Interface tension of Bose-Einstein condensates

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Motivated by recent observations of phase-segregated binary Bose-Einstein condensates, we propose a method to calculate the excess energy due to the interface tension of a trapped configuration. By this method one should be able to numerically reproduce the experimental data by means of a simple Thomas-Fermi approximation, combined with interface excess terms and the Laplace equation. Using the Gross-Pitaevskii theory, we find expressions for the interface excesses which are accurate in a very broad range of the interspecies and intraspecies interaction parameters. We also present finite-temperature corrections to the interface tension which, aside from the regime of weak segregation, turn out to be small.

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I. INTRODUCTION

Soon after the first experimental realization of Bose-Einstein condensation (BEC) in dilute gases, binary BEC mixtures were realized [1–10]. These experiments precipitated a strong theoretical interest, the origin of which is the fact that the multicomponent BEC is not a trivial extension of the single-component BEC [11–30]. Indeed, fundamentally different physics arise on both microscopic and macroscopic levels. Phenomena studied for binary mixtures so far include the quantum tunneling of spin domains [4,5], spin-relaxation processes [4], vortex configurations [2], formation of Feshbach molecules [9], and collective oscillations [3]. Experiments with phase-segregated BEC mixtures were established already in 1998 [6,7]; this triggered many theorists to focus on the observed weakly segregated phases whereby the importance of the interface physics was highlighted several times [18–27].

Also surfaces of single-component BEC gases have gained much attention. Studies are performed on vortices, surface modes, and tunneling phenomena at the border of a trapped single-component BEC [31–34] and on BEC diffraction and van der Waals forces using an optical mirror or evanescent-wave prism [35–37]. Moreover a combination of the interface physics of binary BEC gases and the surface physics near hard walls led to the theoretical prediction of anomalous wetting phase transitions [38].

The clearest observation so far of phase segregation of BEC mixtures was reported by Papp *et al.* (see Ref. [10]) who used a mixture of ^{85}Rb and ^{87}Rb particles. By changing the particle numbers of both species and the intraspecies interactions of the ^{85}Rb particles by use of a Feshbach resonance, many topologically distinct states were encountered. In the phase-segregated regime most trap configurations contained BEC droplets. Papp *et al.* stated that a detailed theoretical understanding of the observed droplet formation is lacking. As an essential first step towards this understanding we present here expressions for the interface tension. Moreover, we also formulate a method by which all trap configurations can be straightforwardly studied by the use of a local density approximation or Thomas-Fermi approximation. At first sight, numerically reproducing the experimentally observed (meta)stable states requires solving the coupled Gross-Pitaevskii (GP) equations for the full three-dimensional system; in such case, a high accuracy is indispensable to capture the important energy contributions near the two-phase boundaries which strongly affect the ground-state topology.

In this work, we argue that it is not necessary to solve the full GP system in order to recover numerically the experimental configurations; instead, one can find the ground state, that is, minimize the total energy of the trapped cloud, by use of the Thomas-Fermi approximation and the expressions for the interface tension which we provide here. This allows an omission of the quantum pressure term which strongly complicates the numerical work. The analytical calculation of the interface tension is nontrivial as it involves solving the binary GP equations (i.e., two coupled nonlinear second-order differential equations). Estimates and analytical expressions were already given in Refs. [21–24] and were relevant to the early experiments on weakly segregated mixtures but irrelevant to the interfaces as observed in Ref. [10] since there segregation is not weak. By developing expansions, we succeed in obtaining analytical expressions for the interface tension which are accurate for almost all parameter regimes.

As a main result we find that, even though the interface tension is not constant throughout the trap, the total excess energy $\Omega_{\mathcal{A}}$ can be reduced to a simple integral of the trapping potential along the interface area $\mathcal{A}$,

$$\Omega_{\mathcal{A}} = \frac{\sqrt{2m_1}}{4\pi\hbar a_{11}} \mathcal{F}(\xi_2/\xi_1, K) \int_{\mathcal{A}} d\mathbf{r} [\mu_1 - U_1(\mathbf{r})]^{3/2}, \qquad (1)$$

where a_{11}, m_1, μ_1, and U_1 are the intraspecies scattering length, the particle mass, the chemical potential, and the applied trapping potential of phase 1. The parameters K and ξ_2/ξ_1 can be expressed in terms of the atomic masses and the interspecies and intraspecies scattering lengths,

$$K = \frac{m_1 + m_2}{2\sqrt{m_1 m_2}} \frac{a_{12}}{\sqrt{a_{11}a_{22}}} \quad \text{and} \quad \xi_2/\xi_1 = \sqrt[4]{\frac{m_1 a_{11}}{m_2 a_{22}}}. \qquad (2)$$

For a broad range of values of ξ_2/ξ_1 and K, the function $\mathcal{F}$ can be written as

$$\mathcal{F}(\xi_2/\xi_1,K) = \frac{\sqrt{2}}{3}(1+\xi_2/\xi_1) - \frac{0.514\sqrt{\xi_2/\xi_1}}{K^{1/4}} - \sqrt{\xi_2/\xi_1}(\xi_2/\xi_1+\xi_1/\xi_2)\left(\frac{0.055}{K^{3/4}}+\frac{0.067}{K^{5/4}}\right)+\cdots. \tag{3}$$

This work is structured as follows. We start off in Sec. II by introducing the GP formalism for binary BECs. After defining the excess energy in a homogeneous and in a trapped system in Sec. III, we find analytical expressions for the interface tension in Sec. IV. We estimate the finite-temperature corrections to the interface tension in Sec. V. In Sec. VI we discuss the experimental relevance of our findings.

II. BINARY BEC SYSTEM

Equilibrium states of a mixture of two dilute BEC gases with order parameters Ψ_1 and Ψ_2 and chemical potentials μ_1 and μ_2, are well modeled using the grand potential,

$$\Omega(\mu_1,\mu_2,V) = \sum_{i=1,2}\left[\int_V d\mathbf{r}\Psi_i^*(\mathbf{r})\left(-\frac{\hbar^2}{2m_i}\nabla^2-\mu_i+U_i(\mathbf{r})\right)\times\Psi_i(\mathbf{r})+\frac{G_{ii}}{2}|\Psi_i(\mathbf{r})|^4\right] + G_{12}\int_V d\mathbf{r}|\Psi_1(\mathbf{r})|^2|\Psi_2(\mathbf{r})|^2, \tag{4}$$

where $G_{ij}=2\pi\hbar^2 a_{ij}(m_i^{-1}+m_j^{-1})$ are the coupling constants and a_{ij} are the s-wave scattering lengths (henceforth $i=1,2$). In view of the derivation of the interface tension, we continue here by assuming vanishing external potentials $U_1=U_2=0$; we reintroduce the external potentials when discussing the surface excess of a trapped system. In the absence of particle flow one can choose the order parameters to be real valued such that the equilibrium pressures for the pure states are

$$P_i = \frac{\mu_i^2}{2G_{ii}}. \tag{5}$$

In order to study phase-segregated states of the two coexisting condensates, we introduce the parameter

$$K \equiv \frac{G_{12}}{\sqrt{G_{11}G_{22}}}, \tag{6}$$

which quantifies the interspecies couplings relative to the average of the intraspecies couplings. It is well known that when K exceeds one, the species become immiscible and only pure phases can exist [22] while phase mixing occurs when $K<1$. Along the two-phase interface, coexistence is ensured by the condition

$$\frac{\mu_1^2}{2G_{11}} = \frac{\mu_2^2}{2G_{22}}. \tag{7}$$

Henceforth, we assume that $K>1$ and that the chemical potentials are such that the bulk pressures are $P_1=P_2\equiv P$. For calculational convenience, we further rescale the order parameters Ψ_1 and Ψ_2 and define the dimensionless wave functions ψ_1 and ψ_2,

$$\Psi_i \equiv \psi_i\sqrt{\frac{\mu_i}{G_{ii}}}. \tag{8}$$

The quantum nature of the system results in a zero-point motion; this determines the typical length scale for density modulations at boundaries, impurities, vortices or solitons. For the pure phases, the resultant length is the healing length ξ_i which is defined as

$$\xi_i \equiv \frac{\hbar}{\sqrt{2m_i\mu_i}}. \tag{9}$$

Without loss of generality, we choose the phases such that $\xi_2/\xi_1\leqslant 1$. As coexistence must occur along the interface, K and ξ_2/ξ_1 can be expressed in terms of the atomic masses and the scattering lengths as given in Eq. (2). Finally, after rescaling the space coordinate to the dimensionless variable $\tilde{\mathbf{r}}\equiv\mathbf{r}/\xi_1$, the reduced time-independent Gross-Pitaevskii (GP) equations are [39,40]

$$\nabla^2\psi_1 = -\psi_1+\psi_1^3+K\psi_1\psi_2^2, \tag{10a}$$

$$(\xi_2/\xi_1)^2\nabla^2\psi_2 = -\psi_2+\psi_2^3+K\psi_2\psi_1^2. \tag{10b}$$

Having established the equations of motion, we continue now by defining the interface tension.

III. DEFINITION OF INTERFACE TENSION AND INTERFACE EXCESS

In order to calculate the interface tension, consider two BEC components in an infinitely large system with translational symmetry in the x-y direction. The presence of phase 1 at $z\to\infty$ and of phase 2 at $z\to-\infty$ imply the following boundary conditions:

$$\psi_1(z=-\infty)=\psi_2(z=\infty)=0, \tag{11a}$$

$$\psi_1(z=\infty)=\psi_2(z=-\infty)=1. \tag{11b}$$

Under these conditions, the first integral of the reduced GP equations (10a) and (10b) is

$$\dot{\psi}_1^2+(\xi_2/\xi_1)^2\dot{\psi}_2^2-K\psi_1^2\psi_2^2+\sum_{i=1,2}\left(\psi_i^2-\frac{\psi_i^4}{2}\right)=\frac{1}{2}, \tag{12}$$

where the overdot denotes the derivative with respect to $\tilde{z}$. Since we work at fixed chemical potentials, the interface tension is the excess grand potential per unit area; this excess is uniquely determined by subtraction of the total grand potential of a volume V containing a pure phase, from the grand potential Ω, that is, $\Omega+PV$. By use of Eqs. (10) and (12) the interface tension can be written as

$$\gamma_{12} = 4P\xi_1 \int_{-\infty}^{+\infty} d\tilde{z}[\dot{\psi}_1^2(\tilde{z}) + (\xi_2/\xi_1)^2 \dot{\psi}_2^2(\tilde{z})] \equiv 4P\xi_1 \mathcal{F}(\xi_2/\xi_1, K). \tag{13}$$

The interface tension in the grand canonical ensemble is exactly 4 times the interface tension in the canonical ensemble as introduced by Ao and Chui [22,41]. Note also that, as opposed to the grand canonical ensemble, the definition of the interface tension in the canonical ensemble is not unique [42]. In Eq. (13), we define the dimensionless function $\mathcal{F}$ which, as is also the case for the normalized profiles ψ_i, only depends on ξ_2/ξ_1 and K since the wave functions are fully determined by the GP equations (10) and the boundary conditions (11). It is clear from Eq. (13) that the excess energy is positive and due to a bending of the normalized wave functions ψ_1 and ψ_2.

One can now straightforwardly generalize the definition of the interface tension to the total excess energy of a trapped system. Therefore, we use a local approximation for the interface tension: We assume the characteristic lengths over which the trapping potentials $U_i(\mathbf{r})$ (for $i=1,2$) vary to be large as compared to the interface thickness. At each point $\mathbf{r}$ along the interface, Eq. (13) then gives the expression for the interface tension $\gamma_{12}(\mathbf{r})$ for condensates at effective chemical potentials $\mu_i - U_i(\mathbf{r})$ $(i=1,2)$. The total excess energy $\Omega_{\mathcal{A}}$ is then obtained by integration over the interface area $\mathcal{A}$, i.e., $\Omega_{\mathcal{A}} = \int_{\mathcal{A}} d\mathbf{r}\, \gamma_{12}(\mathbf{r})$. The function $\mathcal{F}(\xi_2/\xi_1, K)$ can be set outside this integral as it is position independent; indeed, both K and ξ_2/ξ_1 are uniquely determined by the scattering lengths and the particle masses [see Eq. (2)]. This remarkable property implies that, first, along the entire interface in a trap, the interface profiles ψ_1 and ψ_2 are unchanged [determined by Eqs. (10) and (11) only]. This is an exceptional feature of BEC interfaces [43]. Second, it implies that in a trap the local interface tension $\gamma_{12}(\mathbf{r})$ depends on position only through the term $P\xi_1$ as can be seen from Eq. (13). The total excess grand potential is then

$$\Omega_{\mathcal{A}} = 4\mathcal{F}(\xi_2/\xi_1, K) \int_{\mathcal{A}} d\mathbf{r} P(\mathbf{r}) \xi_1(\mathbf{r}), \tag{14}$$

which, using the effective chemical potentials $\mu_i - U_i(\mathbf{r})$ in Eqs. (5) and (9), brings us to Eq. (1) wherein we factorize the total excess energy as a product of two distinct terms: The first is a function of the microscopic gas parameters whereas the last is a position integral of the external potential along the interface area $\mathcal{A}$. The calculation of the function $\mathcal{F}$ constitutes the subject of the next section.

Expression (1) for the total excess energy is our main result. Together with a Thomas-Fermi (TF) approximation in bulk, it forms the core of a simple method to calculate the total energy of the trapped system and therefore to minimize it. The TF approach neglects the energy contributions arising from density gradients and thus gives rise to sharp interfaces, the locus of which is normally taken where two-phase coexistence is satisfied. The latter, however, is invalid when the interface is curved as appears, for example, for droplets. Instead, a difference in pressures appears along the two-phase boundary as expressed by the Laplace equation

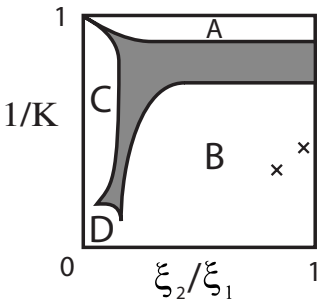

FIG. 1. Regions of validity of the approximations presented in Secs. IV A–IV D in the space of parameters $1/K$ and ξ_2/ξ_1. In the shaded region, the approximations have a low accuracy; the boundaries are drawn on a qualitative basis. The crosses denote values corresponding to the experiments of Ref. [10].

$$P_1 - P_2 = \gamma_{12}(1/R_1 + 1/R_2), \tag{15}$$

with R_1 and R_2 the principal radii of curvature of the interface. It is clear that the difference in pressures along the interface is largest for small droplets. Within a first approach, for large R_1 and R_2, one can take the γ_{12} in Eq. (15) to be the interface tension for a flat interface, calculated by assuming equal pressures on opposite sides of the interface.

Finally, note that, pertaining to the interface tension in a trapped system, it is essential to work at fixed chemical potentials instead of particle numbers and use definition (13) as opposed to the interface tension in the canonical ensemble [22,42].

IV. CALCULATION OF INTERFACE TENSION

In the following four sections A–D, we derive expressions for $\mathcal{F}(\xi_2/\xi_1, K) = \gamma_{12}/(4P\xi_1)$ as expansions for different regimes of ξ_2/ξ_1 and K. The wave functions ψ_1 and ψ_2 must satisfy the boundary conditions (11). The regions of validity of the expansions are outlined (qualitatively) in Fig. 1 where A–D indicate the sections and the shaded region indicates the absence of an accurate approximation. In Fig. 2, we depict typical profiles for the wave functions ψ_1 and ψ_2 which are met in the four considered regimes. First in A, we focus on the case of weak segregation i.e., $K \to 1$. Second, in B, we develop an expansion around the point of strong segregation $1/K \to 0$; the result is expansion (3) which is accurate for a broad range of values. Third, we treat the case of a strong healing length asymmetry, that is, when $\xi_2/\xi_1 \ll 1$, in C. Finally, we study the case of $\xi_2/\xi_1 \ll 1$ in combination with strong segregation $1/K \to 0$ in D.

A. Weak segregation

For the regime of weak segregation, i.e., close to the point where the two phases tend to mix $(K \to 1)$, it was found by Barankov in Ref. [24] that the interface tension varies as

$$\gamma_{12} = 4P\xi_1 \frac{\sqrt{K-1}}{3} \left(\frac{1 - (\xi_2/\xi_1)^3}{1 - (\xi_2/\xi_1)^2} \right). \tag{16}$$

In the case of $\xi_2/\xi_1 = 1$, the same leading behavior was recovered in Refs. [23,44,22] and the square-root behavior as a

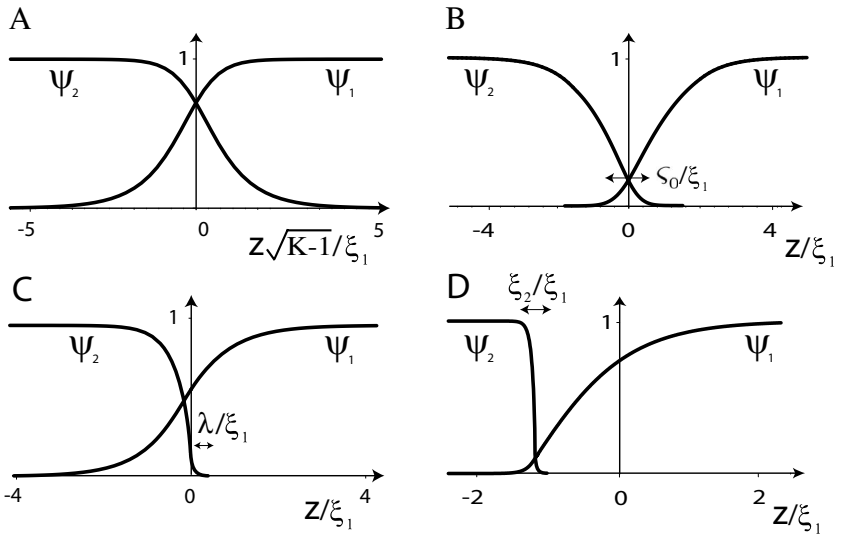

FIG. 2. Typical interface profiles for the four cases which are treated in Secs. IV A–IV D. We indicate the characteristic length scales over which the wave functions vary. (A) Weak segregation regime $K\to 1$ (here with $\xi_2/\xi_1=1$). The relevant length scale is $\xi_1/\sqrt{K-1}$ which is large. (B) Strong segregation regime with $1/K\to 0$ (here with $K=200$ and $\xi_2/\xi_1=1$). The condensates overlap over a length scale ς_0 [see Eq. (17)]. (C) The regime of strong healing length asymmetry $\xi_2/\xi_1\to 0$. When ξ_2/ξ_1 is small but nonzero, ψ_2 vanishes with a tail of length λ [see Eq. (23)]. (D) When both $\xi_2/\xi_1\to 0$ and $1/K\to 0$, the condensates will overlap over a distance ξ_2.

function of $K-1$ arises from simple models as given in Refs. [21,22]. Approximation (16) is exact at $K=1$ but is already 3.6% off at $K=1.1$ when $\xi_2=\xi_1$. Despite this small range of validity, such small values for $K-1$ were realized in the early experiments on phase-segregated ^{87}Rb mixtures [4–7]. On the other hand, the use of an interface tension for determining the excess energy in these experiments is inaccurate as the "interface thickness," that is $\xi_1/\sqrt{K-1}$, is of the same order as the length of variation of the trapping potential; this invalidates the assumption of constant chemical potentials across the interface.

B. Strong segregation

In the following we develop an expansion around the point of strong segregation where $1/K\to 0$. An analogous expansion which originated in a paper by Ginzburg and Landau [45], was used to determine an accurate analytical expression for the interface tension of a normal-superconducting interface [46].

In the limit $1/K\to 0$, species 1 and 2 do not overlap. Their wave functions are easily found using the GP equations (10) and the boundary conditions (11): $\psi_1=\Theta(z)\tanh(z/\sqrt{2}\xi_1)$ and $\psi_2=\Theta(-z)\tanh(-z/\sqrt{2}\xi_2)$, where Θ is the Heaviside function. For a finite but small value of $1/K$, these tanh profiles shift towards each other so as to overlap over a length proportional to $\sqrt{\xi_1\xi_2}/\sqrt[4]{K}$. In this overlap zone, the wave functions are modified due to the interspecies interactions. In Fig. 2(b), we depict such wave functions for the case of $\xi_2/\xi_1=1$. Note that the length of overlap vanishes very slowly when $1/K\to 0$ as it is proportional to $1/\sqrt[4]{K}$. We introduce the following (change of) variables ($i=1,2$):

$$\hat{z}\equiv z/\varsigma_0,\quad \varsigma_0\equiv\frac{\sqrt{\xi_1\xi_2}}{\sqrt[4]{K}},\quad \text{and}\quad \varsigma_i\equiv\varsigma_0/\xi_i. \tag{17}$$

Note that ς_0 has the dimension of length [drawn in Fig. 2(b)] whereas ς_1 and ς_2 are dimensionless. We expand the wave function of phase $i=1,2$ in terms of the parameter ς_i,

$$\psi_i=\psi_i^0+\varsigma_i(\psi_{i1}-\psi_{i1}^0)+\varsigma_i^3(\psi_{i2}-\psi_{i2}^0)+\cdots.$$

We remark that $(\psi_i-\psi_i^0)/\varsigma_i$ is a regular function of ς_i^2. The functions ψ_{i1}^0 and ψ_{i2}^0 are derivable from the asymptotic behavior of ψ_i for $|\hat{z}|\to\infty$ which are shifted tanh profiles,

$$\begin{aligned}\psi_1^0&=\Theta(\hat{z}+\delta_{11}+\varsigma_1^2\delta_{12}+\cdots)\\&\quad\times\tanh\left(\frac{\varsigma_1(\hat{z}+\delta_{11}+\varsigma_1^2\delta_{12}+\cdots)}{\sqrt{2}}\right)\\&\equiv\varsigma_1\psi_{11}^0+\varsigma_1^3\psi_{12}^0+\cdots,\end{aligned} \tag{18a}$$

$$\begin{aligned}\psi_2^0&=\Theta(-\hat{z}+\delta_{21}+\varsigma_2^2\delta_{22}+\cdots)\\&\quad\times\tanh\left(\frac{\varsigma_2(-\hat{z}+\delta_{21}+\varsigma_2^2\delta_{22}+\cdots)}{\sqrt{2}}\right)\\&\equiv\varsigma_2\psi_{21}^0+\varsigma_2^3\psi_{22}^0+\cdots.\end{aligned} \tag{18b}$$

From this expansion, it is clear that ψ_{i1}^0 and ψ_{i2}^0 are first-order and third-order polynomials in $\hat{z}$, respectively. Note that the "absolute shift" can be set to zero at every order without any loss of generality; thus $\delta_{11}=\delta_{21}$ and $\varsigma_1^2\delta_{12}=\varsigma_2^2\delta_{22}$ [46].

Substitution of the expanded wave functions in the GP equations (10) entails four new differential equations,

$$\ddot{\psi}_{11}=\psi_{11}\psi_{21}^2, \tag{19a}$$

$$\ddot{\psi}_{21}=\psi_{21}\psi_{11}^2, \tag{19b}$$

$$\ddot{\psi}_{12}=-\psi_{11}+\psi_{12}\psi_{21}^2+2\psi_{11}\psi_{21}\psi_{22}(\xi_2/\xi_1)^{-2}, \tag{19c}$$

$$\ddot{\psi}_{22} = -\psi_{21} + \psi_{22}\psi_{11}^2 + 2\psi_{21}\psi_{11}\psi_{12}(\xi_2/\xi_1)^2. \quad (19d)$$

Here, the overdots denote the derivative with respect to $\hat{z}$. The solutions of these equations will provide us with the numerical values for the δ's; indeed, the boundary conditions for ψ_{i1} and ψ_{i2} are to tangentially approach ψ_{i1}^0 and ψ_{i2}^0, respectively, for $\hat{z} \to \pm\infty$, and to vanish for $\hat{z} \to \mp\infty$. Now, in the same fashion as the wave functions, one can expand the interface tension,

$$\gamma_{12} = \gamma^0 + \varsigma_0 \sum_{i=1,2} [\gamma_{i1} - \gamma_{i1}^0 + \varsigma_i^2(\gamma_{i2} - \gamma_{i2}^0) + O(\varsigma_i^4)].$$

The zeroth-order term is obtained using (unshifted) tanh profiles such that $\gamma^0 = 4\sqrt{2}P(\xi_1+\xi_2)/3$ [22,24], while

$$\sum_{i=1,2} \gamma_{i1} = 4P\int_{-\infty}^{\infty} d\hat{z}(\dot{\psi}_{11}^2 + \dot{\psi}_{21}^2),$$

$$\sum_{i=1,2} \varsigma_i^2\gamma_{i2} = \frac{8P}{\sqrt{K}}\int_{-\infty}^{\infty} d\hat{z}\left((\xi_2/\xi_1)\dot{\psi}_{11}\dot{\psi}_{12} + \frac{\dot{\psi}_{21}\dot{\psi}_{22}}{(\xi_2/\xi_1)}\right).$$

After long calculations, one can express the interface tension in terms of the spatial shifts δ_{11}, δ_{12}, δ_{21}, and δ_{22}, in a way similar to what was done in Ref. [46],

$$\gamma_{12} = 4P\xi_1\left(\frac{\sqrt{2}}{3}(1+\xi_2/\xi_1) - \frac{(\delta_{11}+\delta_{21})}{3}\frac{\sqrt{\xi_2/\xi_1}}{\sqrt[4]{K}} - \frac{\sqrt{\xi_2/\xi_1}[\delta_{12}(\xi_2/\xi_1) + \delta_{22}(\xi_1/\xi_2)]}{\sqrt[4]{K}\sqrt{K}} + \cdots\right).$$

It is readily seen in the expansion that γ_{12} is symmetrical in ξ_1 and ξ_2, as it must be. As a final step, we extracted numerical values for the δ's from the numerical integration of Eqs. (19). We find that $\delta_{11}=\delta_{21}=0.771$ [46], and, assuming $\xi_2/\xi_1=1$ in Eqs. (19c) and (19d), we obtain $\delta_{12}=\delta_{22}=0.055$. Note that this result is different from δ_2 found in Ref. [46] because the problem at hand is different starting from the first order in ς_i^2. By fitting numerically obtained values for γ_{12} with an additional fitting term of fifth order in $1/\sqrt[4]{K}$, and neglecting the dependence of δ_{12} and δ_{22} on ξ_2/ξ_1, we finally arrive at expression (3).

The accuracy of this expansion is clear from Fig. 3 where we plot Eq. (3) in full lines against the numerically obtained values for $\xi_2/\xi_1=1$ (squares), $\xi_2/\xi_1=1/2$ (triangles), and $\xi_2/\xi_1=1/3$ (dots). Our expansion works very well for K in the interval $[1.5, +\infty]$; moreover, it is good for all three values of ξ_2/ξ_1, which *a posteriori* justifies the neglect of the dependence of δ_{12}, δ_{22} and the fitted higher-order term on ξ_2/ξ_1. Also in Fig. 3, we draw with gray lines Barankov's approximation [16], accurate for values of K between 1 and 1.1.

C. Strong healing length asymmetry

So far, we have constructed expansions around extreme values for the interspecies interaction parameter K. In the following, we will focus on the case when the healing length of species 2 is much smaller than the one of species 1, i.e., when $\xi_2/\xi_1 \ll 1$.

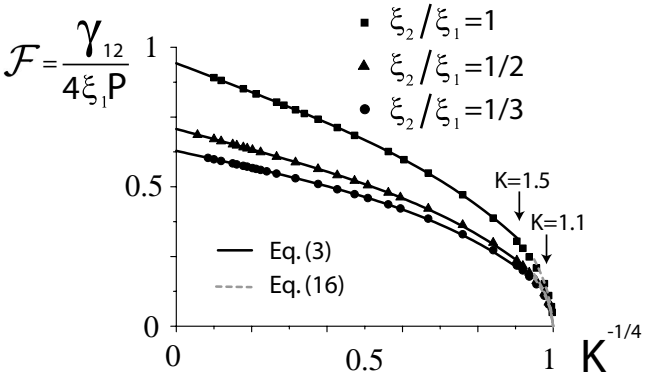

FIG. 3. Values of $\mathcal{F}$ or interface tension γ_{12} in units of $4P\xi_1$, against values of $K^{-1/4}$ where $K=G_{12}/\sqrt{G_{11}G_{22}}$. The squares, triangles, and dots are obtained by numerical integration of the GP equations for $\xi_2/\xi_1=1$, $1/2$ and $1/3$, respectively. The full lines are plots of Eq. (3) and are seen to give an accurate approximation for values of K in the interval $[1.5, \infty]$. The gray lines plot Eq. (16) which is accurate for $K \in [1, 1.1]$.

In the limit of $\xi_2/\xi_1=0$ (and such that $\xi_2^2\ddot{\psi}_2 \to 0$), the GP equations (10) can be reduced to

$$\psi_2^2 = \Theta(-z)(1 - K\psi_1^2), \quad (20a)$$

$$\xi_1^2\ddot{\psi}_1 = \Theta(z)\psi_1(-1+\psi_1^2) + \Theta(-z)\psi_1(K-1)[1-(1+K)\psi_1^2], \quad (20b)$$

from which it follows that the density of phase 2 is slaved to the density of phase 1. The solution to Eq. (20b) is [20]

$$\psi_1 = \Theta(z)\tanh\left(\frac{z+z_1}{\sqrt{2}\xi_1}\right) + \frac{\Theta(-z)\sqrt{2}}{\sqrt{K+1}}\left[\cosh\left(\frac{z+z_2}{\xi_1/\sqrt{K-1}}\right)\right]^{-1}. \quad (21)$$

The constants $z_1>0$ and $z_2<0$ are determined by the continuity of ψ_1 at $z=0$ where $\psi_1^2(0)=1/K$. The wave function ψ_2 is nonzero only when $z<0$ and relates to ψ_1 by Eq. (20a). Near $z=0$ it vanishes with the square-root behavior $\psi_2 \propto \sqrt{-z/\xi_1}$.

The first-order corrections due to a small and nonzero ξ_2/ξ_1 affect only ψ_2, near the origin $z=0$ where $\ddot{\psi}_2$ is large due to the square-root behavior of ψ_2. These corrections will induce wave function ψ_2 to acquire a small tail of length λ which is depicted in Fig. 2(c). We search now for how the GP equation (10b) can be modified to appropriately describe such corrections. We assume that ψ_1 varies little on the length scale λ; this allows us to expand $K\psi_1^2$ in Eq. (10b) around $z=0$ as $K\psi_1^2 \approx 1+Fz/\xi_1$ where $F \equiv \sqrt{2/K}(K-1)$. Sufficiently far from the origin, when $\lambda \ll -z \ll \xi_1$, we want ψ_2 to vary as $\psi_2 \propto \sqrt{-z/\xi_1}$; therefore, we may not throw away the nonlinear term ψ_2^3 in Eq. (10b). By appropriately scaling ψ_2 and z, we find that, for $|z| \ll \xi_1$,

$$\ddot{\bar{\psi}}_2 = \bar{\psi}_2(\bar{z} + \bar{\psi}_2^2), \quad (22)$$

where the overdots denote the derivative with respect to $\bar{z}$ which we define as:

$$\bar{z} \equiv z/\lambda \quad \text{with } \lambda \equiv \xi_2 (F(\xi_2/\xi_1))^{-1/3}, \tag{23}$$

and where the new wave function $\bar{\psi}_2 \equiv \psi_2 (F(\xi_2/\xi_1))^{-1/3}$. For $-\bar{z} \gg \lambda$, the term $\ddot{\bar{\psi}}_2$ in Eq. (22) may be neglected; indeed, doing so results in the solution $\bar{\psi}_2 = \sqrt{-\bar{z}}$. As expected this is in fact $\psi_2 \propto -\sqrt{z/\xi_1}$.

The differential equation which appears in Eq. (22) was encountered earlier by Lundh *et al.* [32] and Dalfovo *et al.* [31] when studying the BEC order parameter at the border of a large harmonic trap. The role of the trapping potential is played here by the interactions with condensate 1.

We briefly sketch how we calculated the interface tension; we refer to Refs. [31,32] for details of the method. To zeroth order in ξ_2/ξ_1, the interface tension is easily found by integration of $\dot{\psi}_1^2$ [see Eq. (13)] with ψ_1 given in Eq. (21). For small and nonzero ξ_2/ξ_1, extra energy contributions arise due to the integral over $\dot{\psi}_2^2$ [see Eq. (13)]. For $-z \gg \lambda$, ψ_2 must be taken from Eqs. (20a) and (21) whereas for $|z| \ll \xi_1$, ψ_2 is the (numerical) solution of Eq. (22). Since these two solutions for ψ_2 are equal in the region $\lambda \ll -z \ll \xi_1$, where $\psi_2 \propto \sqrt{-z/\xi_1}$ the interface tension is well defined. All of the extra energy contributions due to a nonzero ξ_2/ξ_1 can be seen to be of order $(\xi_2/\xi_1)^2$.

Calculations then lead to $\mathcal{F}$ to second order in ξ_2/ξ_1,

$$\begin{aligned}\frac{\gamma_{12}}{4\xi_1 P} = {} & \frac{2}{3}\frac{\sqrt{K-1}}{K+1}\left[1-\left(\frac{K-1}{2K}\right)^{3/2}\right] \\ & + \frac{\sqrt{2}}{3}\left[1+\frac{1}{2}\left(\frac{1}{K}\right)^{3/2}-\frac{3}{2\sqrt{K}}\right] \\ & + \left(\frac{\xi_2}{\xi_1}\right)^2 \frac{\sqrt{K-1}}{3}\left(\frac{K+3}{K+1}\right) + \left(\frac{\xi_2}{\xi_1}\right)^2 \frac{(K-1)}{\sqrt{2K}} \\ & \times \left[-\frac{2}{3}\frac{(K+2)}{(K+1)} + 0.7 + \frac{\ln}{6}\left(\frac{32K(K-1)}{(K+1)^3(\xi_2/\xi_1)^2}\right)\right. \\ & \left. - \operatorname{arctanh}\left(\sqrt{\frac{K-1}{2K}}\right)\right] + \cdots . \end{aligned} \tag{24}$$

Since there are two length scales (λ and ξ_1) over which the density varies, their relation $\lambda \ll \xi_1$ renders difficult the full numerical integration of the GP equations. Accordingly, we could not verify expansion (24) directly.

Conditions for the validity of the above approximation can be derived. First, the linearization of ψ_1 near $z=0$ in Eq. (10b) is justified only when the length over which higher-order corrections to ψ_1 are relevant [that is $(\dot{\psi}_1/\ddot{\psi}_1)(0) \propto \sqrt{K}\xi_1$ is large] as compared to the length over which ψ_2 varies (being λ). Second, corrections to ψ_1 caused by a nonzero ξ_2/ξ_1 can be neglected on $[-\lambda, \infty]$ when, in Eq. (10a), the amplitude $K\psi_2^2$ of the term $K\psi_2^2\psi_1$ [being $K(F(\xi_2/\xi_1))^{2/3}$] is sufficiently small. These conditions of validity amount to

$$\xi_2/\xi_1 \ll \sqrt{K(K-1)} \quad \text{and} \quad \xi_2/\xi_1 \ll \sqrt{K}.$$

Thus, our expansion fails in the regime of strong segregation when $\sqrt{K} \ll \xi_2/\xi_1$ and close to weak segregation when $\sqrt{K-1} \ll \xi_2/\xi_1$. Note that to zeroth order in ξ_2/ξ_1, our expansion (24) agrees with Eq. (16) when $K \to 1$. However, it differs from the expansion (16) by a factor of 2 in the term of order $(\xi_2/\xi_1)^2$.

D. Both strong segregation and strong healing length asymmetry

One may now wonder what happens to the interface tension when both K and $(\xi_2/\xi_1)^{-1}$ are large. When K goes faster to infinity than $(\xi_2/\xi_1)^{-2}$, we will find that expansion (3) is still valid while expansion (24) must be taken in the inverse case. In the following, we focus on the intermediate case when both $(\xi_2/\xi_1)^{-2}$ and K diverge such that $\kappa \equiv [(\xi_2/\xi_1)\sqrt{K}]^{-1}$ remains of order one. To zeroth order in both ξ_2/ξ_1 and K^{-1}, the condensate wave functions do not overlap; seen on a length scale ξ_1, this results in the wave functions $\psi_2 = \Theta(-z)$ and $\psi_1 = \Theta(z)\tanh(z/\sqrt{2}\xi_1)$.

For small and nonzero values for ξ_2/ξ_1 and $1/K$ while $\kappa \equiv [(\xi_2/\xi_1)\sqrt{K}]^{-1}$ is of order one, the condensates overlap. Due to the strong repulsion this happens only within a short region of length ξ_2; over that interval, the value of the wave function ψ_2 varies between zero and one while the value of ψ_1 does not vary much [see Fig. 2(d)]. The latter is only modified close to $z=0$, where, to zeroth order, it vanishes linearly. This brings about the definition of a new wave function ϕ_1,

$$\psi_1 = (\xi_2/\xi_1)\left(\phi_1 - \frac{z'\Theta(z')}{\sqrt{2}}\right) + \Theta(z)\tanh\left(\frac{z}{\sqrt{2}\xi_1}\right).$$

Here we introduced the dimensionless variable $z' \equiv z/\xi_2$ and ϕ_1 must have the asymptotic behavior $\phi_1(z' \to \infty) = z'/\sqrt{2}$ and $\phi_1(z' \to -\infty) = 0$. We can now expand the GP equations (10) in terms of the small parameters $(\xi_2/\xi_1)^2$ and $1/K$ in the overlap interval,

$$\frac{\ddot{\phi}_1}{\phi_1} = \left(\frac{\psi_2}{\kappa}\right)^2 \quad \text{and} \quad \frac{\ddot{\psi}_2}{\psi_2} = -1 + \psi_2^2 + \left(\frac{\phi_1}{\kappa}\right)^2. \tag{25}$$

The overdots denote the derivative with respect to z'. One may notice that these equations are the same as the Ginzburg-Landau equations which are valid in a superconductor when a constant magnetic field is applied parallel to its surface. In that case, the Ginzburg-Landau parameter κ is the ratio of the penetration length of the magnetic field to the coherence length, ψ_2 plays the role of the order parameter of the superconductor and ϕ_1 that of the vector potential (see Ref. [47] for more details, such as the choice of gauge).

By a straightforward calculation, one can rewrite the interface tension equation (13) as an integral over ϕ_1 and ψ_2,

$$\frac{\gamma_{12}}{4\xi_1 P} = \frac{\sqrt{2}}{3} + (\xi_2/\xi_1)\int dz' \left[\left(\dot{\phi}_1 - \frac{1}{\sqrt{2}}\right)^2 + \dot{\psi}_2^2\right], \tag{26}$$

where the overdots denote the derivative with respect to z' and ϕ_1 and ψ_2 are obtained by the Euler-Lagrange equations (25).

An analytical expression for the interface tension of a superconductor-normal interface in case of small κ was obtained by Boulter and Indekeu in Ref. [46]. Using their result, one finds

$$\frac{\gamma_{12}}{4P\xi_1} = \frac{\sqrt{2}}{3} + (\xi_2/\xi_1)\left(\frac{\sqrt{2}}{3} - \frac{0.5140}{[(\xi_2/\xi_1)\sqrt{K}]^{1/2}} - \frac{0.066\,53}{[(\xi_2/\xi_1)\sqrt{K}]^{3/2}} + \frac{0.00107}{[(\xi_2/\xi_1)\sqrt{K}]^{5/2}} + \cdots \right). \quad (27)$$

This approximation is very accurate for values of κ in the interval between 0 and 1 [46]. To first order in κ, Eq. (27) agrees with the interface tension found for $K \to \infty$ as given in Eq. (3).

For large κ, according to standard results, the integral in Eq. (26) goes as $2(1-\sqrt{2})\kappa/3$ such that [48]

$$\frac{\gamma_{12}}{4P\xi_1} = \frac{\sqrt{2}}{3} + \frac{2(1-\sqrt{2})}{3\sqrt{K}} + (\xi_2/\xi_1)O(\kappa^{-1}). \quad (28)$$

Since large κ implies $\xi_2/\xi_1 \ll \sqrt{K}$, this last result is in full accord with the $K \to \infty$ limit in the expansion equation (24). The higher-order corrections to Eq. (28) can also be extracted from Eq. (24).

Note that Eqs. (25) and (27) are valid for all values of κ and may be generally used to numerically integrate the interface tension in the limit under consideration.

V. TEMPERATURE DEPENDENCE OF THE INTERFACE TENSION

At low but nonzero temperature, interface waves will be excited as thermal excitations. In this section, we will consider these and ignore quantum fluctuations. It is common to incorporate the free energy contributions which arise from capillary excitations into a new temperature-dependent interface tension $\gamma_{12}(T)$. Generally, when the interface waves have wave numbers k and frequencies $\omega(k)$, one finds for a three-dimensional system that [49,50]

$$\gamma_{12}(T) = \gamma_{12}(0) + \frac{k_B T}{2\pi} \int_0^\infty \ln(1 - e^{-\hbar\omega(k)/k_B T}) k dk,$$

where $\gamma_{12}(0)$ is the interface tension at zero temperature and the last term embodies a negative correction due to a nonzero temperature. For a flat interface between two BECs, one may obtain the capillary-wave spectrum from the time-dependent GP equations. For sufficiently large wavelengths $k^{-1} \gg \gamma_{12}/P$, one then finds for the modes with in-phase motion of both species [23,24]

$$\omega(k) = k^{3/2} \sqrt{\frac{\gamma_{12}}{m_1 n_1 + m_2 n_2}}, \quad (29)$$

where n_i is the bulk density of phase $i=1,2$. When the temperature T satisfies the condition $k_B T \ll \hbar^2/[2m_i(\gamma_{12}/P)^2]$, only modes with wave numbers satisfying Eq. (29) are thermally excited. The temperature-dependent interface tension then becomes [51]

$$\gamma_{12}(T) = \gamma_{12}(0) - \frac{c(k_B T)^{7/3}}{4\pi\hbar^{4/3}} \left(\frac{m_1 n_1 + m_2 n_2}{\gamma_{12}(0)} \right)^{2/3},$$

where $c \equiv \Gamma(7/2)\zeta(7/2)$ and ζ and Γ are functions.

Taking $n_1 \approx n_2$, $\gamma_{12}(0) \propto \xi_1 P$ and $\mu_1 \approx \mu_2$, one calculates that the relative temperature corrections $[\gamma_{12}(T) - \gamma_{12}(0)]/\gamma_{12}(0)$ are of order $\sqrt{n_1 a_{11}^3}(k_B T/\mu_1)^{7/3}$. It is known that $\sqrt{n_1 a_{11}^3} \ll 1$ is the condition for the GP theory to be applicable; moreover, for the current BEC experiments $k_B T$ is of the same order or less than μ_1 [40].

On the other hand, for a system in the weakly segregated regime, the interface tension varies as $\gamma_{12}(0) \propto \xi_1 P\sqrt{K-1}$ and accordingly vanishes as $K \to 1$. The relative temperature corrections are then of order $(K-1)^{-5/6}\sqrt{n_1 a_{11}^3}(k_B T/\mu_1)^{7/3}$ which may become large as $K \to 1$.

In conclusion, thermal fluctuations of a flat BEC interface do not affect the interface tension at low temperature, except possibly near weak segregation. Note that the calculated temperature dependence of the interface tension does not hold in trapped systems, as the interface modes there are quantized [27,52].

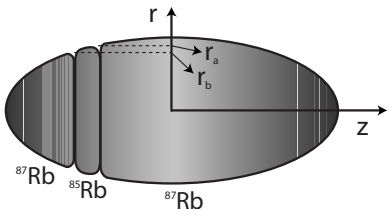

FIG. 4. Cross section of a trapped cloud of BEC mixtures as it was observed in Ref. [10]. Due to phase segregation, ^{85}Rb forms a layer between clouds of ^{87}Rb. In Eq. (30), we calculate the total excess energy due to the presence of the two interfaces.

VI. DISCUSSION

We discuss now the relevance of our results with respect to the recent experiments of Papp *et al.* [10]. Two main values for the scattering lengths of phase-segregated states were reported: One configuration was characterized by $K=3.01$ and $\xi_2/\xi_1=0.84$ such that $\mathcal{F}=\gamma_{12}/(4P\xi_1)=0.434$, while for the other configuration, $K=2.36$ and $\xi_2/\xi_1=0.952$ such that $\mathcal{F}=0.415$. Here species 1 and 2 are ^{85}Rb and ^{87}Rb, respectively. Note that these values for $\mathcal{F}$ are obtained both numerically and with Eq. (3). The values for $\mathcal{F}$ together with Eq. (1) allow a numerical calculation of the interface excess of any trapped configuration.

As an example, we consider now the topology as depicted in Fig. 4 in which a layer of ^{85}Rb BEC is present between clouds of ^{87}Rb. This configuration was experimentally obtained in Ref. [10] by strong radial confinement so as to quench gravitational effects. Particles of phase $i=1,2$ are confined by an anisotropic trapping potential $U_i(r,z) = m_i(\omega_{ri}^2 r^2 + \omega_{zi}^2 z^2)/2$ with $r^2 = x^2 + y^2$. Using Eq. (1), one finds the total excess energy due to the presence of the two interfaces,

$$\Omega_A^{HO} = \mathcal{F}(\xi_2/\xi_1, K) \frac{m_1^2 \omega_{r1}^3 (r_a^5 + r_b^5)}{20\hbar a_{11}}. \quad (30)$$

Here r_a and r_b are the maximal radial coordinates along the two interfaces (see Fig. 4) and $\mathcal{F}=0.415$. Comparing this excess energy Ω_A^{HO} with the total energy E of a gas of 1.4×10^5 ^{87}Rb particles, we obtain that $\Omega_A^{HO}/E \approx 0.03$. This implies that, even for the largest clouds observed in Ref. [10],

the interface excess energy is substantial and must be considered accurately when determining the shape of the ground-state configuration.

Note that in recent experiments on ultracold imbalanced fermion gases, a breaking of the local density approximation was encountered in the sense that the introduction of the interface and its tension was essential in explaining the experiments [53,54].

The formalism presented in this work assumes a local approximation for the interface tension. For this approach to be valid, the interface thickness must be smaller than the length over which the trapping potential varies. Generally, the former length is simply $\xi_1+\xi_2$; however, close to the mixed state (i.e., when $K\to 1$) it is $(\xi_1+\xi_2)/\sqrt{K-1}$ which is larger. On the other hand, the characteristic variation length of the trapping potential of species i is $a_{ho}=\sqrt{\hbar/m_i\bar{\omega}_i}$ with $\bar{\omega}\equiv(\omega_{r,i}^2\omega_{z,i})^{1/3}$. If we consider the configuration of 1.4×10^5 particles with $K=2.36$ and $\xi_2/\xi_1=0.952$, we find that $(\xi_1+\xi_2)/a_{ho}\approx 0.1$ is indeed small at the trap center [10]. Although the coherence lengths diverge at the trap boundary, this divergence is so weak that $\xi_1+\xi_2$ exceeds a_{ho} only in a layer of thickness of 0.5% of the trapping radius. This justifies the use of the local approximation for the interface in the experiments of Ref. [10].

VII. CONCLUSION

We propose a method to calculate the total energy of a trapped phase-segregated BEC mixture. In order to find the bulk energies, one can use a local density approximation or Thomas-Fermi approach. However, with respect to the recent experiments on phase-segregated BEC components [10], the bulk contribution must be supplemented by interface excesses which may have pronounced effects on the ground-state topology. The interface excess energy arises from the presence of the two-phase boundaries, the position of which are determined by the Laplace equation. Using a local approximation for the interface, we write the total excess energy as a simple integral of the trapping potential along the interface [see Eq. (1)]. By use of analytical expansions, we find the interface tension in almost all parameter regimes (see Fig. 1), including the regimes encountered in Ref. [10]. We also study the influence of thermal fluctuations on the interface tension at low temperature and find that their effect is negligible, except possibly close to the mixed state.

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