Self-consistent theory of a homogeneous binary Bose mixture with strong repulsive interspecies interaction

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Multicomponent quantum gases are ideal platforms to study fundamental phenomena arising from the mutual interaction between different constituents. Particularly, due to the repulsive interactions between two species, the system may exhibit a phase separation. We develop a mean-field-based theory for a two-component Bose mixture, which is equivalent to the Hartree-Fock-Bogoliubov approximation, and derive analytical expressions for the phase boundary and miscibility. The majority of existing theories, which are valid only for weakly interacting Bose gases, predict that the phase boundary is determined by the criterion $g_{ab} \leqslant \sqrt{g_{aa}g_{bb}}$ (where g_{ab} is a coupling constant between the components a and b). We show that in the Bose-Einstein condensation phase ($T \leqslant T_c$) the system may remain in a stable and miscible phase also for larger values of g_{ab}, depending on the gas parameter γ and temperature.

I. INTRODUCTION

The investigation of mixtures of two-component Bose gases has been of interest since the experimental realization nearly 25 years ago in JILA [1,2]. Due to the possibility of tuning the interspecies scattering length (a_{ab}) by using Feshbach resonances, two-component quantum fluids exhibit rich physics that is not accessible in a single-component fluid. Theoretical [3,4] and experimental studies [5–13] have revealed that the nature of this physics dramatically depends on the sign of the intercomponent coupling constant of the *s*-wave contact interaction g_{ab}: for $g_{ab} < 0$ ($g_{aa} > 0$, $g_{bb} > 0$), quantum liquid droplets may arise [3,12], while for $g_{ab} > 0$, a phase transition between miscible and immiscible states can occur. In some sense, the situation is similar to two-body physics: when the interparticle interaction is negative, one is mainly interested in the properties of bound states; otherwise one studies scattering angles and cross sections.

In the present work we concentrate only on the case with repulsive interactions ($g_{aa} > 0$, $g_{bb} > 0$, $g_{ab} > 0$) and theoretically study the properties of a two-component homogeneous Bose system, such as stability, miscibility, and a possible phase transition at finite temperature at equilibrium.

Although recent experiments [9,11] do not clearly identify evident signatures of miscible-immiscible transition, the existence of the transition with spatial separation, including zero temperature, has been theoretically proven [14–23]. Particularly, a long time ago, Timmermans [4] proposed to distinguish two types of spatial separation: (1) potential separation, caused by the external trapping potentials in much the same way as gravity can separate fluids of different specific weight, and (2) phase separation, which persists in the absence of external potentials and is similar to separation of immiscible fluids, such as oil and water. In the present work we discuss the system without a trap and study only the phase separation which takes place after crossing the border of instability. We show that the onset of the instability in the system lowers its free energy by the segregation of the components into a phase-separated state.

The origin of this instability is the following. In contrast to a single-component Bose system, a binary mixture of bosons with Bose-Einstein condensation (BEC) has two branches of collective excitations, ω_d and ω_s, corresponding to density c_d and pseudospin sound c_s modes, respectively. The former describes the oscillations of both components in phase, while the latter is responsible for out-of-phase oscillations of the components with respect to each other. For some values of physical parameters (g_{ab}, T) for one of the modes $c_s^2 < 0$, so that this mode grows initially at a rate $|\omega_s|$, which is the indicator of instability [4]. Particularly, at zero temperature, this may happen when the interspecies coupling constant g_{ab} exceeds a critical value $g_c = \sqrt{g_{aa}g_{bb}}$, i.e., $g_{ab} > g_c$. Nowadays this criterion is so widely accepted that some authors consider it even as a definition of miscible ($g_{ab} < \sqrt{g_{aa}g_{bb}}$) or immiscible ($g_{ab} > \sqrt{g_{aa}g_{bb}}$) states [10,24] despite the fact that it was obtained in the rather crude Bogoliubov approximation, which is valid only for very dilute gases, with the gas parameter $\gamma = \rho a^3 \sim 10^{-5}$ [25].

As to the works where some corrections to the Bogoliubov or semiclassical approximations were considered [16,17,22–24], they have mainly two drawbacks: the Hugenholtz-Pines (HP) theorem [26,27] for multicomponent

BECs is not satisfied and/or the anomalous densities, especially intercomponent anomalous pair density, are neglected. As a result, the majority of theoretical approximations lack self-consistency, being valid only for $\gamma \ll 1$. The principal necessity of taking into account anomalous averages for the Bose-condensed phase has been emphasized in Refs. [28–37].

Atomic interactions in gases are modeled by contact potentials expressed through effective scattering lengths, which can be made rather large by means of the Feshbach resonance technique, so that the gas parameter can become quite large [5,38,39]. The aim of the present work is to develop a mean-field-based approximation, without any restriction to the value of $\gamma > 0$, by taking into account the HP theorem, derived for multicomponent BECs in Refs. [27,40], as well as anomalous densities, σ_a, σ_b, and σ_{ab}. For this purpose we start with the standard Hamiltonian of a binary Bose mixture with contact interactions. We use the variational method, similar to that employed in Refs. [35,41–43], which is a variant of the general approach called optimized perturbation theory [44,45]. In the present case, this approach is equivalent to the Hartree-Fock-Bogoliubov (HFB) approximation [46].

It is well known that the usage of the HFB approximation has its own problem, which is called in the literature the Hohenberg-Martin dilemma [47], which is summarized as follows: In the theory based on the standard grand canonical ensemble with spontaneous symmetry breaking, depending on the way of calculation, one obtains either a gap in the spectrum of collective excitations, or local conservation laws together with general thermodynamic relations becoming invalid. Recall that the excitation spectrum, according to the HP theorem, must be gapless. A self-consistent way of solving this dilemma has been advanced in Refs. [28–30] by introducing additional Lagrange multipliers for each component, namely, μ_{0a}, μ_{1a}, μ_{0b}, and μ_{1b}. This choice is directly related to the inclusion of anomalous density. So, when one neglects the anomalous density, μ_0 equals μ_1, while when the anomalous density is taken into account, μ_0 and μ_1 can be fixed from the conditions of minimization of the thermodynamic potential with respect to condensed fractions and from the validity of the generalized HP theorem, respectively [29,46].

Since there is no restriction to the magnitude of the gas parameter in the present approach, our criterion for the stability of a binary Bose system will be more general than the simple inequality $g_{ab} \leqslant \sqrt{g_{aa}g_{bb}}$. Particularly, for a symmetric system with equal masses ($m_a = m_b$) and coupling constants ($g_{aa} = g_{bb} = g$, $g_{ab} = \bar{g}_{ab}g$) at zero temperature we have obtained the phase diagram on the ($\bar{g}_{ab}$, γ) plane which displays that, for moderate values of γ ($\gamma \approx 0.001$), the system may remain stable even at $\bar{g}_{ab} = 1.1$, in contrast to the predictions of the previous studies. At finite temperatures this criterion clearly involves at least three parameters ($\bar{g}_{ab}$, γ, T), which gives us the opportunity to derive a three-dimensional phase diagram for a Bose-condensed two-component homogeneous mixture.

The paper is structured as follows. In Sec. II, we derive general expressions for the free energy, collective excitation spectrum, and the densities. Then, in Sec. III, we discuss the BEC system in more detail. The theory is applied to the symmetric Bose mixture in Sec. IV in order to obtain

quantitative results. In the last section, we present discussions and conclusions.

II. THERMODYNAMIC POTENTIAL AND MAIN EQUATIONS

The Lagrangian density for two-species complex scalar fields ψ and ϕ, with contact self-couplings g_a and g_b and interspecies coupling g_{ab}, is given as

$$L = \psi^\dagger \left(i\partial_t + \frac{\vec{\nabla}^2}{2m_a} + \mu_a \right)\psi - \frac{g_a}{2}(\psi^\dagger\psi)^2$$
$$+ \phi^\dagger \left(i\partial_t + \frac{\vec{\nabla}^2}{2m_b} + \mu_b \right)\phi - \frac{g_b}{2}(\phi^\dagger\phi)^2 - g_{ab}(\psi^\dagger\psi)(\phi^\dagger\phi),$$
$$(1)$$

where the associated chemical potentials are represented by $\mu_{a,b}$ while $m_{a,b}$ represent the masses. In terms of the corresponding s-wave scattering lengths a_s, the coupling constants can be written as $g_{a,b} = 4\pi a_{a,b}/m_{a,b}$, while the cross coupling is $g_{ab} = 2\pi a_{ab}/m_{ab}$, where $m_{ab} = m_a m_b/(m_a + m_b)$ represents reduced mass. Here and below we set $\hbar = 1$, $k_B = 1$.

Note that in the present work only repulsive interactions will be considered, $g_{a,b} \geqslant 0$, $g_{ab} \geqslant 0$. The grand canonical thermodynamic potential Ω can be calculated in the path integral formalism as

$$\Omega = -T \ln Z, \qquad (2)$$

$$Z = \int D\psi^\dagger D\psi D\phi^\dagger D\phi\, e^{-S(\psi^\dagger,\psi,\phi^\dagger,\phi)}, \qquad (3)$$

where the equivalent finite-temperature Euclidean ($\tau = it$) space time action to (1) is given by

$$S = \int_0^\beta d\tau \int d\vec{r} \left\{ \psi^\dagger \hat{K}_a \psi + \phi^\dagger \hat{K}_b \phi + \frac{g_a}{2}(\psi^\dagger\psi)^2 \right.$$
$$\left. + \frac{g_b}{2}(\phi^\dagger\phi)^2 + g_{ab}(\psi^\dagger\psi)(\phi^\dagger\phi) \right\},$$

$$\hat{K}_{a,b} = \frac{\partial}{\partial\tau} - \hat{O}_{a,b}, \quad \hat{O}_{a,b} = \frac{\vec{\nabla}^2}{2m_{a,b}} + \mu_{a,b}. \qquad (4)$$

In Eq. (4) the fields $\psi(\vec{r}, \tau)$ and $\phi(\vec{r}, \tau)$ are periodic in τ with period $\beta = 1/T$. Clearly, this path integral cannot be evaluated exactly due to the terms of fourth order in fields, so an approximation is needed. In the present work, we use the approach sometimes called variational perturbation theory [41,48–50], which is a particular case of optimized perturbation theory [44,45]. For a two-component system, this method involves the following steps.

Step 1. Introduce fluctuating fields $\tilde{\psi}$ and $\tilde{\phi}$ by the Bogoliubov shift:

$$\psi(\vec{r}, \tau) = \sqrt{\rho_{0a}} + \tilde{\psi}(\vec{r}, \tau),$$
$$\phi(\vec{r}, \tau) = \sqrt{\rho_{0b}} + \tilde{\phi}(\vec{r}, \tau), \qquad (5)$$

where the order parameters ρ_{0a} and ρ_{0b} correspond to the condensate fractions of the components a and b, respectively. Note that the Bogoliubov shift is an exact canonical transformation [51], and not an approximation, as sometimes it is stated. For a uniform system at equilibrium, ρ_{0a} and ρ_{0b} are

real variational constants, which are fixed by the minimum of the free energy Ω as $\partial \Omega / \partial \rho_{0,a,b} = 0$, $\partial^2 \Omega / \partial^2 \rho_{0,a,b} \geq 0$ [35]. As to the numbers of uncondensed particles N_{1a} and N_{1b}, they are related to the fields $\tilde{\psi}$ and $\tilde{\phi}$:

$$N_{1a} = V \rho_{1a} = \int d\vec{r} \langle \tilde{\psi}^\dagger(r) \tilde{\psi}(r) \rangle, \qquad (6)$$

$$N_{1b} = V \rho_{1b} = \int d\vec{r} \langle \tilde{\phi}^\dagger(r) \tilde{\phi}(r) \rangle, \qquad (7)$$

so that

$$N_a = \int d\vec{r} \langle \psi^\dagger(r) \psi(r) \rangle, \qquad (8)$$

$$N_b = \int d\vec{r} \langle \phi^\dagger(r) \phi(r) \rangle, \qquad (9)$$

with the normalization conditions $N = N_a + N_b$, $N_a = V \rho_a = V(\rho_{0a} + \rho_{1a})$, and $N_b = V \rho_b = V(\rho_{0b} + \rho_{1b})$, where $N_{a(b)}$ is the number of particles in the component a (b) and N is the particle number in the whole two-component system and V is the total volume of the system. Since we are considering a homogeneous system, the densities ρ_a and ρ_b are uniform.

Step 2. Make the following replacement in the action: $g_a \to \tilde{\delta} g_a$, $g_b \to \tilde{\delta} g_b$, $g_{ab} \to \tilde{\delta} g_{ab}$.

Step 3. Add to the action the term

$$S_\Sigma = (1 - \tilde{\delta}) \int d\tau d\vec{r} \Bigg\{ \Sigma_n^{(a)}(\tilde{\psi}^\dagger \tilde{\psi}) + \Sigma_n^{(b)}(\tilde{\phi}^\dagger \tilde{\phi})$$
$$+ \frac{1}{2} \Sigma_{an}^{(a)}(\tilde{\psi} \tilde{\psi} + \tilde{\psi}^\dagger \tilde{\psi}^\dagger) + \frac{1}{2} \Sigma_{an}^{(b)}(\tilde{\phi} \tilde{\phi} + \tilde{\phi}^\dagger \tilde{\phi}^\dagger)$$
$$+ \Sigma_n^{(ab)}(\tilde{\psi}^\dagger \tilde{\phi} + \tilde{\phi}^\dagger \tilde{\psi}) + \Sigma_{an}^{(ab)}(\tilde{\psi} \tilde{\phi} + \tilde{\phi}^\dagger \tilde{\psi}^\dagger) \Bigg\}, \quad (10)$$

where the variational parameters Σ_n and Σ_{an} can be naturally interpreted as normal and anomalous self-energies, respectively.

Step 4. Now in the Cartesian representation

$$\tilde{\psi} = \frac{1}{\sqrt{2}}(\psi_1 + i \psi_2), \qquad \tilde{\phi} = \frac{1}{\sqrt{2}}(\psi_3 + i \psi_4), \qquad (11)$$

such that

$$\int D \tilde{\psi}^\dagger D \tilde{\psi} D \tilde{\phi}^\dagger D \tilde{\phi} \to \int \prod_{i=1}^{4} D \psi_i, \qquad (12)$$

the action (4) can be written as

$$S = S_0 + S_{\text{free}} + \tilde{\delta} S_{\text{int}}, \qquad (13)$$

$$S_{\text{int}} = S_{\text{int}}^{(1)} + S_{\text{int}}^{(2)} + S_{\text{int}}^{(3)} + S_{\text{int}}^{(4)}, \qquad (14)$$

$$S_0 = \int_0^\beta d\tau \int d\vec{r} \Bigg\{ -\mu_{0a} \rho_{0a} - \mu_{0b} \rho_{0b} + \frac{g_a \rho_{0a}^2}{2}$$
$$+ \frac{g_b \rho_{0b}^2}{2} + g_{ab} \rho_{0a} \rho_{0b} \Bigg\}, \qquad (15)$$

$$S_{\text{free}} = \frac{1}{2} \int_0^\beta d\tau \int d\vec{r} \{ \psi_1 [X_1 + \hat{K}_a] \psi_1 + \psi_2 [X_2 + \hat{K}_a] \psi_2$$
$$+ \psi_3 [X_3 + \hat{K}_b] \psi_3 + \psi_4 [X_4 + \hat{K}_b] \psi_4 + X_5 [\psi_1 \psi_3$$
$$+ \psi_3 \psi_1] + X_6 [\psi_2 \psi_4 + \psi_4 \psi_2] \}, \qquad (16)$$

$$S_{\text{int}}^{(2)} = \frac{1}{2} \int d\tau d\vec{r} \Bigg\{ \sum_{i=1}^{4} \Lambda_i \psi_i^2 + \Lambda_5 (\psi_1 \psi_3 + \psi_3 \psi_1)$$
$$+ \Lambda_6 (\psi_2 \psi_4 + \psi_4 \psi_2) \Bigg\}, \qquad (17)$$

$$S_{\text{int}}^{(4)} = \frac{1}{8} \int d\tau d\vec{r} \{ g_a (\psi_1^2 + \psi_2^2)^2 + g_b (\psi_3^2 + \psi_4^2)^2$$
$$+ 2 g_{ab} (\psi_1^2 + \psi_2^2)(\psi_3^2 + \psi_4^2) \}, \qquad (18)$$

where we have introduced the following notations:

$$X_1 = \Sigma_n^{(a)} + \Sigma_{an}^{(a)} - \mu_{1a}, X_3 = \Sigma_n^{(b)} + \Sigma_{an}^{(b)} - \mu_{1b}, \quad (19)$$

$$X_2 = \Sigma_n^{(a)} - \Sigma_{an}^{(a)} - \mu_{1a}, X_4 = \Sigma_n^{(b)} - \Sigma_{an}^{(b)} - \mu_{1b}, \quad (20)$$

$$X_5 = \Sigma_n^{(ab)} + \Sigma_{an}^{(ab)}, \qquad X_6 = \Sigma_n^{(ab)} - \Sigma_{an}^{(ab)}, \qquad (21)$$

$$\Lambda_1 = -\mu_{1a} - X_1 + 3 g_a \rho_{0a} + g_{ab} \rho_{0b}, \qquad (22)$$

$$\Lambda_2 = -\mu_{1a} - X_2 + g_a \rho_{0a} + g_{ab} \rho_{0b}, \qquad (23)$$

$$\Lambda_3 = -\mu_{1b} - X_3 + 3 g_b \rho_{0b} + g_{ab} \rho_{0a}, \qquad (24)$$

$$\Lambda_4 = -\mu_{1b} - X_4 + g_b \rho_{0b} + g_{ab} \rho_{0a}, \qquad (25)$$

$$\Lambda_5 = -X_5 + 2 g_{ab} \sqrt{\rho_{0a} \rho_{0b}}, \qquad (26)$$

$$\Lambda_6 = -X_6. \qquad (27)$$

Equations (13)–(27) need some comments:

(a) We omit the explicit expressions for $S^{(1)}$ and $S^{(3)}$ since the path integrals including odd powers of fields are zero, e.g., $\int [\prod_{i=1}^{4} D\psi_i] \psi_1 \psi_2^2 e^{-S} = 0$.

(b) Two kinds of chemical potentials, μ_0 and μ_1, are introduced instead of a unique chemical potential μ, such that $\mu_{0a} N_{0a} + \mu_{1a} N_{1a} = \mu_a N_a$. The reason is the following. Actually, the mean-field-based theories of BEC have a long-standing puzzle referred to as the Hohenberg-Martin dilemma [47], which can be explained for a one-component system rather simply. The chemical potential should satisfy the Goldstone theorem and correspond to the minimum of the thermodynamic potential. It has been shown that, when anomalous density, $\sigma \sim \langle \tilde{\psi} \tilde{\psi} \rangle$[1] is accurately taken into account, these two conditions cannot be satisfied simultaneously [29–31]. The solution to this problem has been advanced in Refs. [28–30]. It was shown that, in a system with spontaneous gauge symmetry breaking, the introduction of two chemical potentials makes the theory self-consistent. Naturally, in the normal phase, when $\rho_0 = 0$, $\sigma = 0$, both chemical potentials coincide: $\mu = \mu_0 = \mu_1$.

(c) The six variational parameters $X_1, \ldots, X_6$ should be fixed by the minimization of Ω, e.g., $\partial \Omega / (\partial X_i) = 0$ ($i = 1$–6).

Step 5. Now, passing to the momentum space,

$$\psi_i(\vec{r}, \tau) = \frac{1}{\sqrt{V \beta}} \sum_{n=-\infty}^{\infty} \sum_{k} \psi_i(\omega_n, \vec{k}) e^{i \omega_n \tau + i \vec{k} \vec{r}}, \qquad (28)$$

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[1]See Eq. (46) below.

where $\sum_k = V \int d\vec{k}/(2\pi)^3$ and $\omega_n = 2\pi n T$ is a Matsubara frequency, one may present Eq. (16) as

$$S_{\text{free}} = \frac{(2\pi)^4}{2V\beta} \sum_{\vec{k},\vec{p},m,n} \sum_{i,j=1}^{4} \psi_i(\omega_n, \vec{k}) G_{ij}^{-1}(\omega_n, \vec{k}; \omega_m, \vec{p})$$

$$\times \psi_j(\omega_m, \vec{p}) \delta(\vec{k} + \vec{p}) \delta(\omega_n + \omega_m) \quad (29)$$

with the inverse propagator

$$G^{-1}(\omega_n, \vec{k})$$

$$= \begin{pmatrix} \varepsilon_a(k) + X_1 & \omega_n & X_5 & 0 \\ -\omega_n & \varepsilon_a(k) + X_2 & 0 & X_6 \\ X_5 & 0 & \varepsilon_b(k) + X_3 & \omega_n \\ 0 & X_6 & -\omega_n & \varepsilon_b(k) + X_4 \end{pmatrix}, \quad (30)$$

where $\varepsilon_{a,b}(k) = \vec{k}^2 / 2m_{a,b}$.

Evaluating the determinant of this matrix, we obtain two branches of dispersion:

$$\omega_{1,2}(k) = \sqrt{\frac{E_a^2 + E_b^2}{2} + X_5 X_6 \pm \frac{\sqrt{D}}{2}}, \quad (31)$$

$$D = \left(E_a^2 - E_b^2\right)^2 + 4E_{13}^2 X_6^2 + 4E_{24}^2 X_5^2$$

$$+ 4X_5 X_6 \left(E_a^2 + E_b^2\right), \quad (32)$$

where

$$E_a^2 = (\varepsilon_a(k) + X_1)(\varepsilon_a(k) + X_2), \quad (33)$$

$$E_b^2 = (\varepsilon_b(k) + X_3)(\varepsilon_b(k) + X_4), \quad (34)$$

$$E_{13}^2 = (\varepsilon_a(k) + X_1)(\varepsilon_b(k) + X_3), \quad (35)$$

$$E_{24}^2 = (\varepsilon_a(k) + X_2)(\varepsilon_b(k) + X_4). \quad (36)$$

Step 6. The perturbation scheme is considered as an expansion in powers of $\tilde{\delta}$ by using the propagators

$$G_{ij}(r, \tau; r', \tau') = \frac{1}{V\beta} \sum_{n,\vec{k}} e^{i\vec{k}(r-r')} e^{i\omega_n(\tau-\tau')} G_{ij}(\omega_n, \vec{k}), \quad (37)$$

which are presented explicitly in the Appendix. The expansion parameter $\tilde{\delta}$ will be set to $\tilde{\delta} = 1$ at the end of the calculations.

Step 7. The detailed calculation of the generating functional and hence Ω in the first order of $\tilde{\delta}$ can be performed in the similar way as it has been done in Ref. [35] for the one-component model. Therefore, using the following formulas, where $(x = (\tau, \vec{r}))$,

$$\langle \psi_i(x) \psi_j(x) \rangle = G_{ij}(x, x) = \frac{1}{V\beta} \sum_{\omega_n, \vec{k}} G_{ij}(\omega_n, \vec{k}), \quad (38)$$

$$\left\langle \psi_i^2(x) \psi_j^2(x) \right\rangle = G_{ii}(x, x) G_{jj}(x, x) + 2G_{ij}^2(x, x), \quad (39)$$

$$\left\langle \psi_i^4(x) \right\rangle = 3G_{ii}^2(x, x), \quad G_{ij}(x, x) = G_{ji}(x, x), \quad (40)$$

$$G_{12}(x, x) = G_{14}(x, x) = 0, \quad (41)$$

$$G_{23}(x, x) = G_{34}(x, x) = 0, \quad (42)$$

one obtains

$$\Omega = \Omega_0 + \Omega_{ln} + \Omega_2 + \Omega_4,$$

$$\Omega_0 = V\left\{ -\mu_{0a}\rho_{0a} - \mu_{0b}\rho_{0b} + \frac{g_a\rho_{0a}^2}{2} + \frac{g_b\rho_{0b}^2}{2} + g_{ab}\rho_{0a}\rho_{0b} \right\},$$

$$\Omega_{ln} = \frac{T}{2} \sum_{k,\omega_n} \ln\left[\left(\omega_n^2 + \omega_1^2\right)\left(\omega_n^2 + \omega_2^2\right) \right]$$

$$= \frac{1}{2} \sum_k (\omega_1(k) + \omega_2(k))$$

$$+ T \sum_k \ln(1 - e^{-\beta\omega_1(k)}) + T \sum_k \ln(1 - e^{-\beta\omega_2(k)}),$$

$$\Omega_2 = \frac{1}{2} \sum_{i=1}^{6} A_i \Lambda_i,$$

$$\Omega_4 = \frac{1}{8V}\left\{ g_a\left[3A_1^2 + 3A_2^2 + 2A_1A_2\right] + g_b\left[3A_3^2 + 3A_4^2 + 2A_3A_4\right] \right.$$

$$\left. + 2g_{ab}\left[(A_1 + A_2)(A_3 + A_4) + \frac{A_5^2 + A_6^2}{2} \right] \right\}, \quad (43)$$

where $A_i = V G_{ii}(x, x)$ $(i = 1\text{--}4)$, $A_5 = 2V G_{13}(x, x)$, $A_6 = 2V G_{24}(x, x)$, Λ_i are given by Eqs. (22)–(27), and $G_{ij}(x, x)$ are presented in the Appendix. Feynman diagrams contributing to Ω in the present optimized perturbation theory are illustrated in Refs. [25,52].[2]

The variational parameters are determined by the minimization of the thermodynamic potential $\Omega(X_1, \ldots, X_6)$ as $\partial\Omega(X_1, \ldots, X_6)/\partial X_i = 0$ $(i = 1\text{--}6)$. These equations can be rewritten in the following compact form:

$$X_1 = g_a[3\rho_{0a} + 2\rho_{1a} + \sigma_a] + g_{ab}\rho_b - \mu_{1a},$$

$$X_2 = g_a[\rho_{0a} + 2\rho_{1a} - \sigma_a] + g_{ab}\rho_b - \mu_{1a},$$

$$X_3 = g_b[3\rho_{0b} + 2\rho_{1b} + \sigma_b] + g_{ab}\rho_a - \mu_{1b},$$

$$X_4 = g_b[\rho_{0b} + 2\rho_{1b} - \sigma_b] + g_{ab}\rho_a - \mu_{1b},$$

$$X_5 = 2g_{ab}\sqrt{\rho_{0a}\rho_{0b}} + g_{ab}\frac{\rho_{ab} + \sigma_{ab}}{2},$$

$$X_6 = \frac{g_{ab}}{2}(\rho_{ab} - \sigma_{ab}), \quad (44)$$

where the densities ρ_1 and σ are given in the next section. Note that, in the derivation of Eqs. (44), we used the relation $\partial\Omega_{ln}/\partial X_i = A_i/2$, $i = 1\text{--}6$, which can be checked by using *Mathematica* or MAPLE. In general, the system of Eqs. (44) with the given set of input parameters, such as coupling parameters, and the total densities of atoms is the system of nonlinear algebraic equations with respect to unknown variational parameters $(X_1, \ldots, X_6)$. As it is seen from their definition in Eqs. (19)–(27) the latter can be clearly considered self-energies in the Cartesian representation (11).

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[2]The next order corrections to the present approximation can be found in the similar way as has been developed by Stancu and Stevenson [52] for the simple $\lambda\phi^4$ theory.

A. Normal and anomalous densities

Fluctuating fields $\tilde{\psi}(r)$ and $\tilde{\phi}(r)$ define the density of uncondensed particles in accordance with Eqs. (7). When the Green's functions are known, these densities may be calculated as

$$
\begin{aligned}
\rho_{1a} &= \frac{1}{V} \int d\vec{r} \langle \tilde{\psi}^\dagger(\vec{r}) \tilde{\psi}(\vec{r}) \rangle = \frac{1}{2V} \int d\vec{r} [G_{11}(\vec{r}, \vec{r}) \\
&\quad + G_{22}(\vec{r}, \vec{r})] = \frac{1}{2V}(A_1 + A_2), \\
\rho_{1b} &= \frac{1}{V} \int d\vec{r} \langle \tilde{\phi}^\dagger(\vec{r}) \tilde{\phi}(\vec{r}) \rangle = \frac{1}{2V} \int d\vec{r} [G_{33}(\vec{r}, \vec{r}) \\
&\quad + G_{44}(\vec{r}, \vec{r})] = \frac{1}{2V}(A_3 + A_4).
\end{aligned}
\tag{45}
$$

In general, one may introduce the anomalous

$$
\begin{aligned}
\sigma_a &= \frac{1}{2V} \int d\vec{r} [\langle \tilde{\psi}^\dagger(\vec{r}) \tilde{\psi}^\dagger(\vec{r}) \rangle + \langle \tilde{\psi}(\vec{r}) \tilde{\psi}(\vec{r}) \rangle] \\
&= \frac{1}{2V}(A_1 - A_2), \\
\sigma_b &= \frac{1}{2V} \int d\vec{r} [\langle \tilde{\phi}^\dagger(\vec{r}) \tilde{\phi}^\dagger(\vec{r}) \rangle + \langle \tilde{\phi}(\vec{r}) \tilde{\phi}(\vec{r}) \rangle] \\
&= \frac{1}{2V}(A_3 - A_4),
\end{aligned}
\tag{46}
$$

and "mixed" densities:

$$
\begin{aligned}
\rho_{ab} &= \frac{1}{V} \int d\vec{r} [\langle \tilde{\psi}^\dagger(\vec{r}) \tilde{\phi}(\vec{r}) \rangle + \langle \tilde{\phi}^\dagger(\vec{r}) \tilde{\psi}(\vec{r}) \rangle] \\
&= \frac{1}{V} \int d\vec{r} [G_{13}(\vec{r}, \vec{r}) + G_{24}(\vec{r}, \vec{r})] = \frac{1}{2V}(A_5 + A_6), \\
\sigma_{ab} &= \frac{1}{V} \int d\vec{r} [\langle \tilde{\psi}(\vec{r}) \tilde{\phi}(\vec{r}) \rangle + \langle \tilde{\phi}^\dagger(\vec{r}) \tilde{\psi}^\dagger(\vec{r}) \rangle] \\
&= \frac{1}{2V}(A_5 - A_6).
\end{aligned}
\tag{47}
$$

Clearly, these densities, which are explicitly given in the Appendix, do not depend on the coordinate variables; i.e., they are constants for a uniform system. Physically, the pair densities ρ_{ab} and σ_{ab} describe the processes where, due to the presence of the reservoir, particles are exchanged or pairing correlations emerge between the two components.

From their definition, it is clear that the mixed densities characterize the correlations between the components of a two-component system. To quantify these correlations, one may introduce the overlap parameter η,

$$
\eta = \frac{1}{2\sqrt{N_a N_b}} \int d\vec{r} \{ \langle \psi^\dagger(\vec{r}) \phi(\vec{r}) \rangle + \langle \phi^\dagger(\vec{r}) \psi(\vec{r}) \rangle \}, \tag{48}
$$

where $\psi(\vec{r})$ and $\phi(\vec{r})$ are the field operators of the components a and b, respectively.

Using Eqs. (5), (11), and (44)–(48), one may present η as follows:

$$
\begin{aligned}
\eta &= \frac{1}{\sqrt{N_a N_b}} \int d\vec{r} \sqrt{\rho_{0a} \rho_{0b}} + \frac{1}{2\sqrt{N_a N_b}} \int d\vec{r} \{ \langle \tilde{\psi}^\dagger(\vec{r}) \tilde{\phi}(\vec{r}) \rangle \\
&\quad + \langle \tilde{\phi}^\dagger(\vec{r}) \tilde{\psi}(\vec{r}) \rangle \} = \sqrt{n_{0a} n_{0b}} + \frac{\rho_{ab}}{2\sqrt{\rho_a \rho_b}} = \frac{X_5 + X_6}{2g_{ab}\sqrt{\rho_a \rho_b}},
\end{aligned}
\tag{49}
$$

where n_{0a} and n_{0b} are the normalized condensed fractions, $n_{0a} = \rho_{0a}/\rho_a$, $n_{0b} = \rho_{0b}/\rho_b$. Note that, when the fluctuations are neglected, i.e., $\tilde{\psi} = \tilde{\phi} = 0$, η in Eq. (49) coincides with the miscibility parameter of Refs. [53,54], introduced for nonuniform coupled systems. Particularly, when at least one of the components is in the normal phase, the parameter η is completely defined by the normal pair density, $\eta(T > T_c) = \rho_{ab}/2\sqrt{\rho_a \rho_b} = X_5/g_{ab}\sqrt{\rho_a \rho_b}$.

B. Particular cases of HFB approximation

The presented HFB-type theory is general, so that some well-known approximations to this general theory can be easily derived as particular cases.

(i) Sometimes, one uses the trick (first suggested by Shohno [55]) of omitting anomalous averages, which corresponds to the case when in Eqs. (43) and (44) σ_a, σ_b, and σ_{ab} are omitted by setting $\mu_{0a,b} = \mu_{1a,b} = \mu_{a,b}$. However, as has been shown in a number of publications [28–37], this trick results in a not-self-consistent approach containing paradoxes.

(ii) Bogoliubov and quadratic approximations correspond to the case when, after the shift (5) only quadratic terms of fluctuating fields are kept in the action (4): $S \approx S_0 + S_{\text{free}} + S_{\text{int}}^{(2)}$, with $\tilde{\delta} = 1$. The formal difference is that in the quadratic approximation one has

$$
\Omega^{\text{Bil}} = \Omega_0 + \Omega_{ln}, \tag{50}
$$

where Ω_0 and Ω_{ln} have the same expressions as in Eqs. (43) with the self-energies given by

$$
\begin{aligned}
X_1 &\approx X_1^{\text{Bil}} = 3g_a \rho_{0a} + g_{ab} \rho_{0b} - \mu_a, \\
X_2 &\approx X_2^{\text{Bil}} = g_a \rho_{0a} + g_{ab} \rho_{0b} - \mu_a, \\
X_3 &\approx X_3^{\text{Bil}} = 3g_b \rho_{0b} + g_{ab} \rho_{0a} - \mu_b, \\
X_4 &\approx X_4^{\text{Bil}} = g_b \rho_{0b} + g_{ab} \rho_{0a} - \mu_b, \\
X_5 &\approx X_5^{\text{Bil}} = 2g_{ab}\sqrt{\rho_{0a} \rho_{0b}}, \\
X_6 &\approx X_6^{\text{Bil}} = 0.
\end{aligned}
\tag{51}
$$

In the Bogoliubov approximation, the thermodynamic potential is formally given by Eq. (50), and the self-energies by Eqs. (51), with setting there $\rho_{0a,b} \approx \rho_{a,b}$, i.e., $X_i^{Bog} = X_i^{\text{Bil}}(\rho_{0a} = \rho_a, \rho_{0b} = \rho_b)$. In this case, the equations are uncoupled and the solutions are simple. Actually, both these variants enjoy the same level of accuracy and are valid only for small gas parameters $\gamma \leqslant 10^{-5}$.

Note that, for all above cases the expressions for the energy dispersions as well as for the densities are formally the same as given by Eqs. (31) and (A11)–(A16), respectively.

C. Intermediate summary

Now we are in a position of summarizing the present section. In practical calculations, in the framework of our self-consistent theory, one has to solve the system of, in general, six nonlinear algebraic equations (44) with respect to the variational parameters $[X_1, \ldots, X_6]$ and then evaluate all thermodynamic equilibrium characteristics of the uniform two-component Bose system from $\Omega(X_1, \ldots, X_6)$ given in Eqs. (43). Stability and miscibility properties can be studied

by analyzing the spectrum of collective excitations (31). At a first glance, this procedure, especially solving the system of six nonlinear algebraic equations, seems rather cumbersome. However, in reality the number of the unknown variational parameters $[X_1, \ldots, X_6]$ may be reduced depending on the considered state (BEC or normal phase) and on the existing symmetries in the system. In the next sections we discuss these cases in detail.

III. CONDENSED AND NORMAL PHASES

A. Condensed phase

In this phase, the number of variational parameters is reduced due to the Hugenholtz-Pines theorem [26], which has been extended for multicomponent Bose-Einstein condensates in Refs. [27,40]. For a two-component Bose system, in our notation, it reads

$$\Sigma_n^{(a)} - \Sigma_{an}^{(a)} = \mu_{1a}, \qquad \Sigma_n^{(b)} - \Sigma_{an}^{(b)} = \mu_{1b},$$
$$\Sigma_n^{(ab)} = \Sigma_{an}^{(ab)}, \tag{52}$$

and hence

$$X_2 = 0, \quad X_4 = 0, \quad X_6 = 0, \quad \sigma_{ab} = \rho_{ab}. \tag{53}$$

Therefore, in the BEC phase, instead of six equations, we are left with a system of three equations:

$$\Delta_a \equiv X_1/2 = g_a(\rho_{0a} + \sigma_a) = g_a[\rho_a - \rho_{1a} + \sigma_a]$$
$$\Delta_b \equiv X_3/2 = g_b(\rho_{0b} + \sigma_b) = g_b[\rho_b - \rho_{1b} + \sigma_b]$$
$$\Delta_{ab} \equiv X_5/2 = g_{ab}\sqrt{\rho_{0a}\rho_{0b}} + \frac{g_{ab}}{2}\rho_{ab}. \tag{54}$$

Note that, for the Bose systems with fixed chemical potentials [34], these equations may be rewritten as

$$\Delta_a = \mu_{1a} + 2g_a(\sigma_a - \rho_{1a}) - g_{ab}\rho_b$$
$$\Delta_b = \mu_{1b} + 2g_b(\sigma_b - \rho_{1b}) - g_{ab}\rho_a$$
$$\Delta_{ab} = g_{ab}(\sqrt{\rho_{0a}\rho_{0b}} + \rho_{ab}/2). \tag{55}$$

On the other hand, if the densities are fixed, as in atomic gases, one may determine the chemical potentials from Eqs. (44) and (52) as

$$\mu_{1a} = g_a[\rho_a + \rho_{1a} - \sigma_a] + g_{ab}\rho_b,$$
$$\mu_{1b} = g_b[\rho_b + \rho_{1b} - \sigma_b] + g_{ab}\rho_a. \tag{56}$$

The total chemical potentials defined as $\mu_a = (\partial F/\partial N_a)$ and $\mu_b = (\partial F/\partial N_b)$ (where F is the total free energy of the system) can be calculated as

$$\mu_a\rho_a = \mu_{1a}\rho_{1a} + \mu_{0a}\rho_{0a}, \quad \mu_b\rho_b = \mu_{1b}\rho_{1b} + \mu_{0b}\rho_{0b}, \tag{57}$$

where

$$\mu_{0a} = g_a[\rho_a + \rho_{1a} + \sigma_a] + g_{ab}\left[\rho_b + \frac{\rho_{0b}\sigma_{ab}}{\sqrt{\rho_{0a}\rho_{0b}}}\right],$$
$$\mu_{0b} = g_b[\rho_b + \rho_{1b} + \sigma_b] + g_{ab}\left[\rho_a + \frac{\rho_{0a}\sigma_{ab}}{\sqrt{\rho_{0a}\rho_{0b}}}\right]. \tag{58}$$

The last two equations are derived from $\partial\Omega/\partial\rho_{0a} = 0$ and $\partial\Omega/\partial\rho_{0b} = 0$, where Ω is given by Eq. (43). As is expected,

when one neglects anomalous densities by setting $\sigma_a = \sigma_b = \sigma_{ab} = 0$, then $\mu_{0a} = \mu_{1a} = \mu_a$, $\mu_{0b} = \mu_{1b} = \mu_b$.

With the constraints (53), the dispersions in Eqs. (31) can be rewritten as

$$\omega_{1,2} = \sqrt{\frac{\varepsilon(k)^2}{2}\left(\nu_1^2 + \nu_2^2\right) + 2\varepsilon(k)\Lambda_{1,2}},$$

$$\Lambda_{1,2} = \frac{1}{2}(\Delta_a\nu_1 + \Delta_b\nu_2) \pm \frac{\sqrt{D_s}}{4},$$

$$D_s = 16\nu_1\nu_2\Delta_{ab}^2 + \left(\nu_1^2\varepsilon(k) - \nu_2^2\varepsilon(k) + 2\Delta_a\nu_1 - 2\Delta_b\nu_2\right)^2,$$

$$\omega_1^2 - \omega_2^2 = \varepsilon(k)\sqrt{D_s}, \tag{59}$$

where we introduce the reduced mass $m_R = m_{ab} = m_a m_b / (m_a + m_b)$, and $\nu_1 = m_b/(m_a + m_b)$, $\nu_2 = m_a/(m_a + m_b)$, and $\varepsilon(k) = \vec{k}^2/2m_R$. Decomposing ω_i in powers of momenta gives the sound velocities through the equations

$$\omega_1 = c_1|\vec{k}| + O(k^3), \quad \omega_2 = c_2|\vec{k}| + O(k^3), \tag{60}$$

$$c_1^2 = \frac{\Delta_a m_b + \Delta_b m_a + \sqrt{4m_a m_b \Delta_{ab}^2 + (\Delta_b m_a - \Delta_a m_b)^2}}{2m_a m_b},$$

$$c_2^2 = \frac{\Delta_a m_b + \Delta_b m_a - \sqrt{4m_a m_b \Delta_{ab}^2 + (\Delta_b m_a - \Delta_a m_b)^2}}{2m_a m_b}. \tag{61}$$

The velocities c_1 (c_2) are referred in the literature as density (pseudospin) sound velocities. In a binary superfluid, the density sound corresponds to oscillation of two superfluid components in phase, while the pseudospin sound corresponds to the out-of-phase oscillations [8].

From the last equation it is seen that, when $\Delta_a\Delta_b < \Delta_{ab}^2$, c_2^2 becomes negative, signaling the instability of the system. In particular, applying the Bogoliubov approximation, i.e., setting $\rho_{0a} \approx \rho_a$, $\rho_{0b} \approx \rho_b$, and $\sigma_a = \sigma_b = \rho_{ab} \approx 0$, then from Eqs. (54) one obtains

$$\Delta_a \approx g_a\rho_a, \quad \Delta_b \approx g_b\rho_b, \quad \Delta_{ab} \approx g_{ab}\sqrt{\rho_a\rho_b}, \tag{62}$$

thus arriving at the well-known stability condition $g_a g_b/g_{ab}^2 \geqslant 1$.

Explicit expressions for the densities may be obtained from Eqs. (45)–(47) by setting there $X_2 = X_4 = X_6 = 0$. As is expected, when the intercoupling constant goes to zero, we arrive at the well-known formulas of the single-component case:

$$\rho_{1a}(g_{ab} \to 0) = \frac{1}{V}\sum_k\left[\frac{\Delta_a + \varepsilon_a(\vec{k})}{\omega_a(k)}W_1(k) - \frac{1}{2}\right],$$

$$\rho_{1b}(g_{ab} \to 0) = \frac{1}{V}\sum_k\left[\frac{\Delta_b + \varepsilon_b(\vec{k})}{\omega_b(k)}W_2(k) - \frac{1}{2}\right],$$

$$\sigma_a(g_{ab} \to 0) = -\frac{\Delta_a}{V}\sum_k\frac{W_1(k)}{\omega_a(k)},$$

$$\sigma_b(g_{ab} \to 0) = -\frac{\Delta_b}{V}\sum_k\frac{W_2(k)}{\omega_b(k)},$$

$$\rho_{ab}(g_{ab} \to 0) = \sigma_{ab}(g_{ab} \to 0) = 0,$$

$$c_1^2 = \Delta_b/m_b, \quad c_2^2 = \Delta_a/m_a, \tag{63}$$

where $W_{a,b}(k) = 1/2 + 1/(e^{\omega_{a,b}(k)\beta} - 1)$, $\omega_{a,b} = \sqrt{\varepsilon_{a,b}(k)(\varepsilon_{a,b}(k) + 2\Delta_{a,b})}$.

In the above discussion, we have assumed that both components are in the BEC state. In the next section, we consider the case where the whole system is in the normal phase; hence there is no the HP theorem.

B. Normal phase

The general criterion of miscibility or immiscibility is prescribed by the behavior of the spectrum of collective excitations. To be miscible, a binary Bose mixture has to possess all real branches of the collective spectrum positive (nonnegative). In the case of a Bose-condensed system, the global gauge symmetry is broken and the spectra of single-particle and collective excitations coincide [56]. However, for a normal (uncondensed) system, these spectra are different. The positiveness of the single-particle spectrum, defined by the poles of the single-particle Green's function, tells us that, on the level of single-particle properties, the system is stable, but this tells us nothing about whether it is mixed or separated. The spectrum of collective excitations of a normal system is defined by the poles of the second-order Green's function or the poles of dynamic susceptibility (response function). The mixture separates when the lowest branch of the collective spectrum crosses zero.

First, let us prove that the binary normal Bose mixture at $T > T_c$ enjoys a stable single-particle spectrum that is positive at any temperature and the values of local interaction parameters, independently of whether the system is mixed or separated.

By definition, in the normal phase $\rho_{0a} = \rho_{0b} = \sigma_a = \sigma_b = \sigma_{ab} = 0$, and hence $\rho_{1a} = \rho_a$, $\rho_{1b} = \rho_b$, $\mu_{0a} = \mu_{1a} = \mu_a$, $\mu_{0b} = \mu_{1b} = \mu_b$, $X_6 = X_5$, $X_2 = X_1$, and $X_4 = X_3$. Thus, the main Eqs. (44) are simplified as

$$X_1 = 2\rho_a g_a + \rho_b g_{ab} - \mu_a \equiv -\mu_{\text{eff}}^{(a)},$$
$$X_3 = 2\rho_b g_b + \rho_a g_{ab} - \mu_b \equiv -\mu_{\text{eff}}^{(b)}, \qquad (64)$$
$$X_5 = \tfrac{1}{2}\rho_{ab} g_{ab},$$

where the densities are given by the equations

$$\rho_{1a} = \rho_a = \frac{1}{V} \sum_k \left\{ \frac{\left(X_5^2 E_b + E_a \omega_1^2 - E_a E_b^2\right) f(\omega_1)}{\sqrt{D}\omega_1} \right.$$
$$\left. + \frac{\left(X_5^2 E_b + E_a \omega_2^2 - E_a E_b^2\right) f(\omega_2)}{\sqrt{D}\omega_2} \right\},$$

$$\rho_{1b} = \rho_b = \frac{1}{V} \sum_k \left\{ \frac{\left(X_5^2 E_a + E_b \omega_1^2 - E_a^2 E_b\right) f(\omega_1)}{\sqrt{D}\omega_1} \right.$$
$$\left. + \frac{\left(X_5^2 E_a + E_b \omega_2^2 - E_a^2 E_b\right) f(\omega_2)}{\sqrt{D}\omega_2} \right\},$$

$$\rho_{ab} = \frac{2X_5}{V} \sum_k \left\{ \frac{\left(-X_5^2 + E_a E_b + \omega_1^2\right) f(\omega_1)}{\sqrt{D}\omega_1} \right.$$
$$\left. - \frac{\left(-X_5^2 + E_a E_b + \omega_2^2\right) f(\omega_2)}{\sqrt{D}\omega_2} \right\},$$

$$\eta = \frac{\rho_{ab}}{2\sqrt{\rho_a \rho_b}}, \quad f(x) = 1/(e^{\beta x} - 1). \qquad (65)$$

Then the dispersion relations (31) reduce to the form

$$\omega_{1,2} = \sqrt{\frac{E_a^2 + E_b^2}{2} + X_5^2 \pm \frac{\sqrt{D}}{2}},$$
$$D = (E_a + E_b)^2 \left[4X_5^2 + (E_a - E_b)^2\right], \qquad (66)$$

with

$$E_a = \varepsilon_a(k) - \mu_{\text{eff}}^{(a)}, \quad E_a = \varepsilon_b(k) - \mu_{\text{eff}}^{(b)}. \qquad (67)$$

This spectrum is real and positive, provided the expression under the square root does not become negative. It is convenient to test the positiveness of the expression $\omega_1^2 \omega_2^2$. Then from Eq. (66) one easily obtains the condition

$$\omega_1^2 \omega_2^2 = \left(E_a E_b - X_5^2\right)^2 \geqslant 0. \qquad (68)$$

Since ω_1 is positive, both ω_1^2 and ω_2^2 are positive simultaneously for any g_{ab} and temperature $T \geqslant T_c$; hence the spectra are real and positive.

Note that, when $g_{ab} = 0$, Eqs. (65) turn into the well-known expressions

$$\rho_{1a} = \rho_a = \frac{1}{V} \sum_k \frac{1}{e^{\beta(\varepsilon_a(k) - \mu_{\text{eff}}^{(a)})} - 1},$$
$$\rho_{1b} = \rho_b = \frac{1}{V} \sum_k \frac{1}{e^{\beta(\varepsilon_b(k) - \mu_{\text{eff}}^{(b)})} - 1}, \qquad (69)$$

where $\mu_{\text{eff}}^{(a)} = \mu_a - 2\rho_a g_a$.

The spectrum of collective excitations of a binary mixture of normal components has been studied in the random-phase approximation in Ref. [57]. In that approximation, for the case of contact interactions, the dynamic condition for mixture stability is found to coincide with the inequality $g_{ab}^2 < g_a g_b$, being practically independent of temperature.

C. Near critical temperature

Let T_c^a and T_c^b be the BEC transition temperatures for the corresponding components. For concreteness, we assume that $T_c^a \leqslant T_c^b$. In fact, T_c^a corresponds to the point where the effective chemical potential vanishes, $\mu_{\text{eff}}^{(a)} = -X_1 = 0$. From the stability condition $\Delta_a \Delta_b > \Delta_{ab}^2$, that is, $X_5^2 \leqslant X_1 X_3$, it is understood that the system can be stable only for $X_5 = 0$, with the sound velocities

$$c_1^2 = \frac{\Delta_b}{m_b} \geqslant 0, \quad c_2^2 = 0. \qquad (70)$$

This temperature can be evaluated from Eqs. (69) as

$$\rho_{1a} = \rho_a = \frac{1}{V} \sum_k \frac{1}{e^{\varepsilon_a(k)/T_c^a} - 1}. \qquad (71)$$

From this equation it is seen that in the present approximation, like in many versions of mean-field approximations [25], there is no shift of critical temperature due to intercomponent coupling constant g_{ab}, i.e., $T_c(g_{ab}) = T_c(g_{ab} = 0)$.

For completeness, at the end of this section we present explicit expressions for the free energy $F = \Omega + \mu N = \Omega +$

$\mu_a N_a + \mu_b N_b$, which has the form

$$F(T < T_c) = F_0 + F_{ZM} + F_T,$$

$$F_0 = \frac{V\rho_a^2 g_a}{2}\left(1 + n_{1a}^2 - \tilde{m}_a^2 - 2n_{1a}\tilde{m}_a\right) + \frac{V\rho_b^2 g_b}{2}$$

$$\times \left(1 + n_{1b}^2 - \tilde{m}_b^2 - 2n_{1b}\tilde{m}_b\right) + \frac{V}{2}\rho_a\rho_b(2 - \tilde{m}_{ab}^2),$$

$$F_{ZM} = \frac{1}{2}\sum_k\left\{\omega_1 + \omega_2 - \varepsilon_k - \Delta_a - \Delta_b\right.$$

$$\left. + \frac{\nu_2^2\Delta_a^2 + \nu_1^2\Delta_b^2 + 4\Delta_{ab}^2\nu_1\nu_2}{2\nu_1\nu_2\varepsilon(k)}\right\},$$

$$F_T = T\sum_k[\ln(1 - e^{-\omega_1\beta}) + \ln(1 - e^{-\omega_2\beta})],$$

$$F(T > T_c) = Vg_a\rho_a^2 + Vg_b\rho_b^2 + g_{ab}V\rho_a\rho_b + F_T, \qquad (72)$$

where $n_{1a} = \rho_{1a}/\rho_a$, $\tilde{m}_a = \sigma_a/\rho_a$, $\tilde{m}_{ab} = \sigma_{ab}/\rho_a$, and the dispersions ω_1 and ω_2 for the BEC and normal phases are given in Eqs. (59) and (66), respectively. The explicit expressions for F_{ZM}, referred in the literature as zero mode energy, can be found, e.g., in Refs. [3,58]. Note that the present approach includes by itself not only the Lee-Huang-Yang (LHY) term [59], but also the corrections beyond the LHY approximation due to taking account of anomalous densities. Particularly, the LHY term can be obtained expanding F_{ZM} in powers of the coupling parameters.

Concluding the present section, let us summarize the conditions of stability for a two-component uniform Bose system:

(i) At temperatures below the critical one, when the system is in the condensed phase, the mixture is stable, provided the general condition

$$\frac{\Delta_a(\gamma, T)\Delta_b(\gamma, T)}{\Delta_{ab}^2(\gamma, T)} \geqslant 1 \qquad (73)$$

holds. Here the self-energies $\Delta_a(\gamma, T)$, $\Delta_b(\gamma, T)$, and $\Delta_{ab}(\gamma, T)$ are the solutions to Eqs. (54).

(ii) The inequality (73) may be replaced by

$$\frac{g_a g_b}{g_{ab}^2} \geqslant 1 \qquad (74)$$

for very dilute gases, where the Bogoliubov approximation is valid.

In the next section it will be shown that, for a balanced symmetric Bose mixture, the inequality (73) may be represented as an expansion in powers of γ.

IV. BALANCED SYMMETRIC BOSE MIXTURES

The case of a binary superfluid gas with two symmetric components consisting of ^{23}Na in an equal mixture of two hyperfine ground states has been recently realized experimentally by Kim *et al.* [8]. So we assume that $g_a = g_b = g$, $g_{ab} = \bar{g}_{ab}g_a$, $m_a = m_b = m$, $\varepsilon_a(k) = \varepsilon_b(k) = \varepsilon(k) = k^2/2m$, and $\rho_a = \rho_b = \rho/2$, where $N = \rho V$ is the total number of atoms in the mixture. Note that, treating the anomalous averages, we resort to the standard way of regularization by employing the method of counterterms that is equivalent to the dimensional regularization [25,46].

A. Zero temperature

At zero temperature, the densities are simplified to

$$n_{1a} = \frac{\rho_{1a}(T=0)}{\rho_a} = \frac{\rho_{1b}(T=0)}{\rho_a} = \frac{1}{2V\rho_a}\sum_k\left\{\frac{\Delta_a + \varepsilon(k) + \Delta_{ab}}{2\omega_1} + \frac{\Delta_a + \varepsilon(k) - \Delta_{ab}}{2\omega_2} - 1\right\} = \frac{m^3(c_1^3 + c_2^3)}{6\pi^2\rho_a} = n_{1b},$$

$$\tilde{m}_a = \frac{\sigma_a(T=0)}{\rho_a} = \frac{\sigma_b(T=0)}{\rho_b} = -\frac{1}{2V\rho_a}\sum_k\left\{\frac{\Delta_a + \Delta_{ab}}{2\omega_1} + \frac{\Delta_a - \Delta_{ab}}{2\omega_2} - \frac{\Delta_a}{\varepsilon(k)}\right\} = 3n_{1a}(T=0), \qquad (75)$$

$$n_{ab} = \frac{\rho_{ab}(T=0)}{\sqrt{\rho_a\rho_b}} = \frac{1}{2V\rho_a}\sum_k\left\{\frac{\varepsilon(k) + \Delta_a + \Delta_{ab}}{\omega_1} - \frac{\varepsilon(k) + \Delta_a - \Delta_{ab}}{\omega_2}\right\} = \frac{m^3(c_1^3 - c_2^3)}{3\pi^2\rho_a}, \quad \tilde{m}_{ab} = \frac{\sigma_{ab}(T=0)}{\sqrt{\rho_a\rho_b}} = n_{ab},$$

where we have introduced the sound velocities

$$c_{1,2}^2 = (\Delta_a \pm \Delta_{ab})/m, \qquad (76)$$

which satisfy the following equations, derived from Eqs. (55) and (61):

$$c_1^3 - c_2^3(\bar{g}_{ab} - 1) - \frac{3\pi^2 c_1^2}{gm^2} + \frac{3\pi^2\rho_a(\bar{g}_{ab} + 1)}{m^3} = 0,$$

$$c_1^3 + c_2^3(\bar{g}_{ab} + 1) - \frac{3\pi^2 c_2^2}{gm^2} - \frac{3\pi^2\rho_a(\bar{g}_{ab} - 1)}{m^3} = 0. \qquad (77)$$

These equations can be rewritten in the dimensionless form as

$$s_1^3 + (1 - \bar{g}_{ab})s_2^3 - \frac{3\pi s_1^2}{4} + \frac{3\pi^2\gamma(\bar{g}_{ab} + 1)}{2} = 0,$$

$$s_1^3 + (1 + \bar{g}_{ab})s_2^3 - \frac{3\pi s_2^2}{4} - \frac{3\pi^2\gamma(\bar{g}_{ab} - 1)}{2} = 0, \qquad (78)$$

where $\gamma = \rho a_s^3$, $\rho = 2\rho_a$ is the total density of the whole binary system, $a_s = mg/4\pi$, and $s_{1,2} = c_{1,2}ma_s$. From the Bogoliubov approximation, it is known that the system becomes unstable for $\bar{g}_{ab} > 1$. Here we study the problem of possible corrections to this criterion due to quantum fluctuations.
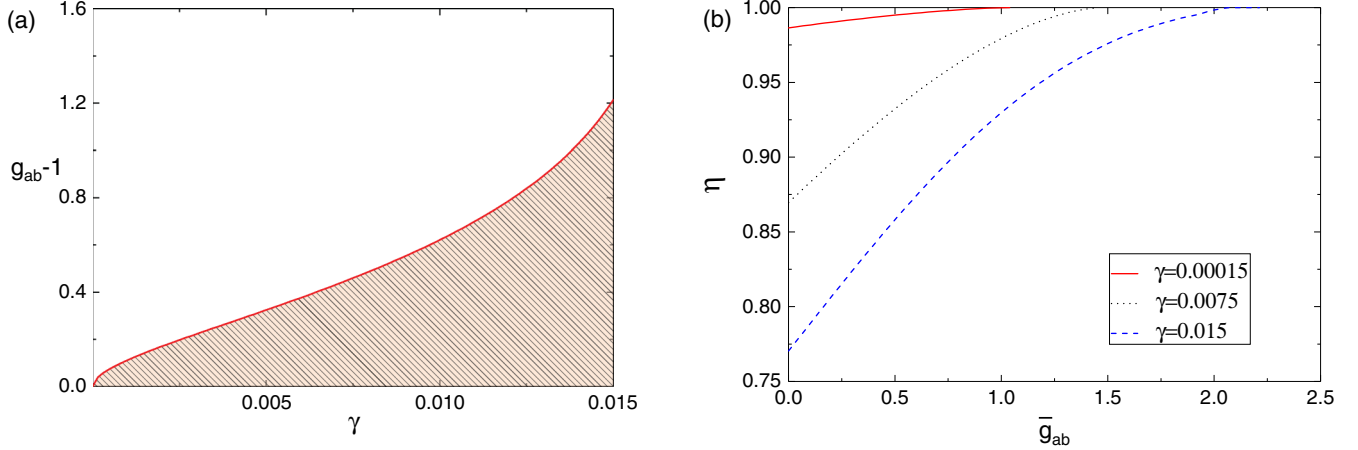
FIG. 1. (a) The phase diagram of a symmetric binary Bose system with repulsive interactions at zero temperature. The shaded region corresponds to the stable, miscible phase. (b) Overlap parameter η vs $\bar{g}_{ab} = g_{ab}/g$ for three different values of the gas parameter: $\gamma = 0.15 \times 10^{-3}$ (solid line), $\gamma = 0.75 \times 10^{-2}$ (dotted line), and $\gamma = 0.15 \times 10^{-1}$ (dashed line).

To find the answer to this question one has to consider the dispersions:

$$\omega_1^2 = \varepsilon(k)[\varepsilon(k) + 2(\Delta_a + \Delta_{ab})],$$
$$\omega_2^2 = \varepsilon(k)[\varepsilon(k) + 2(\Delta_a - \Delta_{ab})]. \tag{79}$$

It is seen that the boundary of stability is defined by the condition $\Delta_a = \Delta_{ab}$, since for $\Delta_a < \Delta_{ab}$ the sound velocity c_2 becomes negative. This is also seen from the general condition $\Delta_a \Delta_b \leqslant \Delta_{ab}^2$, with $\Delta_a = \Delta_b$. In other words, the boundary of stability in the phase diagram $(\bar{g}_{ab}, \gamma)$ lies on the line $c_2 = 0$, i.e., $s_2(\bar{g}_{ab}^*, \gamma^*) \equiv 0$. From Eqs. (78), one obtains

$$(s_1^*)^3 - \frac{3\pi}{8}(s_1^*)^2 + \frac{3\pi^2\gamma^*}{2} = 0,$$

$$\bar{g}_{ab}^* = \frac{(s_1^*)^2}{4\pi\gamma^*}, \tag{80}$$

where the asterisk indicates the threshold values of the parameters, corresponding to the boundary of stability for the symmetric binary mixture. In Fig. 1(a), we present the phase diagram on the $(\bar{g}_{ab}, \gamma)$ plane (solid line). It is seen that, due to quantum fluctuations, the system at $T = 0$ remains stable even, for example, at $\bar{g}_{ab}^*(\gamma \approx 0.013) \approx 1.9$. This is one of the main results of the present work.

For small γ, one may use the following expansion for $\bar{g}_{ab}^*$:

$$\bar{g}_{ab}^* = 1 + \frac{16\sqrt{\gamma}}{3\sqrt{\pi}} + \frac{128\gamma}{3\pi} + \frac{3584\gamma^{3/2}}{9\pi^{3/2}} + O(\gamma^{5/2}), \tag{81}$$

in order to obtain the stability condition in the form

$$g_{ab} \leqslant g_a\left[1 + \frac{16\sqrt{\gamma}}{3\sqrt{\pi}} + O(\gamma)\right], \tag{82}$$

which is valid for $\gamma \leqslant 0.005$.

The overlap parameter for the symmetric case at $T = 0$ has the form

$$\eta = n_{0a} + \frac{n_{ab}}{2} = 1 - n_{1a} + \frac{n_{ab}}{2} = 1 - \frac{2s_2^3}{3\pi^2\gamma}, \tag{83}$$

where we use Eqs. (75) and (76). On the boundary of stability, $s_2 = s_2^* = 0$, and η reaches its maximum value $\eta = 1$ [see Fig. 1(b)].

Close to the phase transition point, the condensed fraction can be presented as

$$n_0^*(T=0) = 1 - \frac{\rho_{1a}}{\rho_a}\bigg|_{\bar{g}_{ab}\to\bar{g}_{ab}^*} = 1 - \frac{8\sqrt{\gamma}}{3\sqrt{\pi}} - \frac{64\gamma}{3\pi} + O(\gamma^{3/2}). \tag{84}$$

In Fig. 2(a), we present the condensed fraction vs $\bar{g}_{ab}$. It is seen that intercomponent repulsion g_{ab} tends to destroy BEC, repelling the condensed particles.

The present work would not be complete without a comparison with the experiment performed by Kim *et al.* [8]. The authors studied the mixture of atoms with two hyperfine ground states of ^{23}Na and measured the sound velocities $c_1 = 3.23$ mm/s and $c_2 = 0.70$ mm/s by fixing the relative coupling constant $\bar{g}_{ab} = 0.93$ and the gas parameter $\gamma \approx 1.4 \times 10^{-6}$. For this set of parameters from Eqs. (77), we get the following values for the sound velocities: $c_1 = 3.91$ mm/s, $c_2 = 0.75$ mm/s, which are rather close to the experimental data. To make further prediction, we have calculated the relative sound velocity c_2/c_1 vs $\bar{g}_{ab}$ for three different values of γ. The results are presented in Fig. 2(b). It is seen that c_2/c_1 reduces with increasing $\bar{g}_{ab}$ and vanishes at $\bar{g}_{ab} = \bar{g}_{ab}^*$, where the phase separation occurs.

B. Finite temperature BEC in a balanced symmetric binary mixture

Setting $m_a = m_b = m$, $\rho_a = \rho_b = \rho/2$, $g_a = g_b = g$, and $g_{ab} = \bar{g}_{ab}g$ in Eqs. (A11)–(A16), we can obtain the following
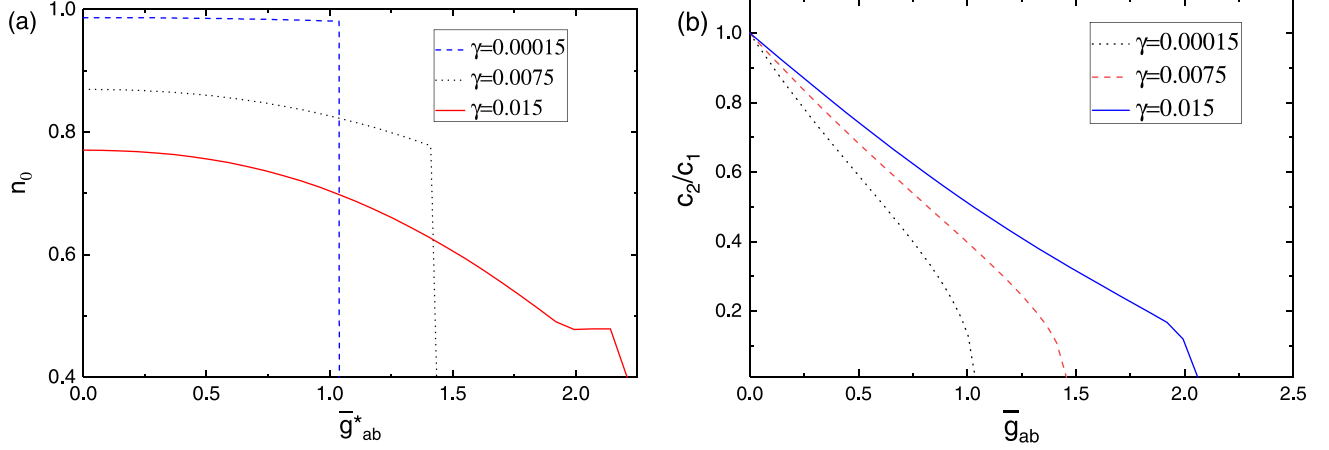
FIG. 2. (a) The condensed fraction $[n_0 = \rho_0/(\rho/2)]$ at zero temperature vs $\overline{g}_{ab} = g_{ab}/g$ in the interval $0 < \overline{g}_{ab} < \overline{g}_{ab}^*(\gamma)$ for different values of γ. (b) The relative sound velocity c_2/c_1 vs $\overline{g}_{ab}$ for different values of γ at $T = 0$.

expressions for the densities at finite temperatures,

$$
n_{1a} = \frac{\rho_{1a}}{\rho_a} = \frac{m^3(c_1^3 + c_2^3)}{6\pi^2 \rho_a} + \frac{1}{2V\rho_a} \sum_k \left[\frac{mc_1^2 + \varepsilon(k)}{\omega_1} f(\omega_1) \right.
$$
$$
\left. + \frac{mc_2^2 + \varepsilon(k)}{\omega_2} f(\omega_2) \right],
$$

$$
\tilde{m}_a = \frac{\sigma_a}{\rho_a} = \frac{m^3(c_1^3 + c_2^3)}{2\pi^2 \rho_a} - \frac{m}{2V\rho_a} \sum_k \left[c_1^2 f(\omega_1) + c_2^2 f(\omega_2) \right],
$$

$$
n_{ab} = \frac{\rho_{ab}}{\rho_a} = \frac{m^3(c_1^3 - c_2^3)}{3\pi^2 \rho_a} + \frac{1}{V\rho_a} \sum_k \left[\frac{c_1^2 m + \varepsilon(k)}{\omega_1} f(\omega_1) \right.
$$
$$
\left. + \frac{c_2^2 m + \varepsilon(k)}{\omega_2} f(\omega_2) \right], \tag{85}
$$

as well as for the overlap parameter η,

$$
\eta = 1 - \frac{m^3 c_2^3}{3\pi^2 \rho_a} - \frac{1}{V\rho_a} \sum_k \frac{mc_2^2 + \varepsilon(k)}{\omega_2} f(\omega_2), \tag{86}
$$

where the dispersions, given in terms of the sound velocities, are

$$
\omega_{1,2} = \sqrt{\varepsilon(k)\big(\varepsilon(k) + 2mc_{1,2}^2\big)}. \tag{87}
$$

Note that close to the critical temperature, where $c_2 = 0$ and $\omega_2 = \varepsilon(k)$, the overlap parameter η tends to zero:

$$
\eta(T \to T_c) = 1 - \frac{1}{\rho_a V} \sum_k \frac{1}{e^{\varepsilon(k)/T_c} - 1} = 1 - 1 = 0, \tag{88}
$$

as is shown for the general case in Sec. III. As to the main equations (54) they are simplified as

$$
\Delta_a = \Delta_b = \frac{m}{2}\big(c_1^2 + c_2^2\big) = g\rho_a[1 - n_{1a} + \tilde{m}_a],
$$

$$
\Delta_{ab} = \frac{m}{2}\big(c_1^2 - c_2^2\big) = g\overline{g}_{ab}\rho_a \left[1 - n_{1a} + \frac{n_{ab}}{2} \right]. \tag{89}
$$

For practical calculations, it is convenient to solve the system of the following dimensionless equations:

$$
s_1^3 + s_2^3 - \frac{3\pi}{8}\big(s_1^2 + s_2^2\big) + \frac{3\pi^2\gamma}{2} - \frac{3\pi^2 a_s}{2mV}
$$
$$
\times \sum_k \left[\frac{a_s^2 m\varepsilon(k) + 2s_1^2}{\omega_1} f(\omega_1) \right.
$$
$$
\left. + \frac{a_s^2 m\varepsilon(k) + 2s_2^2}{\omega_2} f(\omega_2) \right] = 0,
$$

$$
s_1^2 - s_2^2 + \frac{8\overline{g}_{ab}s_2^3}{3\pi} - 4\pi\overline{g}_{ab}\gamma + \frac{8\pi\overline{g}_{ab}a_s}{mV}
$$
$$
\times \sum_k \frac{s_2^2 + a_s^2 m\varepsilon(k)}{\omega_2} f(\omega_2) = 0, \tag{90}
$$

where $\omega_{1,2} = \varepsilon^2(k) + 2\varepsilon(k)s_{1,2}^2/ma_s^2$, with respect to the dimensionless sound velocities $s_i = c_i m a_s$, and then evaluate the densities from Eqs. (85) and (86).

In the previous section we studied the boundary of stability [Fig. 1(a)] at zero temperature. As is clear, at finite temperature the stability condition $\Delta_a(\overline{g}_{ab}, \gamma, T) \leqslant \Delta_{ab}(\overline{g}_{ab}, \gamma, T)$ can also be violated. Now the stability becomes lost at a certain point with $\overline{g}_{ab} = \overline{g}_{ab}^*$ for a given gas parameter γ and temperature T. At this point, according to Eqs. (89), we have $c_2 = 0$ and hence $\overline{g}_{ab}^*$ satisfies the following equation:

$$
\overline{g}_{ab}^* = \frac{v_1^2}{2(1 - t^{3/2})}, \tag{91}
$$

where we use the identity

$$
\frac{1}{V} \sum_k f(\omega_2) = \frac{1}{V} \sum_k \frac{1}{e^{\varepsilon(k)\beta} - 1} = \rho_a t^{3/2}, \tag{92}
$$

with $t = T/T_c$ and $T_c = 2\rho_a^{2/3}\pi/mn\eta(3/2)^{2/3} \approx 2.08\gamma^{2/3}/a_s^2 m$. Along the line of the stability boundary, the reduced sound velocity in Eq. (91) is $v_1 = ma_s c_1/\sqrt{2\pi\gamma}$, and the
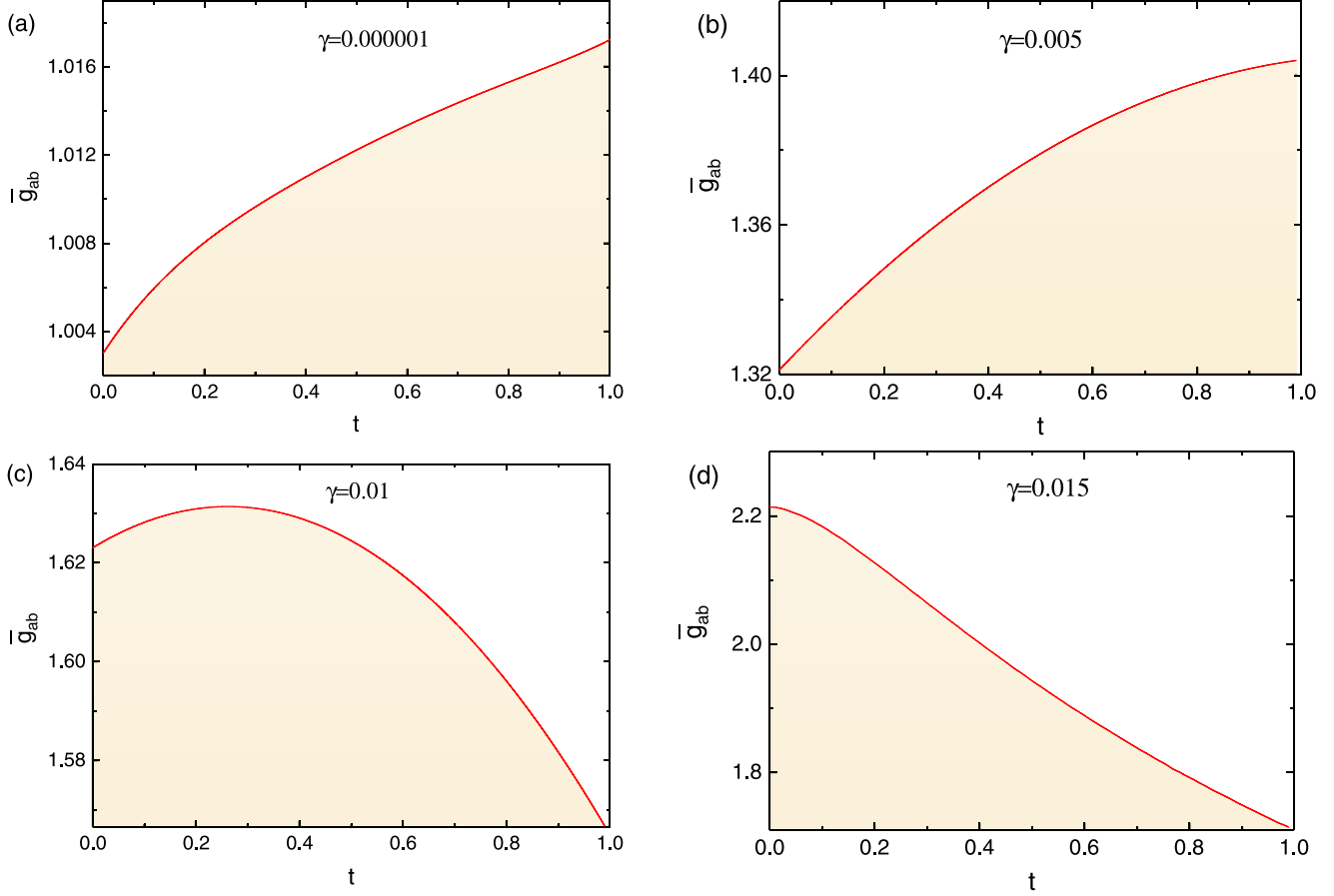
FIG. 3. Phase diagram of the balanced symmetric two-component Bose mixture on the $(\overline{g}_{ab} = g_{ab}/g, t = T/T_c)$ plane for different gas parameters: (a) $\gamma = 0.000001$, (b) $\gamma = 0.005$, (c) $\gamma = 0.01$, and (d) $\gamma = 0.015$. The shaded region corresponds to a stable miscible state.

densities are given by the following equations:

$$1 - \frac{v_1^2}{2} + \frac{4v_1^3}{3}\sqrt{\frac{2\gamma}{\pi}} - \frac{t^{3/2}}{2}$$
$$- \frac{a_s}{Vm\gamma}\sum_k \frac{(a_s^2\varepsilon(k)m + 4\pi v_1^2\gamma)}{\omega_1}f(\omega_1) = 0, \quad (93)$$

$$n_{1a}^* = \frac{t^{3/2}}{2} + \frac{2}{3}\sqrt{\frac{2\gamma}{\pi}}v_1^3$$
$$+ \frac{a_s}{\pi\gamma V}\sum_k \frac{(2\pi\gamma v_1^2 + \varepsilon(k)ma_s^2)}{\omega_1}f(\omega_1) = 0, \quad (94)$$

$$\tilde{m}_a^* = \frac{2v_1^3\sqrt{2\gamma}}{\sqrt{\pi}} - \frac{2a_s\pi v_1^2}{mV}\sum_k \frac{1}{\omega_1}f(\omega_1), \quad (95)$$

$$n_{ab}^* = -t^{3/2} + \frac{4v_1^3}{3}\sqrt{\frac{2\gamma}{\pi}}$$
$$+ \frac{2a_s}{m\gamma V}\sum_k \frac{(2\pi\gamma v_1^2 + \varepsilon(k)ma_s^2)}{\omega_1}f(\omega_1). \quad (96)$$

The equation for η^* is simplified as

$$\eta^* = \eta(c_2 = 0) = 1 - t^{3/2} \neq 0, \quad (97)$$

where we use Eqs. (86) and (92).

In Fig. 3, we present the phase diagram of a symmetric two-component BEC on the $(\overline{g}_{ab}, t)$ plane for four values of γ. It is seen that instability can occur at any temperature below the critical one depending on $g_{ab} = \overline{g}_{ab}g$. For example, at $t = 0.5$ the system remains in a miscible, stable phase before $\overline{g}_{ab}$ reaches the value $\overline{g}_{ab}^* = 1.625$ for $\gamma = 0.01$. Increasing further $\overline{g}_{ab}$ at this temperature leads to the phase transition to an immiscible but stable phase which has lower energy. It is seen from Fig. 3(a) that for small γ the threshold value of $\overline{g}_{ab}$ is close to unity in agreement with the Bogoliubov prediction, and it increases with increasing γ due to the quantum corrections. Below $\overline{g}_{ab} < \overline{g}_{ab}^*$, the system is miscible and stable.

In Fig. 4, we plot the overlap parameter $\eta(t)$ for different values of $\overline{g}_{ab}$ and γ. As is seen, η is close to unity near zero temperature, and rapidly decreases by increasing the temperature, to vanish at $T = T_c$.

In Fig. 5 we present the chemical potential on the whole range of temperatures ($t = T/T_c$) for different values of $\overline{g}_{ab}$. It is seen that the modification of μ due to $\overline{g}_{ab}$ is rather large both in Bose-condensed ($T < T_c$) and normal ($T > T_c$) phases.

V. DISCUSSION AND CONCLUSIONS

We have developed a self-consistent mean-field theory for a binary homogeneous mixture of two-component Bose systems. This theory, being conserving and gapless, imposes
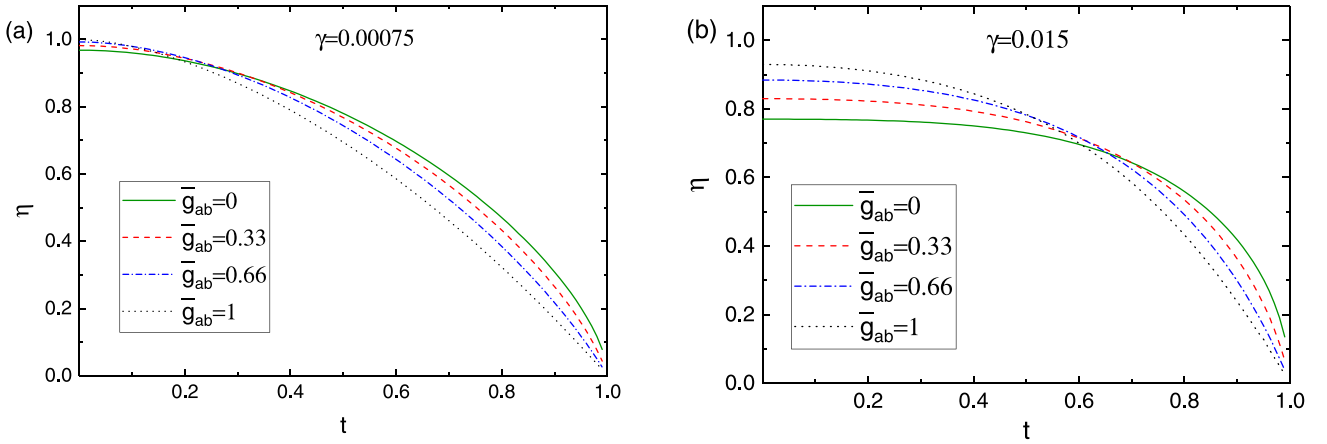
FIG. 4. The overlap parameter vs temperature for (a) $\gamma = 7.5 \times 10^{-3}$ and (b) $\gamma = 0.015$.

no restriction on the gas parameter γ, and hence it is valid for arbitrary strong interactions g_{ab}. The theory satisfies the generalized HP theorem and takes into account anomalous densities σ_a, σ_b, and σ_{ab}. The presented approach is a kind of a self-consistent Hartree-Fock-Bogoliubov approximation; hence it is the most general mean-field approximation. Therefore, as particular cases it includes other known mean-field

approximations, such as the Shohno model, quadratic, and Bogoliubov approximations. For numerical analysis, we have considered the balanced symmetric configuration of a two-component mixture of Bose gases. We have obtained the phase diagram for this system at zero as well as at finite temperatures for arbitrary gas parameters. The phase diagram at zero temperature on the (g_{ab}, γ) plane shows that the system
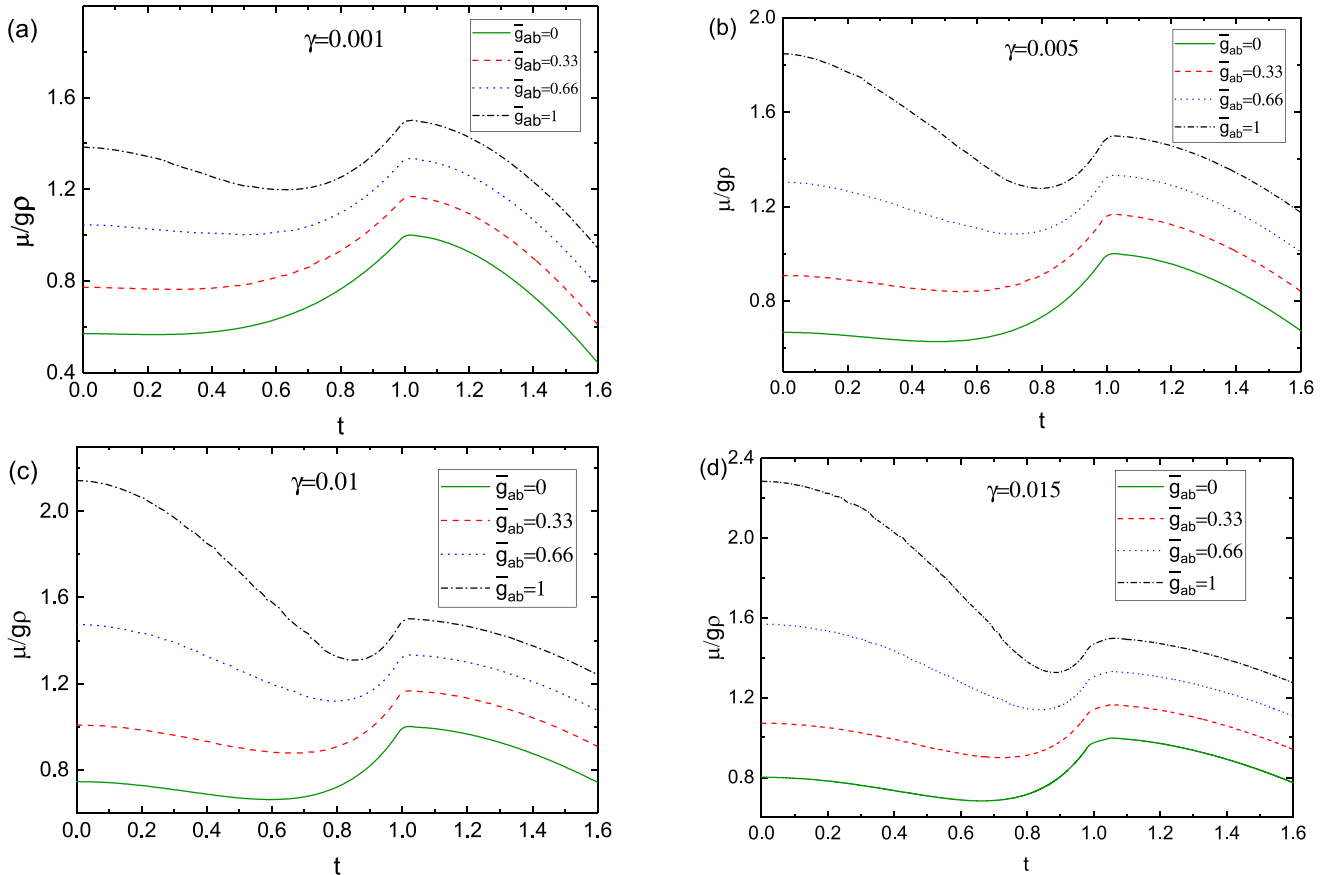
FIG. 5. Reduced chemical potential, $\mu/g\rho$, in the whole range of the dimensionless temperatures $t = T/T_c$ for different values of $\overline{g}_{ab}$ and γ.

may remain stable and miscible even at $g_{ab}/g_{aa} > 1$, provided the anomalous densities are properly taken into account. Comparing this phase diagram with that at finite temperature (g_{ab}, γ, T), we see that the finite temperature can transform the phase-separated two-component BECs at $T = 0$ to a miscible state. This conclusion is in good agreement with the works by Roy *et al.* [17], Ota *et al.* [23], and Shi *et al.* [15]. Our numerical results are also in good agreement with experimental works [8,9], although new experimental measurements for larger values of the interspecies coupling and γ are required.

The increase of the region of miscibility, due to the proper taking account of anomalous averages and temperature, can be understood remembering that these characteristics take into consideration the existence of quantum and temperature fluctuations. In the system, there are different competing factors. From one side, the repulsive interspecies interactions intend to separate the mixture. From the other side, larger interactions induce larger anomalous averages, and the larger amount of uncondensed particles, which characterizes the increasing quantum fluctuations. Both quantum as well as thermal fluctuations are favorable for mixing. Under the given interactions, fluctuations facilitate the process of mixing. This is why the system may be immiscible when fluctuations are absent but becomes miscible in the presence of fluctuations. As an example of the influence of thermal fluctuations, it is possible to consider the role of temperature in the thermodynamic miscibility conditions at weak interactions, when the free energies of mixed and separated states are compared. Taking into account that the difference in the entropy between the mixed and separated states is due to the mixing entropy, one obtains [51] the miscibility condition

$$g_{ab} - \sqrt{g_{aa}\, g_{bb}} < -\frac{2T}{\rho} \sum_i n_i \ln n_i \qquad \left(n_i \equiv \frac{N_i}{N} \right),$$

where ρ is the average density of the mixed system. As is evident, finite temperatures do facilitate the mixing, so that at zero temperature the system can be immiscible, while at finite temperature it can become miscible.

The definition of the energy dispersion as well as the identification of points of instability, introduced in Secs. II and III, requires some clarification. Actually, for this purpose we have exploited first-order Green's functions (30). However, strictly speaking, these parameters should be related to the poles of the full interacting Green's function, given by the Dyson equation $\widehat{G}^{-1} = \widehat{G}_0^{-1} - \widehat{\Sigma}$, where $\widehat{G}_0$ is the "noninteracting" Green's function and $\widehat{\Sigma}$ is the self-energy operator [60]. In the present approach $\widehat{G}_0$ does not coincide with that of an ideal gas, but effectively takes into account two-body interactions via variational parameters [$X_1, \ldots, X_6$].

It will be quite interesting to study a nonsymmetric, e.g., imbalanced two-component Bose mixture, where quasimagnetic transitions may also take place [23]. Moreover, as has been recently claimed by Naidon and Petrov [61], for un-

equal interspecies interaction or unequal masses the mixed phase can form bubbles with a tunable population. This will be the next task for the application of our theory, since the ground-state physics can be qualitatively understood from the arguments valid for a homogeneous system. However, in the case of real systems in a trap phase separation can be suppressed in the inhomogeneous system due to quantum pressure effects [62].

APPENDIX A: THE GREEN'S FUNCTIONS AND THE DENSITIES

Here we present the explicit expressions for the Green's function $G_{ij}(\omega_n, \vec{k})$ ($i, j = 1$–4) and the related densities. By inversion of $G_{ij}^{-1}(\omega_n, \vec{k})$ given in Eq. (30) one obtains

$$G_{11}(\omega_n, \vec{k}) = \frac{W_2 W_3 W_4 + W_2 \omega_n^2 - X_6^2 W_3}{\tilde{D}}, \qquad \text{(A1)}$$

$$G_{12}(\omega_n, \vec{k}) = -\frac{(W_3 W_4 + \omega_n^2 + X_5 X_6)\omega_n}{\tilde{D}}, \qquad \text{(A2)}$$

$$G_{13}(\omega_n, \vec{k}) = -\frac{W_2 X_5 W_4 - X_6^2 X_5 - \omega_n^2 X_6}{\tilde{D}}, \qquad \text{(A3)}$$

$$G_{14}(\omega_n, \vec{k}) = -\frac{(X_5 W_2 + W_3 X_6)\omega_n}{\tilde{D}}, \qquad \text{(A4)}$$

$$G_{22}(\omega_n, \vec{k}) = \frac{W_1 W_3 W_4 + W_1 \omega_n^2 - W_4 X_5^2}{\tilde{D}}, \qquad \text{(A5)}$$

$$G_{23}(\omega_n, \vec{k}) = -\frac{(X_6 W_1 + X_5 W_4)\omega_n}{\tilde{D}}, \qquad \text{(A6)}$$

$$G_{24}(\omega_n, \vec{k}) = -\frac{W_3 X_6 W_1 - X_6 X_5^2 - \omega_n^2 X_5}{\tilde{D}}, \qquad \text{(A7)}$$

$$G_{33}(\omega_n, \vec{k}) = \frac{W_4 W_1 W_2 + W_4 \omega^2 - X_6^2 W_1}{\tilde{D}}, \qquad \text{(A8)}$$

$$G_{34}(\omega_n, \vec{k}) = -\frac{(W_1 W_2 + \omega_n^2 + X_5 X_6)\omega_n}{\tilde{D}}, \qquad \text{(A9)}$$

$$G_{44}(\omega_n, \vec{k}) = \frac{W_3 W_1 W_2 + W_3 \omega_n^2 - X_5^2 W_2}{\tilde{D}}, \qquad \text{(A10)}$$

where $\tilde{D} = (\omega_n^2 + \omega_1^2)(\omega_n^2 + \omega_2^2)$, $\omega_n = 2\pi nT$, $\omega_{1,2}$ are given in the main text, and $W_1 = \varepsilon_a(k) + X_1$, $W_2 = \varepsilon_a(k) + X_2$, $W_3 = \varepsilon_b(k) + X_3$, $W_4 = \varepsilon_b(k) + X_4$, $X_5 = X_{13}$, and $X_6 = X_{24}$.

Below we present explicit expressions for the densities defined in Eqs. (45)–(47):

$$\rho_{1a} = \frac{1}{2\sqrt{D}\omega_1(k)\omega_2(k)V} \sum_k \big([X_6^2 W_3 + W_2 \omega_1^2(k) - W_2 W_3 W_4 - W_1 W_3 W_4 + X_5^2 W_4 + W_1 \omega_1^2(k)]\omega_2(k)\tilde{W}_1(k)$$

$$+ [-X_6^2 W_3 - W_2 \omega_2^2(k) + W_2 W_3 W_4 + W_1 W_3 W_4 - X_5^2 W_4 - W_1 \omega_2^2(k)]\omega_1(k)\tilde{W}_2(k)\big), \qquad \text{(A11)}$$

$$\rho_{1b} = \frac{1}{2\sqrt{D}\omega_1(k)\omega_2(k)V} \sum_k \left(\left[X_6^2 W_1 + W_4\omega_1^2(k) - W_1 W_2 W_3 - W_1 W_2 W_4 + X_5^2 W_2 + W_3\omega_1^2(k) \right]\omega_2(k)\tilde{W}_1(k) \right.$$
$$\left. + \left[-X_6^2 W_1 - W_4\omega_2^2(k) + W_1 W_2 W_3 + W_1 W_2 W_4 - X_5^2 W_2 - W_3\omega_2^2(k) \right]\omega_1(k)\tilde{W}_2(k) \right), \tag{A12}$$

$$\sigma_a = \frac{1}{2\sqrt{D}\omega_1(k)\omega_2(k)V} \sum_k \left(\left[X_6^2 W_3 + W_2\omega_1^2(k) - W_2 W_3 W_4 + W_1 W_3 W_4 - X_5^2 W_4 - W_1\omega_1^2(k) \right]\omega_2(k)\tilde{W}_1(k) \right.$$
$$\left. + \left[-X_6^2 W_3 - W_2\omega_2^2(k) - W_1 W_3 W_4 - W_2 W_3 W_4 - W_2\omega_2^2(k) + X_5^2 W_4 + W_1\omega_2^2(k) \right]\omega_1(k)\tilde{W}_2(k) \right), \tag{A13}$$

$$\sigma_b = \frac{1}{2\sqrt{D}\omega_1(k)\omega_2(k)V} \sum_k \left(\left[X_6^2 W_1 + W_4\omega_1^2(k) + W_1 W_2 W_3 - W_1 W_2 W_4 - -X_5^2 W_2 - W_3\omega_1^2(k) \right]\omega_2(k)\tilde{W}_1(k) \right.$$
$$\left. + \left[-X_6^2 W_1 - W_4\omega_2^2(k) - W_1 W_2 W_3 + W_1 W_2 W_4 + X_5^2 W_2 + W_3\omega_2^2(k) \right]\omega_1(k)\tilde{W}_2(k) \right), \tag{A14}$$

$$\rho_{ab} = \frac{1}{\sqrt{D}\omega_1(k)\omega_2(k)V} \sum_k \left(\left[-X_6^2 X_5 + W_1 W_3 X_6 + W_2 W_4 X_5 + \omega_1^2(k)X_6 + X_5\omega_1^2(k) - X_5^2 X_6 \right]\omega_2(k)\tilde{W}_1(k) \right.$$
$$\left. + \left[X_6^2 X_5 - W_1 W_3 X_6 - W_2 W_4 X_5 - \omega_2^2(k)X_6 - X_5\omega_2^2(k) + X_5^2 X_6 \right]\omega_1(k)\tilde{W}_2(k) \right), \tag{A15}$$

$$\sigma_{ab} = \frac{1}{\sqrt{D}\omega_1(k)\omega_2(k)V} \sum_k \left(\left[-X_6^2 X_5 - W_1 W_3 X_6 + W_2 W_4 X_5 + \omega_1^2(k)X_6 - X_5\omega_1^2(k) + X_5^2 X_6 \right]\omega_2(k)\tilde{W}_1(k) \right.$$
$$\left. + \left[X_6^2 X_5 + W_1 W_3 X_6 - W_2 W_4 X_5 - x\omega_2^2(k)X_6 - X_5\omega_2^2(k) + X_5^2 X_6 \right]\omega_1(k)\tilde{W}_2(k) \right), \tag{A16}$$

where $\tilde{W}_{1,2}(k) = 1/2 + f(\omega_{1,2}(k))$, and D, $\omega_{1,2}(k)$ are given in Eqs. (31)–(36).

Note that, in practical calculation of momentum integrals, adequate counterterms should be included similar to $c_\rho = -1/2$ (for ρ_1), and $c_\sigma = \Delta/2\varepsilon_k$ (for σ) used in the one-component case.

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