Fermi-Bose mixture across a Feshbach resonance

Luca Salasnich$^{1,2}$ and Flavio Toigo$^2$

$^1$CNR-INFM and CNISM, Unità di Milano, Via Celoria 16, 20133 Milano, Italy
$^2$Dipartimento di Fisica “G. Galilei” and CNISM, Università di Padova, Via Marzolo 8, 35131 Padova, Italy

We study a dilute mixture of degenerate bosons and fermions across a Feshbach resonance of the Fermi-Fermi scattering length $a_F$. This scattering length is renormalized by the boson-induced interaction between fermions and its value is crucial to determine the phase diagram of the system. For the mixture in a box and a positive Bose-Fermi scattering length, we show that there are three possibilities: a uniform single mixed phase, a purely fermionic phase coexisting with a mixed phase, and a purely fermionic phase coexisting with a purely bosonic one. As $1/a_F$ is increased from a negative value to the Feshbach resonance ($1/a_F = 0$) the region of pure separation increases and the other two regions are strongly reduced. Above the Feshbach resonance ($1/a_F > 0$), pairs of Fermi atoms become Bose-condensed molecules. We find that these molecules are fully spatially separated from the bosonic atoms when $1/a_F$ exceeds a critical value. For a negative Bose-Fermi scattering length we deduce the condition for collapse, which coincides with the onset of dynamical instability of the fully mixed phase. We consider also the mixture in a harmonic trap and determine the conditions for partial demixing, full demixing and collapse. The experimental implications of our results are investigated by analyzing mixtures of $^6$Li–$^{23}$Na and $^{40}$K–$^{87}$Rb atoms.

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I. INTRODUCTION

The regime of deep Fermi degeneracy is now actively studied with ultracold vapors of $^6$Li and $^{40}$K atoms. Experiments on two-hyperfine-state Fermi gases [1, 2, 3, 4] are concentrated across a Feshbach resonance, where a crossover from a Bardeen-Cooper-Schrieffer (BCS) superfluid to a Bose-Einstein condensate (BEC) of molecular pairs has been predicted [5, 6, 7]. Experimental and theoretical investigations of the Fermi cloud across the BCS-BEC crossover have been devoted to density profiles [8, 9, 10], collective excitations [8, 9, 11, 12, 13, 14, 15, 16], condensate fraction [17, 18, 19, 20], free expansion [1, 4, 21] and vortices [22, 23].

An interesting issue is the inclusion of Bose atoms, like $^{23}$Na or $^{87}$Rb isotopes, in the Fermi cloud. Trapped boson-fermion mixtures, with Fermi atoms in a single hyperfine state, have been investigated by various authors both theoretically [24, 25, 26, 27, 28, 29, 30, 31, 32] and experimentally [33, 34, 35]. Very recently McNamara et al. [36, 37] have reported the observation of simultaneous quantum degeneracy in a completely spin polarized dilute gaseous mixture of $^3$He and $^4$He in their first excited metastable states [37].

The purpose of this paper is to carry out a study of the miscibility of a Fermi-Bose mixture with the Fermi atoms in two equally populated hyperfine states across a Feshbach resonance of the Fermi-Fermi scattering length. Since the density of spin up and spin down fermions is bound to be the same, this three-component system behaves effectively as a two-component mixture: a superfluid Fermi gas and a Bose-Einstein condensate.

First we consider the mixture in a box. For a positive Bose-Fermi scattering length we show that, depending on the total number densities $n_F$ and $n_B$ of the Fermi and Bose components, there are three possible minimum energy configurations: a uniform phase with bosons and fermions fully mixed, a purely fermionic phase coexisting with a purely bosonic one, and a purely fermionic phase coexisting with a mixed phase. We find that the region in the $n_F - n_B$ plane where each one of the three is stable, strongly depends on the effective Fermi-Fermi scattering length. In addition, we find that when the Bose-Fermi scattering length is negative, collapse is driven by the dynamical instability of the homogeneous mixture.

We discuss also the mixture under harmonic confinement. In this case the conditions for partial demixing, full demixing and collapse crucially depend on the sign of the Bose-Fermi scattering length, the ratio between the Bose-Fermi and the Bose-Bose scattering lengths, and the number of atoms involved. We analyze the experimental implications of our results by considering mixtures of $^6$Li–$^{23}$Na and $^{40}$K–$^{87}$Rb atoms as examples.

II. RENORMALIZED SCATTERING LENGTH

It has been recently shown [15, 16, 38, 39] that at zero temperature the energy density of a uniform and dilute Fermi superfluid, composed by two equally populated spin states, can be written in the BCS-BEC crossover as

$$\mathcal{E} = \frac{3}{5} A n_F^{5/3} f(y),$$

where $A = \hbar^2 (3\pi^2)^{2/3} / (2m_F)$ and $m_F$ is the mass of a fermionic atom. The universal function $f(y)$ depends on the inverse interaction parameter $y = (k_F a_F)^{-1}$, where $a_F$ is the Fermi-Fermi scattering length, $n_F$ is the Fermi number density and $k_F = (3\pi^2 n_F)^{1/3}$ is the Fermi wave...
vector. In the experiments on the BCS-BEC crossover the scattering length $a_F$ is changed by using an external magnetic field (Feshbach resonance technique) and may be varied from large negative to large positive values \[1, 2, 3, 4\]. In these experiments the effective range of the interaction between fermions is much smaller than the mean interparticle distance and so the Fermi cloud may be considered as dilute. In the weakly attractive regime ($y \ll -1$) there is a BCS Fermi gas of weakly bound Cooper pairs and the universal function $f(y)$ has the asymptotic behavior $f(y) = 1 + 10/(9\pi y) + O(1/y^3)$ \[15, 16, 38\]. In the so-called unitarity limit ($y = 0$) one expects that the energy per particle is proportional to that of a non-interacting Fermi gas with a coefficient $f(0) = 0.42$ \[40\]. In the weak-coupling BEC regime ($y \gg 1$), there is instead a weakly repulsive Bose gas of fermions \[38, 39\] and the univ- eral function $f(y)$ has the asymptotic behavior $f(y) = 5a_M/(18\pi a_F y) + O(1/y^3)$ \[15, 16, 38\]. Actually the formula $a_M = 0.6a_F$ has been analytically derived for a weakly-interacting gas of dimers \[41\] but it seems to work well also in the strongly-interacting limit \[38\].

In the present work we investigate the effect of Bose atoms mixed with the two-hyperfine-state gas of fermions by using the two different analytical forms Eq. (2) and Eq. (3) of the universal function $f(y)$ proposed by Kim and Zubarev \[15\] and by Manini and Salasnich \[16\] to fit the numerical results from Monte Carlo (MC) simulations \[38, 39\] and obeying the above asymptotic expressions.

The formula proposed by Kim and Zubarev is a $[2/2]$ Padé approximant

$$f(y) = d_0 + \frac{d_1 y + d_2}{y^2 + d_3 y + d_4}, \quad (2)$$

where the values of the five parameters $d_i$ are reported in Ref. \[15\]. Manini and Salasnich slightly improved the fit to the available MC data \[38, 39\] by using a different parametrization, i.e.

$$f(y) = \alpha_1 - \alpha_2 \arctan \left( \frac{\alpha_3}{\alpha_4 + y} \right), \quad (3)$$

with the values of the parameters $\alpha_i$ and $\beta_j$ reported in Ref. \[16\].

At zero temperature a dilute gas of bosons, with density $n_B$, mass $m_B$ and interaction strength $g_B$, is a Bose-Einstein condensate, with a coherence length $\xi_B$ given by $\xi_B = \hbar/(2m_B g_B)$, where $c_B = (g_B n_B / m_B)^{1/2}$ is the bosonic sound velocity. Note that the strength $g_B$ is given by $g_B = 4\pi \hbar^2 a_B/m_B$, where $a_B$ is the Bose-Bose scattering length. Already back in the 1960’s, in connection with dilute solutions of $^3$He in superfluid $^4$He, it was realized that \[42\] the Fermi-Fermi scattering length is renormalized by the density fluctuations of the bosons and that this renormalization may lead to a BCS state even when the Fermi-Fermi bare interaction is repulsive. A thorough analysis \[26, 27, 28, 29\] of the renormalization of the Fermi-Fermi scattering length in Fermi-Bose mixtures of ultracold atomic gases has been provided in recent years. Viverit \[29\] has shown that, quite remarkably, in the dilute mixture and under the condition $k_F \xi_B \ll 1$, the renormalized scattering length of the Fermi-Fermi interatomic potential does not depend on the densities of the atomic species but only on their interaction strengths according to

$$a_F' = a_F - \frac{m_B g_B^2}{4\pi \hbar^2 g_B} \Theta(n_B), \quad (4)$$

where $g_B = 4\pi \hbar^2 a_B/m_B$ is the Bose-Fermi interaction strength, $a_B$ its scattering length and $m_B = 2m_B m_F/(m_B + m_F)$ the reduced mass. Heaviside’s function $\Theta(n_B)$ merely states that the renormalization occurs only where $n_B \neq 0$.

In Fig. 1 we plot the renormalized $1/a_F'$ as a function of the inverse bare scattering length $1/a_F$, according to Eq. (4). Fig. 1 shows that the Bose-Fermi interaction strength $g_B$ drives the system into the non-interacting regime ($1/a_F' = \pm \infty$) when $1/a_F = g_B^2 m_F/(g_B 4\pi \hbar^2) = (8/(9\pi)^{1/3})(g_B g_B^2)$. As previously stressed, the renormalization formula (4) holds if $k_F \xi_B \ll 1$, which may be satisfied only when $g_B$ is positive since it is equivalent to

$$n_B \ll \left( \frac{2m_B g_B}{m_F A} \right)^{3/2} n_B^{3/2}. \quad (5)$$

In the following we will use adimensional densities: for fermions $n_F = n_F g_B^6 (A^2 g_B^2)^{1/2}$ and for bosons $n_B = n_B g_B^2/4\pi \hbar^2$, so that Eq. (5) becomes $n_F \ll \alpha n_B^{3/2}$, where $\alpha = (2m_B g_B/(m_F g_B^2))^{3/2}$. In the case of a mixture of $^6$Li and $^{23}$Na atoms, where $g_B/g_B \approx 0.84$ \[23\], one finds $\alpha \approx 27$, while for a mixture of $^{40}$K and $^{87}$Rb atoms, where $g_B/g_B \approx -4.56$ \[43\], one gets $\alpha \approx 1$. In
both cases the range of densities where this inequality is valid is sufficiently large to allow experimental tests on the predictions of the following sections. Note that measuring lengths in units of \( g_B^{1/2}/(Ag_B) \), Eq. (4) becomes

\[
a_F' = a_F - (9\pi)^{1/3}/8 \approx a_F - 0.38; \text{ working near the Feshbach resonance (} a_F' = a_F = \infty \text{)} the renormalization of the Fermi-Fermi scattering length is very small.
\]

The Eq. (4) is valid for both negative and positive \( a_F \) under the condition [5] provided that a Fermi-Fermi bound state is not formed [29]. We expect that the effect of renormalization is negligible close to the resonance also on the BEC side of the BCS-BEC crossover, where indeed there is the molecular bound state made of two Fermi atoms in different hyperfine states. Thus, studying the BCS-BEC crossover, in the BEC side (\( a_F > 0 \)) we take \( a_F' = a_F \) and work only close to the Feshbach resonance.

Of course this issue deserves further investigations which are beyond the scope of the present paper.

### III. HOMOGENEOUS FERMI-BOSE MIXTURE

We consider a dilute mixture of \( N_B \) bosons and \( N_F \) fermions in a box of volume \( V \). As previously stated, the fermions are equally distributed in two hyperfine states and can be considered as a single superfluid Fermi system whose energy density is given by Eq. (1). Here and in the following we will use a local density approximation and assume that the interaction parameter \( y \) entering the universal function \( f(y) \) depends on the renormalized s-wave scattering length between fermions \( y = (k_F a_F')^{-1}. \)

In our treatment of the BCS-BEC crossover we use \( a_F' \) given by Eq. (4) for \( a_F < 0 \) and \( a_F' = a_F \) for \( a_F > 0 \). The energy density of a uniform, homogeneously mixed phase of condensate bosons and superfluid fermions can then be written as

\[
\mathcal{E} = \frac{3}{5} A n_F^{5/3} f(y) + \frac{1}{2} g_B n_F^2 + g_B n_B n_F ,
\]

where \((1/2)g_B n_F^2\) is the energy density of a Bose-Einstein condensate while \( g_B n_B n_F \) is the contribution from the Bose-Fermi interaction. \( a_B \) and \( a_F \) are not significantly modified by the medium if the diluteness conditions \( A n_F^{5/3} \ll 1 \) and \( a_B n_F^{5/3} \ll 1 \) are satisfied [28, 29, 44, 45], therefore we use them their bare values.

The mixed phase is energetically stable if its energy is a minimum with respect to small variations of the densities \( n_F \) and \( n_B \), while the total number of fermions and bosons are held fixed. To get the equilibrium densities one must then minimize the function

\[
\tilde{\mathcal{E}} = \mathcal{E} - \mu_F n_F - \mu_B n_B ,
\]

where \( \mu_F \) and \( \mu_B \) are Lagrange multipliers (imposing that the numbers of fermions and bosons are fixed) which may be identified with the Fermi and Bose chemical potentials. Setting the derivatives of \( \tilde{\mathcal{E}} \) with respect to \( n_F \) and \( n_B \) equal to zero, one finds:

\[
\mu_F = \frac{A}{n_F^{2/3}} \left( f(y) - \frac{1}{5} f'(y) \right) + g_B n_B , \quad (8)
\]

\[
\mu_B = g_B n_B + g_B n_F . \quad (9)
\]

The solution of Eqs. (8) and (9) gives a minimum if the corresponding Hessian of \( \tilde{\mathcal{E}} \) is positive, i.e. if:

\[
\frac{\partial^2 \tilde{\mathcal{E}}}{\partial n_F^2} \frac{\partial^2 \tilde{\mathcal{E}}}{\partial n_B^2} - \left( \frac{\partial^2 \tilde{\mathcal{E}}}{\partial n_F \partial n_B} \right)^2 > 0 , \quad (10)
\]

implying:

\[
n_F < \left( \frac{2}{3} \right)^3 \left( \frac{A g_B}{g_B n_F} \right)^3 \left( f(y) - \frac{3}{5} g_B f(y) + \frac{1}{10} g_B f''(y) \right)^3 . \quad (11)
\]

(Notice that \( n_F \) appears also in the right side of the inequality via \( y = ((3\pi^2 n_F)^{1/3} a_F')^{-1} \). The solution of this inequality gives the region in the parameters’ space where the homogeneous mixed phase is dynamically stable. Dynamical stability, corresponding to a local minimum of \( \tilde{\mathcal{E}} \) is a necessary but not sufficient condition for the energetic stability (also called thermodynamical stability at non-zero temperatures) which requires instead the global minimum of \( \tilde{\mathcal{E}} \). In fact, we shall show that there could exist inhomogeneous, two-phase, configurations with energy lower than that of the uniform, one-phase, configuration considered in Eq. (3). In Fig. 2 we plot the region of dynamical stability of the homogeneous mixture in the plane \((1/a_F', n_F)\), where \( a_F' \) is given by Eq. (4) for \( a_F < 0 \) and \( a_F' = a_F \) for \( a_F > 0 \). The solid line corresponds to the parametrization of Eq. (2) for \( f(y) \) in solving the equality in (11), while the dashed line follows from Eq. (3).

Fig. 2 shows that in the BCS regime \((1/a_F' \ll -1)\) the critical density \( n_F \) is close to \((2/3)^3\). Near the unitarity limit \((1/a_F' = 1/a_F = 0)\) the critical density strongly reduces and the homogeneous mixture is no longer stable for sufficiently large \(1/a_F' > 0\). This is not surprising because for a positive \( a_F' \), where \( a_F' = a_F \), the Fermi component becomes a gas of Bose-condensed molecules of mass \(2m_F\), which likes to separate from the atoms of mass \( m_B \). As shown in Fig. 2, there exists an upper critical value of \(1/a_F'\) for the stability of the homogeneous mixture. The existence of such upper critical value can be explained by the following simple analytical argument: in the deep BEC regime one treats a homogeneous Bose-Bose mixture as composed of atoms with mass \( m_B \) and molecules with mass \( m_M = 2m_B \) and interaction strength \( g_M = 4\pi\hbar^2 a_M/m_M \) with \( a_M = 0.6a_F' \), but \( a_F' = a_F \). Then, from the stability condition \( g_B^{1/3} < g_B g_M^{1/3} / 4 \), one finds the critical value at vanishingly small fermion density as \( 1/a_F = 1/a_F' = \pi/(3\pi^2)^{2/3}(Ag_B / g_B^{1/3}) = 0.20(Ag_B / g_B^{1/3}). \) This is exactly the value where both solid and dashed lines of Fig. 2 meet the \( n_F = 0 \) axis.
Thus the sound velocity has two branches and the homogeneous mixture becomes dynamically unstable when the lower branch becomes imaginary.

IV. TWO-PHASE FERMI-BOSE MIXTURE

The Bose and Fermi components can form distinct phases, which we label by the index $i$. If we ignore interpenetration effects, a possible phase-separated configuration is described by the number $I$ of phases present, the bosonic densities $n_{B,i}$, the fermionic densities $n_{F,i}$ in each phase, and the fractions $v_i$ of the total volume they occupy. Since the total number of particles is given, the following relations must hold:

$$n_F = \sum_{i=1}^{I} n_{F,i} v_i, \quad n_B = \sum_{i=1}^{I} n_{B,i} v_i, \quad \sum_i v_i = 1.$$  

and $\sum_i v_i = 1$. When $I = 1$ we have the case of a homogeneous mixture discussed in the previous section. The other possibility for the system we are considering is $I = 2$ [17]. In this case the total energy is the sum of the contributions due to fermions, to bosons and to their mutual interaction:

$$\mathcal{E} = \sum_{i=1}^{2} v_i \left[ \frac{3}{5} A n_{F,i}^{5/3} f_i + \frac{1}{2} g_B n_{B,i}^2 + g_{BF} n_{B,i} n_{F,i} \right],$$  

with $f_i = f(y_i)$ and $y_i = (3\pi^2 n_{F,i})^{1/3} a_F^n$, where $a_F^n$ is given for $a_F < 0$ by Eq. (4) properly renormalizing the scattering length between fermions in regions where there are bosons. For $a_F > 0$ we set $a_F^n = a_F$. Note that we have omitted contributions from interface effects since they should be negligible if the system is in a large box [18]. Equilibrium requires the equality of the pressures in each phase:

$$P_i = \frac{2}{5} A n_{F,i}^{5/3} \left( f_i - \frac{1}{2} y_i f_i' \right) + \frac{1}{2} g_B n_{B,i}^2 + g_{BF} n_{B,i} n_{F,i},$$  

where $f_i' = f'(y_i)$, and moreover the equality of the chemical potentials of each species:

$$\mu_{F,i} = A n_{F,i}^{2/3} \left( f_i - \frac{1}{5} y_i f_i'' \right) + g_{BF} n_{B,i},$$  

for fermions and:

$$\mu_{B,i} = g_B n_{B,i} + g_{BF} n_{F,i},$$  

for bosons. If the boson density $n_{B,i}$ is non-zero in both phases, then the chemical potentials $\mu_{B,i}$ must be equal. If the density of one species vanishes in one phase, then its chemical potential in that phase must be higher than in the other. For example, if the boson density is zero in one phase, then the boson chemical potential in that phase must be higher than in the other one, i.e.

$$\mu_{B,i} > \mu_{B,3-i} \quad \text{if } n_{B,i} = 0.$$  

Moreover, the asymptotic behavior of the universal function $f(y) \sim 1/y + O(1/y^{5/3})$ for large $y$, implies that the boundary of the stability region in Fig. 2 reaches the axis $n_F = 0$ with a positive slope. As a consequence there must be an interval of $1/a_F^n$ values where the stability region has both a lower and an upper bound in $n_F$. Numerically, one finds that this reentrant behaviour of the stability line occurs for values between $0.20(A g_B/g_{BF}^2)$ and $0.28(A g_B/g_{BF}^2)$ by using Eq. (3) (see the dashed line in the inset of Fig. 2)) and between $0.20(A g_B/g_{BF}^2)$ and $0.22(A g_B/g_{BF}^2)$, but with much smaller Fermi densities using Eq. (2) (see the solid line).

It is interesting to observe that the inequality [14] can be written as

$$n_F < \frac{g_B m_F}{g_{BF}^2} c_F^2,$$

where $c_F = v_F \left( f(y) - \frac{4}{3} y f'(y) + \frac{17}{10} y^2 f''(y) \right)^{1/2} / \sqrt{3}$ is the sound velocity of the superfluid Fermi component, with $v_F = \sqrt{2A A_{F}^{2/3} / m_F}$ the Fermi velocity. The sound velocity $c_{BF}$ of the Fermi-Bose mixture can be easily obtained following a procedure similar to the one suggested in Ref. [16] for a two-component Bose-Einstein condensate. One finds:

$$c_{BF} = \frac{1}{\sqrt{2}} \sqrt{c_B^2 + c_F^2 \pm \sqrt{(c_B^2 - c_F^2)^2 + 4g_{BF}^2 m_B m_F n_B n_F}},$$

where $c_B = \sqrt{g_B n_B / m_B}$ is the sound velocity of the Bose gas. Thus the sound velocity has two branches and

![FIG. 2: Region of dynamical stability of the homogeneous mixture in the plane $(1/a_F^n, n_F)$. Solid line: obtained with the universal function $f(y)$ derived by Kim and Zubarev [12]. Dashed line: obtained with the universal function $f(y)$ derived by Manini and Salasnich [10]. In the inset there is a zoom of the region with positive Fermi-Fermi scattering length $a_F^n$, where $a_F^n = a_F$. The fermionic density $n_F$ is in units of $A^2 g_B / g_{BF}^2$ and the scattering length $a_F^n$ is in units of $g_{BF}^2/(A g_B)$.](image)
The same is of course true for fermions.

Thus, one has to distinguish four cases of equilibrium, which must be analyzed one by one:

(i) Two pure phases: The bosons and fermions are completely separated corresponding to \( n_{F,1} = 0, n_{B,2} = 0 \) and \( n_{B,1} \neq 0, n_{F,2} \neq 0 \).

(ii) A mixed phase and a purely fermionic one: The boson density vanishes in one region corresponding to \( n_{F,1} \neq 0, n_{B,2} = 0 \) and \( n_{B,1} \neq 0, n_{F,2} \neq 0 \).

(iii) A mixed phase and a purely bosonic one: The fermion density vanishes in one region corresponding to the conditions \( n_{F,1} = 0, n_{B,2} \neq 0 \) and \( n_{B,1} \neq 0, n_{F,2} \neq 0 \).

(iv) Two mixed phases: All densities \( n_{B,1}, n_{F,1} \) and \( n_{B,2}, n_{F,2} \) are different from zero, while \( n_{B,1} \neq n_{B,2} \) and \( n_{F,1} \neq n_{F,2} \).

The analysis of these four cases is similar to that performed for the Fermi-Bose mixture with a single fermionic hyperfine state by Viverit, Pethick and Smith [28] and also by Das [30], who investigated the one-dimensional mixture. In our problem the presence of the universal function \( f(y) \) increases the complexity of the algebraic manipulations.

We leave out the algebra and discuss the results as a function of the inverse scattering length. First of all, the analysis shows that the cases (iii) and (iv) are not realizable. Thus, a separation into two phases, each with different, non-zero, concentrations of bosons and fermions is never in equilibrium, nor is one with a purely bosonic phase and a mixed one. The cases (i) and (ii) are instead possible if \( g_{BF} > 0 \), while for \( g_{BF} < 0 \) these configurations are unstable.

In Fig. 3 we plot the phase diagrams \((n_B, n_F)\) of the Fermi-Bose mixture for three values of the bare s-wave scattering length \( a_F \) and \( g_{BF} > 0 \). In the figure there are the results obtained by using Eq. 4 to model the universal function \( f(y) \). Very similar results are obtained by using Eq. 2. Above the dot-dashed line there are two pure phases where bosons and fermions are completely demixed and therefore \( a'_F = a_F \). Between the dot-dashed line and the solid line there is a mixed phase with a fermion scattering length renormalized by the presence of the bosons and a purely fermionic one where \( a'_F = a_F \). Below the solid line bosons and fermions are homogeneously mixed. Fig. 3 shows that, as \( 1/a_F \) is increased from a negative value to the Feshbach resonance \((1/a_F = 1/a'_F = 0)\), the region of pure separation increases, while the other two are strongly reduced. This effect is stronger above the Feshbach resonance \((1/a_F > 0 \) and \( a'_F = a_F \)) where pairs of Fermi atoms become Bose-condensed molecules. As expected from the dynamical stability analysis of the previous section, when \( 1/a_F \) exceeds a critical value the region of pure separation occupies the whole phase diagram. This critical value is \( 1/a_F = 0.28(A g_B/g_{BF}^2) \) according to Eq. 4 and it is instead \( 1/a_F = 0.22(A g_B/g_{BF}^2) \) using the Eq. 2.

As discussed in the previous section, a physical consequence of the asymptotic behavior of \( f(y) \) for \( y \to +\infty \) is the existence of an interval of \( 1/a_F \), where the re-
gion of dynamical stability of the mixed phase has not only an upper bound in the fermion density but also a lower bound. By using Eq. (3) this happens for $0.20 (A_{BF}/g_{BF}^2) \leq 1/a_F \leq 0.28 (A_{BF}/g_{BF}^2)$. In Fig. 4 we plot the phase diagram obtained with Eq. (3) and $1/a_F = 0.25$. As in Fig. 3, the dark grey region of the diagram is where the fully mixed configuration is dynamically and energetically stable. In Fig. 4 there are domains, indicated as hatched regions, where none of the possible configurations is dynamically and energetically stable. Obviously, in these domains the total energy is no longer given by Eq. (15) and the role of the interface may be relevant. There is a similar effect for $g_{BF} < 0$. In fact, for $g_{BF} < 0$ only the single homogeneous phase, where bosons and fermions are fully mixed, is stable: in Fig. 3 and in Fig. 4, this region is in between the two dashed lines, and it is independent on $n_B$. In the other regions of the phase diagram all the configurations are unstable, and presumably this corresponds to a collapse where fermions and bosons are clumped together [28].

Our predictions can be verified by using alkali-metal atoms. For the Fermi-Bose mixture of $^6$Li atoms and $^{23}$Na atoms one has $A_{BF} = 30 a_0$, where $a_0 = 0.53 \times 10^{-10}$ m is the Bohr radius [29]. In this case it is easy to find that the scaling units of $n_F$ and $n_B$, i.e. $(A_{BF}/g_{BF})^3$ and $A_{BF}^2/g_{BF}^2$, are both about $10^8 \mu m^{-3}$. For the Fermi-Bose mixture of $^{40}$K atoms and $^{87}$Rb atoms one has instead $A_{BF} = -284 a_0$ [30] and the scaling units are about $10^2 \mu m^{-3}$ for fermions and about $10^5 \mu m^{-3}$ for bosons. From these densities and Fig. 3 it follows that in the unitarity limit ($1/a_F = 0$) the mixing-demixing transition can be obtained for instance in a mixture of $\sim 10^6$ $^6$Li atoms and $\sim 10^6$ $^{23}$Na atoms in a volume of $\sim 0.5 \mu m^3$. These numbers of atoms are already realized in experiments with ultra-cold alkali-metal atoms.

V. INCLUSION OF AN EXTERNAL POTENTIAL

In actual experiments, the ultra-cold atoms are usually trapped by an external harmonic potential. For simplicity we consider the same spherical harmonic potential

$$U(r) = \frac{1}{2} K r^2$$

acting on fermions and bosons, where $K = m_F \omega_F^2 = m_B \omega_B^2$ is the elastic constant and $\omega_F$ and $\omega_B$ are the corresponding harmonic frequencies. The energy functional of the mixture can be written as

$$E = \int \left\{ \frac{\hbar^2}{2m_F} \left( \nabla \sqrt{n_F(r)} \right)^2 + \frac{\hbar^2}{2m_B} \left( \nabla \sqrt{n_B(r)} \right)^2 + \mathcal{E}(n_F(r), n_B(r)) + U(r) n_F(r) + U(r) n_B(r) \right\} d^3r$$

where $\mathcal{E}(n_F(r), n_B(r))$ is given by Eq. (6) while the gradient terms give the quantum pressure for bosons and the von Weizsäcker contribution to the kinetic energy of fermions with a nonuniform density. By minimizing the energy with a fixed number $N_B$ of bosons and $N_F$ of fermions we get

$$\mu_F = -\frac{\hbar^2}{2m_F} \frac{\nabla^2 \sqrt{n_F(r)}}{\sqrt{n_F(r)}}$$

$$+ A n_F(1) \left( \frac{1}{5} f'(y(r)) \right) + g_{BF} n_B(r) + U(r),$$

$$\mu_B = -\frac{\hbar^2}{2m_B} \frac{\nabla^2 \sqrt{n_B(r)}}{\sqrt{n_B(r)}} + g_B n_B(r) + g_{BF} n_F(r) + U(r),$$

where $y(r) = (3\pi^2 n_F(r))^{1/3} a_F^{-1}$. Again $a_f' = a_F$ in the case of full denixing and also for $a_F > 0$. The presence of a harmonic external potential $U(r)$ strongly modifies the conditions for demixing. Clearly, due to the harmonic confinement partial denixing is always possible. For instance, with $g_{BF} = 0$ both Fermi and Bose clouds occupy the center of the trap but the effective radii can be quite different and in this case denixing will appear far from the center of the trap. Such conditions can be estimated analytically from the previous equations (22) and (23) within the Thomas-Fermi (TF) approximation, i.e. neglecting von Weizsäcker and quantum-pressure terms. This is a good approximation when $g_B > 0$ and $N_F$ and $N_B$ are large [41, 50]. For $g_{BF} = 0$ the TF approximation gives $R_B = (15 g_{BF} N_B/(4 \pi m_B \omega_B^2))^{1/5}$ for the effective radius of the Bose cloud. The effective radius $R_F$ of the Fermi cloud depends instead on $1/a_F'$. For $1/a_F' \ll -1$ (BCS regime) one finds $R_F = (48 N_F)^{1/6} \hbar/(m_F \omega_F^2)$; for $1/a_F' = 0$ (unitarity limit) one finds $R_F = f(0)^{1/4} (48 N_F)^{1/6} \hbar/(m_F \omega_F^2)$; for $1/a_F' = 1/a_F \gg 1$ (BEC regime) one finds $R_F = (0.60)^{1/5} (15 g_f' N_B/(32 \pi m_F \omega_F^2))^{1/5}$, where $g_f' = 4 \pi a_f'/m_F$. Also for $g_{BF} > 0$ partial denixing is possible by varying the number of atoms. This is the typical situation of the $^6$Li-$^{23}$Na mixture where $g_{BF}/g_B = 0.84$. In Fig. 5(a) we plot the density profiles of the Bose and Fermi clouds obtained in the unitarity limit $1/a_F' = 0$ with $N_B = 10^6$ and $N_F = 10^5$. In this case the radii of the two clouds are very similar but, as shown in Fig. 5(b) where $N_B = 10^6$ and $N_F = 5 \times 10^6$, by increasing the number $N_F$ of fermions one produces partial denixing with Bose and Fermi atoms in the center of the trap and an external shell of fermions. The results of Fig. 5 have been obtained by inserting the Thomas-Fermi density of fermions, $n_F(r)$, into Eq. (23). In this way one gets the following nonlinear Schrödinger equation

$$\left[ -\frac{\hbar^2}{2m_B} \frac{\nabla^2}{\sqrt{n_B(r)}} + U(r) + g_B n_B(r) + g_{BF} n_F(r) \right] \psi(r) = \mu_B \psi(r),$$

(24)
where \(n_B(r) = |\psi(r)|^2\) and \(\psi(r)\) is the macroscopic wave function of the Bose condensate. We have solved this equation by considering its time-dependent version and using a finite-difference Crank-Nicholson method with imaginary time [51].

Usually both Fermi and Bose atoms occupy the center of the trap, but under some conditions one of the two species can be expelled from the center. In particular, as suggested by Mølmer [24], if the bosonic cloud is practically independent on the fermions, one may get the density profile of bosons as

\[
n_B(r) \approx \frac{1}{g_B} (\mu_B - U(r)) ,
\]

by neglecting the quantum-pressure term in Eq. (23).

Inserting this result into Eq. (22) one gets the following TF formula for the fermionic density profile \(n_F(r)\):

\[
A n_F(r)^{2/3} \left( f(y(r)) - \frac{1}{5} f''(y(r)) \right) \approx \mu_F - \frac{g_{BF}}{g_B} \mu_B - U(r) \left( 1 - \frac{g_{BF}}{g_B} \right) ,
\]

where the terms proportional to \(g_{BF}\) are absent in regions with vanishing \(n_B(r)\). This formula shows that if \(g_{BF}/g_B < 1\) the fermions will occupy the center of the trap together with bosons. Instead, if \(g_{BF}/g_B > 1\) the fermions are expelled from the center of the trap and form a shell outside the Bose condensate, i.e. there is a core of bosons surrounded by a shell of fermions. In Fig. 5(c) we show the profiles of the \(^6\)Li–\(^{87}\)Rb mixture with the artificial value \(g_{BF}/g_B = 5\) and setting \(N_B = 10^6\) and \(N_F = 10^5\). It this case the fermionic cloud is expelled from the center of the trap. This effect is more clearly shown in Fig. 5(d) where we set \(N_B = 10^6\) and \(N_F = 5 \times 10^5\). Note that by using a much larger value of the ratio \(g_{BF}/g_B\) we find full demixing.

For the \(^{87}\)Rb–\(^{40}\)K mixture the Bose-Fermi scattering length is attractive, i.e. \(g_{BF} < 0\). In this case the Fermi atoms are mixed with the Bose atoms up to the collapse. As verified by various authors [24, 34, 52, 53] with a Fermi-Bose mixture and with fermions in a unique hyperfine state, the collapse point is well described by the local density approximation at the point where the dynamical instability sets up. In our case this point is obtained from Eq. (11) as

\[
n_F(0) = \left( \frac{2}{3} \right)^3 \left( \frac{A g_B}{g_{BF}} \right)^3 \left( f(y^c(0)) - \frac{3}{5} y^c(0) f''(y^c(0)) \right) + \frac{1}{10} y^c(0)^2 f''(y^c(0)) \left( \frac{g_{BF}}{g_B} \right) ,
\]

where \(y^c(0) = ((3\pi^2 n_F(0))^{1/3} a_F)^{-1}\) and \(n_F(0)\) is the critical density at the center of the trap above which there is the collapse. The plot of \(n_F(0)\) as a function of \(1/a_F^2\) is precisely the solid (dashed) curve of Fig. 2 taking \(f(y)\) from Eq. (2) (Eq. (3)). Using the most recent available data on the \(^{40}\)K–\(^{87}\)Rb mixture [35] we predict that in the deep BCS regime \((1/a_F^2 \ll -1)\) the critical fermionic density is \(n_F^c(0) = 140 \mu m^{-3}\), while in the unitarity limit \((1/a_F^2 = 0)\) it reduces to \(n_F^c(0) = 10 \mu m^{-3}\).

VI. CONCLUSIONS

We have investigated a Fermi-Bose mixture with the Fermi atoms in two equally populated hyperfine states. In particular, we have analyzed the mixture as the Fermi-Fermi scattering length is varied across a Feshbach resonance by using two efficient parametrizations of the universal function \(f(y)\), which characterizes the BCS-BEC crossover. We have found that the phase diagram of the system strongly depends on the Fermi-Fermi scattering length. The conditions for demixing and collapse have been studied in a box and also in a harmonic trap by using a density functional approach. Our results suggest that in the unitarity limit, where the renormalized scattering length of the Fermi-Fermi interaction goes to infinity, demixing or partial demixing can be observed using a mixture of \(^6\)Li and \(^{23}\)Na atoms. Collapse can be instead obtained using a mixture of \(^{40}\)K and \(^{87}\)Rb atoms and varying the fermionic density of the system. Many interesting issues regarding Fermi-Bose mixtures across a Feshbach resonance remain to be investigated both the-
oetically and experimentally. Among them there are finite-temperature effects and population imbalance of fermions in the two spin states.

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