial t} v_j(\boldsymbol{r}, t) - \hat{h}_j^* v_j(\boldsymbol{r}, t). \qquad (4)$$

Here we have applied the linear Bogoliubov transformation for $\tilde{\psi}$

$$\tilde{\psi}_j(\boldsymbol{r}, t) = \sum_n u_{nj}(\boldsymbol{r}, t)(\alpha_n + \beta_n) + v_{nj}^*(\boldsymbol{r}, t)(\alpha_n^\dagger + \beta_n^\dagger), \qquad (5)$$

where α_n, β_n are bosonic operators annihilating quasiparticles in the quantum state n. There is a sum rule,

$$\sum_n [u_{nj}(\boldsymbol{r}, t) u_{nj}^*(\boldsymbol{r}', t) - v_{nj}(\boldsymbol{r}, t) v_{nj}^*(\boldsymbol{r}', t)] = \delta(\boldsymbol{r} - \boldsymbol{r}'), \qquad (6)$$

which retains the Bose commutation relations for all operators.

In the homogeneous system with no external fields the excitation wavefunctions are plane waves

$$u_{\boldsymbol{k},j}(\boldsymbol{r},t) = u_{\boldsymbol{k},j}\exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r} - \mathrm{i}E(\boldsymbol{k})t], \tag{7}$$

$$v_{\boldsymbol{k},j}(\boldsymbol{r},t) = v_{\boldsymbol{k},j}\exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r} - \mathrm{i}E(\boldsymbol{k})t]. \tag{8}$$

The condensate wavefunction is $(\boldsymbol{r},t)$ independent in this case, $\phi_j(\boldsymbol{r},t) \equiv \phi_j$. Solving two GP equations one obtains the chemical potentials as

$$\begin{aligned} \mu_1 &= Vn_1 + Wn_2 \\ \mu_2 &= Un_2 + Wn_1, \end{aligned} \tag{9}$$

and solving four BdG equations one determines the excitation spectrum, $E(\boldsymbol{k})$, from

$$\mathrm{Det}\begin{bmatrix} \xi_1(\boldsymbol{k}) - E(\boldsymbol{k}) & V_k\phi_1^2 & W_k\phi_1\phi_2^* & W_k\phi_1\phi_2 \\ V_k\phi_1^{*2} & \xi_1(\boldsymbol{k}) + E(\boldsymbol{k}) & W_k\phi_1^*\phi_2^* & W_k\phi_1^*\phi_2 \\ W_k\phi_1^*\phi_2 & W_k\phi_1\phi_2 & \xi_2(\boldsymbol{k}) - E(\boldsymbol{k}) & U_k\phi_2^2 \\ W_k\phi_1^*\phi_2^* & W_k\phi_1\phi_2^* & U_k\phi_2^{*2} & \xi_2(\boldsymbol{k}) + E(\boldsymbol{k}) \end{bmatrix} = 0. \tag{10}$$

Here $\xi_1(\boldsymbol{k}) = k^2/2m_1 + V_k n_1$, $\xi_2(\boldsymbol{k}) = k^2/2m_2 + U_k n_2$, V_k, U_k, W_k are the Fourier components of $V_{11}(\boldsymbol{r})$, $V_{22}(\boldsymbol{r})$ and $V_{12}(\boldsymbol{r})$, respectively, $V \equiv V_0$, $U \equiv U_0$ and $W \equiv W_0$, and $n_j = |\phi_j|^2$ the condensate densities. There are two branches of excitations with the dispersion

$$E_{1,2}(\boldsymbol{k}) = 2^{-1/2}\left(\epsilon_1^2(\boldsymbol{k}) + \epsilon_2^2(\boldsymbol{k}) \pm \sqrt{[\epsilon_1^2(\boldsymbol{k}) - \epsilon_2^2(\boldsymbol{k})]^2 + \frac{4k^4}{m_1 m_2}W_k^2 n_1 n_2}\right)^{1/2}, \tag{11}$$

where $\epsilon_1(\boldsymbol{k}) = \sqrt{k^4/(4m_1^2) + k^2 V_k n_1/m_1}$ and $\epsilon_2(\boldsymbol{k}) = \sqrt{k^4/(4m_2^2) + k^2 U_k n_2/m_2}$ are Bogoliubov's modes of two components. If the interactions are short-ranged (hard-core) repulsions, so that $V_k = V$, $U_k = U$ and $W_k = W$, the spectrum, equation (11), is that of [10, 13]. In the long-wave limit both branches are soundlike with the sound velocities

$$s_{1,2} = 2^{-1/2}\left(Vn_1/m_1 + Un_2/m_2 \pm \sqrt{[Vn_1/m_1 - Un_2/m_2]^2 + 4W^2 n_1 n_2/(m_1 m_2)}\right)^{1/2}. \tag{12}$$

The lowest branch becomes unstable ($s_2 < 0$) if $W > \sqrt{UV}$. When $W = \sqrt{UV}$ this branch is quadratic in the long-wave limit

$$E_2(\boldsymbol{k}) = \frac{k^2}{2(m_1 m_2)^{1/2}}\sqrt{\frac{Vn_1m_1 + Un_2m_2}{Vn_1m_2 + Un_2m_1}}. \tag{13}$$

If $m_1 = m_2 = m$ it becomes 'collisionless' [10], i.e. $E_2(\boldsymbol{k}) = k^2/2m$.

The finite-ranged interactions drastically change the whole spectrum. In the extreme case of the long-range Coulomb interaction, $V(\boldsymbol{k}) = 4\pi q_1^2/k^2$, $U(\boldsymbol{k}) = 4\pi q_2^2/k^2$ and $W(\boldsymbol{k}) = 4\pi q_1 q_2/k^2$, the upper branch is the geometric sum of the familiar plasmon modes [14] for $k \to 0$,

$$E_1(\boldsymbol{k}) = \sqrt{\frac{4\pi q_1^2 n_1}{m_1} + \frac{4\pi q_2^2 n_2}{m_2}}, \tag{14}$$

while the lowest branch is

$$E_2(\boldsymbol{k}) = \frac{k^2}{2(m_1 m_2)^{1/2}}\sqrt{\frac{q_1^2 n_1 m_1 + q_2^2 n_2 m_2}{q_1^2 n_1 m_2 + q_2^2 n_2 m_1}}. \tag{15}$$

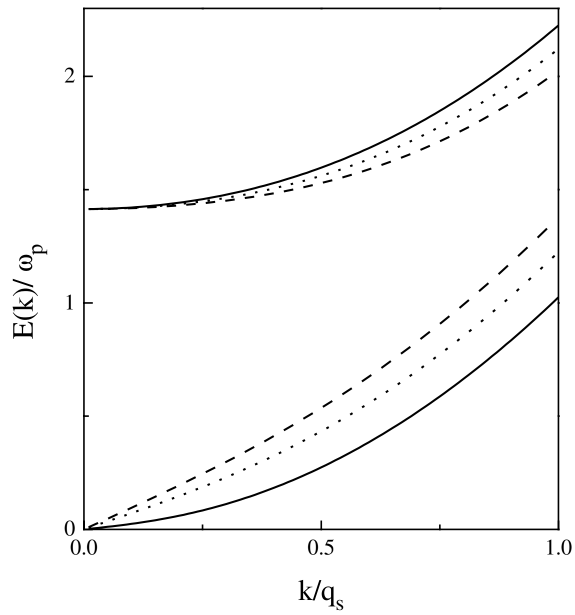

Figure 1. The excitation energy spectrum of the two-component BEC with the long-range repulsive and hard-core interactions. In this plot $n_1 = n_2 = n$, $m_1 = m_2$ and $U = V = \omega_p$, $q_1 = q_2 = e$. Different curves correspond to the different values of $W/V = 0.1$ (dashed curve), 0.5 (dotted curve) and 0.95 (solid curve). Excitation energy is measured in units of the plasma frequency $\omega_p = (4\pi ne^2/m)^{1/2}$ and momentum k is measured in inverse screening length $q_s = (16\pi e^2 nm)^{1/4}$.

Remarkably, this mode is 'collisionless' at *any* charges of the components if $m_1 = m_2$ (figure 1). It corresponds to a low-frequency oscillation in which two condensates move in antiphase with one another, in contrast with the usual optical high-frequency plasmon, equation (14), in which the components oscillate in phase. The mode is similar to the acoustic plasmon (AP) mode in the electron–ion [15] and electron–hole [16] plasmas. However, different from these normal-state APs with a linear dispersion, the AP of BEC mixtures has quadratic dispersion in the long-wavelength limit. We conclude that while the Coulomb Bose condensate is a superfluid (according to the Landau criterion), the mixture of two Coulomb Bose condensates is not. More generally the interaction might include both the long-range repulsion and the hard-core interaction as in the case of bipolarons or any other preformed bosonic pairs [6]. Combination of the two interactions, i.e. $V_{\boldsymbol{k}}, U_{\boldsymbol{k}}, W_{\boldsymbol{k}} \propto$ constant + $1/k^2$, transforms the lowest quadratic mode into the Bogoliubov sound. Hence, a two-component condensate of bipolarons is a superfluid.

Finally, let us discuss the phase-segregated state of the two-component nonconverting mixture with the hard-core interactions when $W > \sqrt{UV}$ [17][3]. In this case the chemical potentials determined in equation (9) are no longer correct. Minimizing the free energy with respect to the equilibrium concentration we find the densities $n'_1 = n_1 + \sqrt{U/V}n_2$ and $n'_2 = n_2 + \sqrt{V/U}n_1$ of two separated phases. The phase boundary is described by two coupled one-dimensional

[3] The condition $W > \sqrt{UV}$, where the lowest branch of the spectrum equation (12) becomes unstable, coincides with the condition where compressibility of the system becomes negative, $|\partial\mu_i/\partial n_j| < 0$. Phase segregation also exists in the case of the *Coulomb + hard-core* interaction. In this case the condition where the spectrum equation (11) becomes unstable depends on the plasma frequency. This shows that the higher-order corrections to the chemical potential due to the Coulomb interaction are crucial.

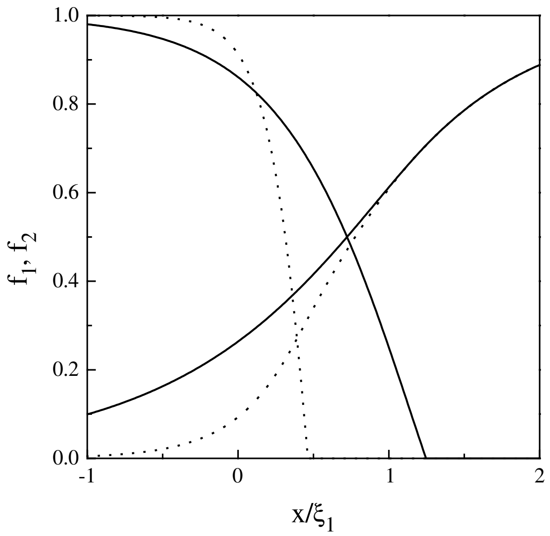

Figure 2. Density profiles of two phase-separated condensates near the boundary for $r = 2$ (solid curve) and $r = 10$ (dotted curve).

GP equations, equation (2) (similar equations have been discussed previously in [17]),

$$\frac{\mathrm{d}^2 f_1}{\mathrm{d}x^2} + f_1 - f_1^3 - r f_1 f_2^2 = 0 \tag{16}$$

and

$$\kappa \frac{\mathrm{d}^2 f_2}{\mathrm{d}x^2} + f_2 - f_2^3 - r f_2 f_1^2 = 0, \tag{17}$$

where we introduce two real dimensionless order parameters, $f_1 = \phi_1/\sqrt{n_1'}$ and $f_2 = \phi_2/\sqrt{n_2'}$, and measure length in units of the coherence length $\xi_1 = (2m_1 V n_1')^{-1/2}$. Parameter $r \equiv W/\sqrt{UV}$ is larger than unity, and $\kappa = m_1 V n_1'/m_2 U n_2'$ is the ratio of two coherence lengths squared. One can solve these equations analytically in the limit $\kappa \to 0$, where two coherence lengths differ significantly or in the case where $r \to \infty$. In the limit $\kappa \to 0$ the first term in the second equation is negligible, so $f_2 = 0$ if $r f_1^2 > 1$, and $f_2 = \sqrt{1 - r f_1^2}$ if $r f_1^2 < 1$. Substituting this solution into the first equation and using $\mathrm{d}f_1/\mathrm{d}x = F(f)$, one can reduce equation (16) to an integrable first-order differential equation. The solution satisfying the boundary conditions, $f_1 = 1$ at $x = \infty$ and $f_1 = 0$ at $x = -\infty$, is

$$f_1(x) = \Theta(x - x_1)\tanh(x/\sqrt{2}) + \Theta(x_1 - x)\frac{\sqrt{2}}{(r+1)^{1/2}\cosh[(r-1)^{1/2}(x - x_2)]}, \tag{18}$$

$$f_2(x) = \Theta(x_1 - x)\left(1 - \frac{2r}{(r+1)\cosh^2[(r-1)^{1/2}(x - x_2)]}\right)^{1/2}, \tag{19}$$

where $\Theta(x)$ is the Θ-function, $\tanh(x_1/\sqrt{2}) = r^{-1/2}$ and $\cosh[(r-1)^{1/2}(x_1 - x_2)] = \sqrt{2r/(r+1)}$. Interestingly the *largest* coherence length (in our case ξ_1) determines the profile of *both* order parameters. The inter-component mutual repulsion (r) only slightly changes the characteristic lengths, as shown in figure 2.

In contrast with the previous studies [13, 17, 18], BdG equations allow us to investigate the possibility of localized excitations near the boundary in the mixture (localized waves).

The quasiparticle eigenstates of the phase-segregated condensate are determined by the *inhomogeneous* BdG equations, (3) and (4). Here we restrict the analysis by surface excitations at the boundary between two condensates in the limit $r \to \infty$. Substituting equations (18) and (19) into (3) and (4), we obtain four coupled linear differential equations. In the limit $r \to \infty$ the equations are decoupled in pairs, so that one can solve only first two equations at $x > 0$. Integration of the equations near zero provides the boundary condition $u_1(0) = v_1(0) = 0$. Then a simple analysis shows that there are no excitations localized near the boundary in that limit.

This conclusion seems to be quite general for any gapless Bose liquid. For example, one can consider a single-component hard-core Bose gas with attractive impurity potential placed at the origin $x = 0$, so that the GP equation is

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + f - f^3 + \alpha\delta(x) = 0, \tag{20}$$

where $\alpha > 0$ is the (dimensionless) strength of the potential. The solution is $f(x) = \coth[(|x| + x_0)/\sqrt{2}]$ where $\sinh(x_0/2^{3/2}) = 1/\alpha$. Substituting this solution into the BdG equations, (3) and (4), one can see that localized excitations do not appear even in this case. The condensate density increases at $x = 0$ and effectively screens out the attractive potential. However, localized excitations could appear in the gapped Bose liquid, like the charged Bose gas. In this case they are formed below the plasma frequency.

In conclusion, we have derived the BdG equations and the excitation spectrum of the two-component BEC with an arbitrary interaction between bosons, including long- and short-range forces. We have found the spectrum of optical and acoustic plasmons. In the case of the Coulomb interaction alone the AP has quadratic dispersion in contrast with the linear dispersion in normal two-component plasmas. Solving GP equations for segregated condensates we have found the boundary profile, and shown that localized surface waves do not exist for the strongly repulsive components.

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References

[1] Anderson M H *et al* 1995 *Science* **269** 198
[2] Davis K B *et al* 1995 *Phys. Rev. Lett.* **75** 3969
[3] Bradley C C *et al* 1995 *Phys. Rev. Lett.* **75** 1687
[4] Mewes M-O *et al* 1997 *Phys. Rev. Lett.* **78** 582
[5] Hagley E W *et al* 1999 *Science* **283** 1706
[6] Alexandrov A S and Mott N F 1994 *Rep. Prog. Phys.* **57** 1197
[7] Bogoliubov N 1947 *J. Phys. USSR* **11** 23–32
[8] Edwards M *et al* 1996 *Phys. Rev.* A **53** R1950
[9] Busch Th *et al* 1997 *Phys. Rev.* A **56** 2978
[10] Goldstein E V *et al* 2000 *Phys. Rev. Lett.* **85** 5030
[11] Alexandrov A S, Beere W H and Kabanov V V 1996 *Phys. Rev.* B **54** 15 363
[12] Alexandrov A S and Kabanov V V 1999 *Phys. Rev.* B **59** 13 628
[13] Ao P and Chui S T 2000 *J. Phys. B: At. Mol. Opt. Phys.* **33** 535
[14] Foldy L L 1961 *Phys. Rev.* **124** 649
[15] Tonks L and Langmuir I 1929 *Phys. Rev.* **33** 195
[16] Pines D and Schrieffer J R 1961 *Phys. Rev.* **124** 1387
[17] Ao P and Chui S T 1998 *Phys. Rev.* A **58** 4836
[18] Ho Tin-Lun and Shenoy V B 1996 *Phys. Rev. Lett.* **77** 3276
Graham R and Wells D 1998 *Phys. Rev.* A **57** 484