

Stable and unstable regimes in Bose-Fermi mixtures with attraction between components

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The collapse of a trapped boson-fermion mixture with attraction between bosons and fermions is investigated in the framework of the effective Hamiltonian for the Bose system. The properties of an ^{87}Rb and ^{40}K mixture are analyzed quantitatively at $T=0$. We find numerically solutions of the modified Gross-Pitaevskii equation which continuously go from the stable to the unstable branch. We discuss how the conditions for the onset of collapse are related to the macroscopic properties of the system. A comparison with the case of a Bose condensate of the atomic ^7Li system is given.

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I. INTRODUCTION

Bose-Einstein condensation in ultracold atomic gas clouds with repulsive and attractive interatomic interactions [1–3] has been the subject of intense theoretical and experimental interest in recent years. Besides the studies using bosonic atoms, growing interest is focused on the cooling of fermionic atoms [4]. Cooling of trapped fermionic atoms to a temperature regime where a Fermi gas can be considered as degenerate has been possible by sympathetic cooling in the presence of a second boson or fermion component. Quantum degeneracy was first reached with mixtures of bosonic ^7Li and fermionic ^6Li atoms [5,6]. Later, successful cooling of mixtures of ^{23}Na and ^6Li [7], as well as ^{87}Rb and ^{40}K [8,10] to ultralow temperatures was achieved. The Bose gas, which can be cooled evaporatively, is used as a coolant for a fermionic system that is in physical contact and thermal equilibrium with the cold Bose gas.

Collision interactions between the bosons and fermions greatly affect the properties of the degenerate mixture. Theoretical considerations predict the phenomenon of component separation for systems with a positive coupling constant [11]. Instabilities and significant modification of the properties of the individual components in the case of boson-fermion attraction [12,13] were predicted. The effect of density fluctuations in a Bose condensate on the fermion-fermion interaction with relevant implications for the achievement of fermionic superfluidity has been investigated in [14]. The presence of a sufficiently attractive boson-fermion interaction can bring about the formation of stable fermionic bright solitons [15].

The simultaneous collapse of the two species has been observed in a ^{40}K - ^{87}Rb mixture by Modugno and co-workers [8] (see also [9]). K and Rb atoms were prepared in doubly polarized states $|F=9/2, m_F=9/2\rangle$ and $|2, 2\rangle$, respectively. As the number of bosons is increased there is an instability value N_{Bc} at which a discontinuous leakage of the bosons and fermions occurs, and collapse of boson and fermion clouds is observed. The collapse was found for the following critical numbers of bosons and fermions: $N_{Bc} \approx 10^5$; $N_{Kc} \approx 2 \times 10^4$. For investigating the stability diagram of the K-Rb system a

mean-field model of Gross-Pitaevskii (GP) type coupled to the Thomas-Fermi equation for fermions has been used [12,16–18]. The ground state and the stability of the system against collapse were considered with an imaginary-time evolution scheme. The signature of the instability is the failure of the convergence procedure toward the ground state of the system, characterized by an indefinite growth of the central density [17].

In this paper we study the instability and collapse of a trapped boson-fermion mixture due to the boson-fermion attractive interaction, using the effective Hamiltonian for the Bose system [19,20]. The effective Hamiltonian incorporates the three-particle elastic collisions induced by the boson-fermion interaction. We analyze quantitatively properties of the ^{87}Rb and ^{40}K mixture with an attractive interaction between bosons and fermions at $T=0$. The stability of this system on the basis of a variational condensate wave function was studied in [20], and good agreement with experiment [8] was found. We estimate the instability boson number N_{Bc} for the collapse transition by numerical calculation of the modified GP equation and give a comparison with a similar picture in a single Bose condensate with attractive interaction. Our instability analysis involves the dependences of the chemical potential μ and the number of boson particles N on the value of the central density n_c of the Bose condensate wave function $\phi(\mathbf{r})$. Considerations based on the n_c dependence were introduced earlier in Ref. [21] for studying the stability of a Bose condensate of atomic ^7Li in a magnetic trap at nonzero temperature. The calculations [21] confirmed that the gas becomes mechanically unstable when the free energy of the system as a function of the central density of the gas approaches a maximum value. In our case we present arguments based on a second variation of the energy functional. We consider explicitly those variations of the condensate wave function $\delta\phi(\mathbf{r})$ that reveal an instability point of the energy functional, and relate these variations to a broad class of variations which does not preserve the normalization.

II. EFFECTIVE BOSE HAMILTONIAN

First of all we briefly discuss the effective boson Hamiltonian [19,20]. Our starting point is the functional-integral

representation of the grand-canonical partition function of the Bose-Fermi mixture. It has the form [22,23]

$$Z = \int D[\phi^*]D[\phi]D[\psi^*]D[\psi] \exp\left(-\frac{1}{\hbar}[S_B(\phi^*, \phi) + S_F(\psi^*, \psi) + S_{int}(\phi^*, \phi, \psi^*, \psi)]\right)$$

and consists of an integration over a complex field $\phi(\tau, \mathbf{r})$, which is periodic on the imaginary-time interval $[0, \hbar\beta]$, and over the Grassmann field $\psi(\tau, \mathbf{r})$, which is antiperiodic on this interval. Therefore, $\phi(\tau, \mathbf{r})$ describes the Bose component of the mixture, whereas $\psi(\tau, \mathbf{r})$ corresponds to the Fermi component. The term describing the Bose gas has the form

$$S_B(\phi^*, \phi) = \int_0^{\hbar\beta} d\tau \int d\mathbf{r} \left[\phi^*(\tau, \mathbf{r}) \left(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m_B} + V_B(\mathbf{r}) - \mu_B \right) \phi(\tau, \mathbf{r}) + \frac{g_B}{2} |\phi(\tau, \mathbf{r})|^4 \right].$$

Because the Pauli principle forbids s -wave scattering between fermionic atoms in the same hyperfine state, the Fermi-gas term can be written in the noninteracting form

$$S_F(\psi^*, \psi) = \int_0^{\hbar\beta} d\tau \int d\mathbf{r} \left[\psi^*(\tau, \mathbf{r}) \left(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m_F} + V_F(\mathbf{r}) - \mu_F \right) \psi(\tau, \mathbf{r}) \right].$$

The term describing the interaction between the two components of the Fermi-Bose mixture is

$$S_{int}(\phi^*, \phi, \psi^*, \psi) = g_{BF} \int_0^{\hbar\beta} d\tau \int d\mathbf{r} |\psi(\tau, \mathbf{r})|^2 |\phi(\tau, \mathbf{r})|^2,$$

where $g_B = 4\pi\hbar^2 a_B/m_B$, $g_{BF} = 2\pi\hbar^2 a_{BF}/m_I$, $m_I = m_B m_F/(m_B + m_F)$, m_B and m_F are the masses of bosonic and fermionic atoms respectively, and a_B and a_{BF} are the s -wave scattering lengths of boson-boson and boson-fermion interactions. The K and Rb atoms in the trap are in potentials with an elongated symmetry (λ -trap asymmetry parameter)

$$V_B(\mathbf{r}) = \frac{m_B \omega_B^2}{2} (\rho^2 + \lambda z^2), \quad V_F(\mathbf{r}) = \frac{m_F \omega_F^2}{2} (\rho^2 + \lambda z^2).$$

The trap parameters ω_B and ω_F are chosen in such a way that $m_B \omega_B^2/2 = m_F \omega_F^2/2$, so $\omega_F = \sqrt{m_B/m_F} \omega_B$. The parameters μ_B and μ_F are the chemical potentials for the Bose and Fermi systems, respectively. The chemical potential of an ideal Fermi gas in a trap is $\mu_F = \hbar \omega_F (6\lambda N_F)^{1/3}$ [24].

The integral over the Fermi fields,

$$Z_F = \int D[\psi^*]D[\psi] \exp\left(-\frac{1}{\hbar}[S_F(\psi^*, \psi) + S_{int}(\phi^*, \phi, \psi^*, \psi)]\right),$$

is Gaussian; we can calculate this integral and obtain the partition function of the Fermi system as a functional of the Bose field $\phi(\tau, \mathbf{r})$,

$$Z_F = \exp\left(-\frac{1}{\hbar} S_{eff}\right); \quad S_{eff} = \int_0^{\hbar\beta} d\tau \int d\mathbf{r} f_{eff}(|\phi(\tau, \mathbf{r})|).$$

Due to the Pauli principle (quantum pressure) the radius of the Bose condensate is much smaller than the radius of the Fermi cloud $R_F \approx \sqrt{\mu_F/V_0}$. As a result one can use an expansion in powers of $V_F(\mathbf{r})/\mu_F$ and obtain the effective Hamiltonian in the form

$$H_{eff}[\phi] = \int d\mathbf{r} \left(\frac{\hbar^2}{2m_B} |\nabla \phi|^2 + [V_{eff}(\mathbf{r}) - \mu_B] |\phi|^2 + \frac{g_{eff}}{2} |\phi|^4 + \frac{g_{eff}^{BF}}{3} |\phi|^6 \right), \quad (1)$$

where

$$V_{eff} = k_0 \frac{m_B \omega_B^2}{2} r^2, \quad k_0 = \left(1 - \frac{3}{2} \kappa \mu_F^{1/2} g_{BF}\right), \quad \kappa = \frac{\sqrt{2} m_F^{3/2}}{3 \pi^2 \hbar^3}$$

$$g_{eff} = g_B - \frac{3}{2} \kappa \mu_F^{1/2} g_{BF}^2, \quad g_{eff}^{BF} = \frac{3\kappa}{8 \mu_F} g_{BF}^3.$$

The first three terms in (1) have the conventional Gross-Pitaevskii [25] form, and the last term is a result of the boson-fermion interaction. The interaction with the Fermi gas leads to modification of the trapping potential. For an attractive fermion-boson interaction the system behaves as if it was confined in a magnetic trapping potential with larger frequencies than the actual ones, in agreement with experiment [8]. The boson-fermion interaction also induces an additional attraction between the Bose atoms that does not depend on the sign of g_{BF} . The last term in the H_{eff} (1) corresponds to three-particle *elastic* collisions induced by the boson-fermion interaction. In contrast with *inelastic* three-body collisions, which result in the recombination and removal of particles from the system [26,27], this term for $g_{BF} < 0$ leads to increase of the gas density in the center of the trap in order to lower the total energy.

III. NUMERICAL PROCEDURE

To simplify the algebra we introduce dimensionless variables for the spatial coordinate, the energy, and the wave function as

$$\mathbf{r} = a_{\perp} \mathbf{r}', \quad E = \hbar \omega_{\perp} E', \quad \phi(\mathbf{r}) = \frac{1}{\sqrt{a_{\perp}^3}} \phi'(\mathbf{r}'),$$

where the typical length and energy of the harmonic external potential are $a_{\perp} = \sqrt{\hbar/m_B \omega_{\perp}}$, $\hbar \omega_{\perp} = \hbar \omega_B$.

The effective Hamiltonian takes the form (the primes are omitted)

$$H_{eff} = \int \left[\frac{1}{2} |\nabla \phi|^2 + \left(k_0 \frac{\rho^2 + \lambda z^2}{2} - \mu_B \right) |\phi|^2 + \frac{u}{4} |\phi|^4 + \frac{v}{6} |\phi|^6 \right] d^3 r + \int \mathcal{E}_{eff}(\phi(\mathbf{r}), \nabla \phi(\mathbf{r}), \mu_B) d^3 r, \quad (2)$$

where we introduced dimensionless parameters $u = 2g_{eff}/a_{\perp}^3 \hbar \omega_{\perp}$ and $v = 2g_{eff}^{BF}/a_{\perp}^6 \hbar \omega_{\perp}$. The wave function ϕ is normalized to the number of atoms in the condensate $\int d^3r |\phi(\mathbf{r})|^2 = N$. In the $T \rightarrow 0$ limit considered, N coincides with the total number of bosonic atoms in the trap. The explicit form of the ground-state wave function is obtained by minimizing the energy functional. The first-order variation of the energy functional gives the modified Gross-Pitaevskii equation

$$\left(-\frac{\nabla^2}{2} + k_0 \frac{\rho^2 + z^2}{2} - \mu_B + \frac{u}{2} |\phi|^2 + \frac{v}{2} |\phi|^4 \right) \phi = 0. \quad (3)$$

The parameters of the ^{87}Rb and ^{40}K mixture with an attractive interaction between the bosons and the fermions are the following [8]: $a_B = 5.25$ nm, $a_{BF} = -21.7_{-4.8}^{+4.3}$ nm. The magnetic potential had an elongated symmetry, with harmonic oscillation frequencies for Rb atoms $\omega_{\perp} = \omega_B = 2\pi \times 215$ Hz and $\omega_{B,z} = \lambda \omega_B = 2\pi \times 16.3$ Hz. At these parameter values the characteristic length $a_{\perp} = 735$ nm, the chemical potential for the fermions $\mu_F \approx 31 \hbar \omega_B$, $\omega_F \approx 1.47 \omega_B$, $k_0 = 1.07$, $u = 0.11$, and $v = -0.0003$. Because k_0 differs from unity only by a small amount we shall approximate k_0 by 1. Since we look for the ground state of Eq. (3) the function $\phi(\mathbf{r})$ can be treated as real.

To clarify the main features of the instabilities of the system we consider the isotropic picture when the problem can be considered effectively as one dimensional. The case of nonspherical symmetry of the trap is recovered at the end by multiplying the critical number of bosons N_c by the reverse trap asymmetry ratio $1/\lambda$.

Equation (3) can be written as ($\mu \equiv \mu_B$)

$$\Delta \phi = (r^2 - 2\mu + u\phi^2 + v\phi^4)\phi. \quad (4)$$

Solutions of Eq. (4) will be compared to those for the single-component Bose condensate with attractive interactions. As an example of a Bose system with attractive interaction we choose ^7Li [28]. The s -wave scattering length is $a = -27.3a_0$, where a_0 is the Bohr radius. The transverse frequency is $\omega_{\perp}/2\pi = 163$ Hz, so the corresponding characteristic length is $a_{\perp} = 2.97 \times 10^{-4}$ cm and $u = 8\pi a/a_{\perp} = -0.012$.

It is convenient to look for the numerical solutions of Eq. (4) as a function of the central density $n_c = \phi^2(0)$. Numerical integration of Eq. (4) with boundary conditions

$$\phi'(0) = 0, \quad \phi(r) \rightarrow 0, \quad r \rightarrow \infty, \quad (5)$$

defines the family of solutions $\phi(r, n_c)$ depending on the central density; the chemical potential $\mu(n_c)$ being also a function of n_c . The consideration of n_c as an input parameter (except for μ) enables us to find solutions in the region of instability and to go continuously from the stable to the unstable branch in the parameter space. This approach differs from an imaginary-time scheme [29], where the stability is indicated by requiring a convergence procedure to the final value. Solving Eq. (4), one can easily estimate the effective energy E_{eff} corresponding to the functional (2) and the ground-state energy $E = E_{eff} + \mu N$, both as functions of the central density n_c .

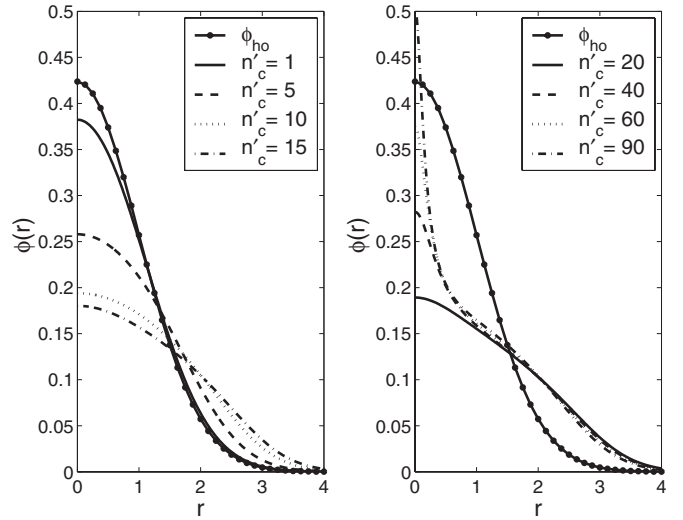


FIG. 1. Evolution of the profile of the bosonic condensate wave function $\phi(r)$ with increasing central density n'_c . The radius r is in units of a_{\perp} . We plot $\phi(r)/\sqrt{N}$, so that the curves are normalized to 1.

The derivative $d\phi(r, n_c)/dn_c$ is of especial interest, because it determines a change in the number of particles through the variation in the central density n_c ,

$$\frac{dN}{dn_c} = 2 \int d^3r \phi(r, n_c) \frac{d\phi(r, n_c)}{dn_c}.$$

The condition $dN/dn_c = 0$ results in the appearance of a zero mode in the density fluctuations and indicates the onset of instability [21].

It is convenient to consider $\phi(r, n_c)$ and $d\phi(r, n_c)/dn_c$ as functions of the rescaled central density parameter $n'_c = |u|n_c$. The results are plotted in Figs. 1 and 2 where $\phi(r, n_c)/\sqrt{N}$ is shown; the distance r is given in units of a_{\perp} . We integrate Eq. (4) for different values of μ . Solutions satisfying the boundary conditions (5) exist for two values of

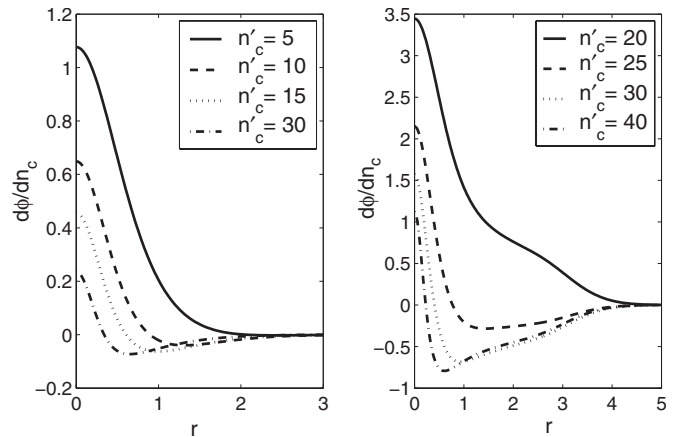


FIG. 2. Evolution of derivative $d\phi(r, n_c)/dn_c$ at various values of central density n'_c . The radius r is in units of a_{\perp} . Normalization of $\phi(r)$ is the same as in Fig. 1. Left panel is for the ^7Li system, and right panel for the BF mixture.

$\mu(n_c)$ where the first solution corresponds to the stable branch (left panel of Fig. 1) and the second one to the unstable solution (right panel of Fig. 1). By changing n_c we can continuously go from one branch to the other one. The solutions corresponding to the other values of μ are unphysical: they are oscillating and exponentially growing.

Figure 1 shows the evolution of the profile of the condensate wave function with increasing central density. For comparison, the solution for the isotropic harmonic oscillator, $\phi_{ho} = \pi^{-3/4} \exp(-r^2/2)$, which corresponds to the ground state of the ideal Bose gas ($u=0, v=0$), is also shown. For $n'_c \lesssim 20$, one sees behavior characteristic of a Bose gas with repulsion, namely, the cloud density becomes more flat at the trap center, with increasing radius of the boson cloud. For $n'_c \gtrsim 20$, the solution changes qualitatively: the central density begins to increase as n'_c is increased. Figure 2 shows the evolution of the derivative $d\phi(r, n_c)/dn_c$ for the ${}^7\text{Li}$ system with attractive interaction ($u < 0$) (the left panel) and for the boson-fermion (BF) mixture (the right panel). The behavior of the BF mixture at relatively high densities ($n'_c \gtrsim 20$) has similar features with the ${}^7\text{Li}$ system. When n'_c increases there is a continuous change of the shape of the function $d\phi/dn_c$. It acquires a negative minimum at $r \lesssim a_\perp$, which results in a saturation and a maximum in the $N(n_c)$ dependence.

To relate the conditions for stability of a system toward small changes in its density profile with the corresponding conditions for thermodynamic functions, let us consider the total energy E as a functional of the condensate wave function $\phi(\mathbf{r})$ and its gradient $\nabla\phi(\mathbf{r})$

$$E = \int d^3r \mathcal{E}(\phi(\mathbf{r}), \nabla\phi(\mathbf{r})) \quad (6)$$

where $\mathcal{E}(\phi(\mathbf{r}), \nabla\phi(\mathbf{r})) = \mathcal{E}_{eff}(\phi(\mathbf{r}), \nabla\phi(\mathbf{r}), \mu) + \mu|\phi(\mathbf{r})|^2$.

The first-order variation δE should be considered with the constraint

$$\delta N = 0, \quad N = \int d^3r |\phi(\mathbf{r})|^2. \quad (7)$$

As usual we broaden the class of allowable variation using the Lagrange procedure with multiplier μ ,

$$E_{eff} = E - \mu N, \quad \delta E_{eff} = 0.$$

The effective energy density contains one more variable μ : $\mathcal{E}_{eff} = \mathcal{E}_{eff}(\phi(\mathbf{r}), \nabla\phi(\mathbf{r}), \mu)$ and the functional E_{eff} coincides with the effective Hamiltonian (2). At $T=0$ the functional E is nothing but the free energy of the system, and E_{eff} is the thermodynamic potential $\Omega = F - \mu N$.

The energies E and E_{eff} can be considered functions of n_c through the functions

$$\phi(r) = \phi(r, n_c), \quad \delta\phi = \frac{d\phi(r, n_c)}{dn_c}, \quad (8)$$

which are solutions of Eq. (4). The first-order variations $\delta E(\phi, \delta\phi)$ and $\delta E_{eff}(\phi, \delta\phi, \mu)$ considering the functions (8) are nothing but the first derivatives of the functions $E(n_c)$ and $E_{eff}(n_c)$.

From Eqs. (2) and (4) one has

$$\frac{\delta E_{eff}}{\delta\phi(r)} = 0, \quad \frac{\partial \mathcal{E}_{eff}}{\partial \mu} = -\phi^2.$$

Taking into account Eq. (6) we obtain

$$\frac{\delta E}{\delta\phi(r)} = 2\mu\phi.$$

Using these equalities we have the following simple relations [21]:

$$\frac{dE}{dn_c} = \int d^3r \frac{\delta E}{\delta\phi(r)} \frac{d\phi}{dn_c} = \mu(n_c) \frac{dN}{dn_c}, \quad (9)$$

$$\frac{dE_{eff}}{dn_c} = \int d^3r \left(\frac{\delta E_{eff}}{\delta\phi(r)} \frac{d\phi}{dn_c} + \frac{\partial \mathcal{E}_{eff}}{\partial \mu} \frac{d\mu}{dn_c} \right) = -\frac{d\mu}{dn_c} N(n_c), \quad (10)$$

which relates the extremum points of $E(n_c)$ and $E_{eff}(n_c)$ with the extrema of $\mu(n_c)$ and $N(n_c)$. Note that the variations (8) do not satisfy the constraint (7), which holds only when $dN/dn_c = 0$. It means that (8) forms a broader class of variations and include those of them that do not conserve the number of particles.

Now we relate the behavior of $\mu(n_c)$ and $N(n_c)$ with the second-order variation $\delta^2 E_{eff}(\phi, \delta\phi, \nabla\delta\phi, \mu)$ taking it for the functions (8). It is related to $d^2 E_{eff}/dn_c^2$ through the equality

$$\begin{aligned} \frac{d^2 E_{eff}}{dn_c^2} &= \delta^2 E_{eff}(n_c) + \int \left(2 \frac{\partial^2 \mathcal{E}_{eff}}{\partial\phi\partial\mu} \frac{d\phi(r, n_c)}{dn_c} \frac{d\mu}{dn_c} \right. \\ &\quad \left. + \frac{\partial \mathcal{E}_{eff}}{\partial \mu} \frac{d^2 \mu}{dn_c^2} \right) d^3r. \end{aligned}$$

Taking into account that $\partial^2 \mathcal{E}_{eff}/\partial\phi\partial\mu = -2\phi$ we obtain the simple relation

$$\delta^2 E_{eff}(n_c) = \frac{d\mu(n_c)}{dn_c} \frac{dN}{dn_c}. \quad (11)$$

Equation (11) shows that there is a simple connection between $\delta^2 E_{eff}(n_c)$ (taken on a particular class of variation) and the behavior of $\mu(n_c)$ and $N(n_c)$. At the point of instability of the system, where $dN/dn_c = 0$, the second variation $\delta^2 E_{eff}(n_c)$ is equal to zero. As for the second variation of functional E , one can write the equality

$$\delta^2 E(n_c) = \frac{d\mu(n_c)}{dn_c} \frac{dN}{dn_c} + 2\mu(n_c) \int \left(\frac{d\phi(r, n_c)}{dn_c} \right)^2 d^3r,$$

which involves an additional term.

IV. RESULTS AND DISCUSSION

To compare the qualitative behavior and the properties near the collapse transition of the ${}^7\text{Li}$ system with those of the BF mixture, we have calculated the functions $\mu(n'_c)$, $N(n'_c)$, and $E(n'_c)$. These are shown in the left panels in Figs. 3 and 4, respectively. The right panels show the dependen-

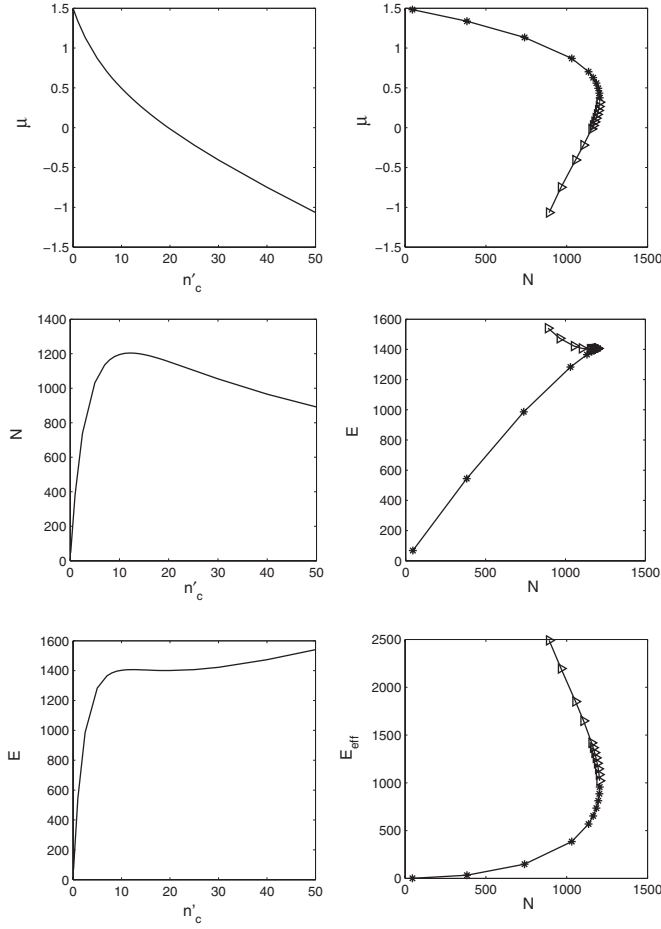


FIG. 3. ${}^7\text{Li}$ system behavior. Left panels: Chemical potential μ , number of particles N , and ground-state energy E as functions of rescaled central density n'_c . Right panels: Chemical potential μ , ground-state energy E , and effective ground-state energy E_{eff} as functions of number of particles, N . Functions μ , E , and E_{eff} are given in units of $\hbar\omega_{\perp}$.

cies of μ , E , and E_{eff} on the number of particles. The function $\mu(n'_c)$ for the ${}^7\text{Li}$ system (Fig. 3) gives no sign of a singularity near the collapse transition. The same can be said about $E_{\text{eff}}(n'_c)$ due to Eq. (10). However, there is a common feature in the behaviors of ${}^7\text{Li}$ and the BF mixture, namely, $N(n'_c)$ and $E(n'_c)$ exhibit local extrema. These extrema occur at $n'_{c0} \approx 12$ for the ${}^7\text{Li}$ system, and at $n'_{c0} \approx 23$ for the BF mixture. These values of central densities correspond to the onset of instabilities of the systems toward collapse. This feature was recognized in Ref. [21] and connected with the presence of a zero-mode fluctuation of density at this point.

The extremum for ${}^7\text{Li}$ is very wide in n'_c . The extrema of $N(n'_c)$ and $\mu(n'_c)$ can be related to those of $E(n'_c)$ and $E_{\text{eff}}(n'_c)$ due to Eqs. (9) and (10). The functions $\mu(N)$, $E(N)$, and $E_{\text{eff}}(N)$ have forms characteristic of multivalued behavior. In Figs. 3 and 4 curves with asterisks (triangles) are those parts of μ , E , and E_{eff} with $n'_c < n'_{c0}$ ($n'_c > n'_{c0}$).

At $n'_c \approx 23$ the behavior of the BF mixture is similar to that of the Bose gas with repulsion. Numerical results show [30,31] that the density profile $n(\mathbf{r})$ can be accurately described in the framework of the Thomas-Fermi (TF) approxi-

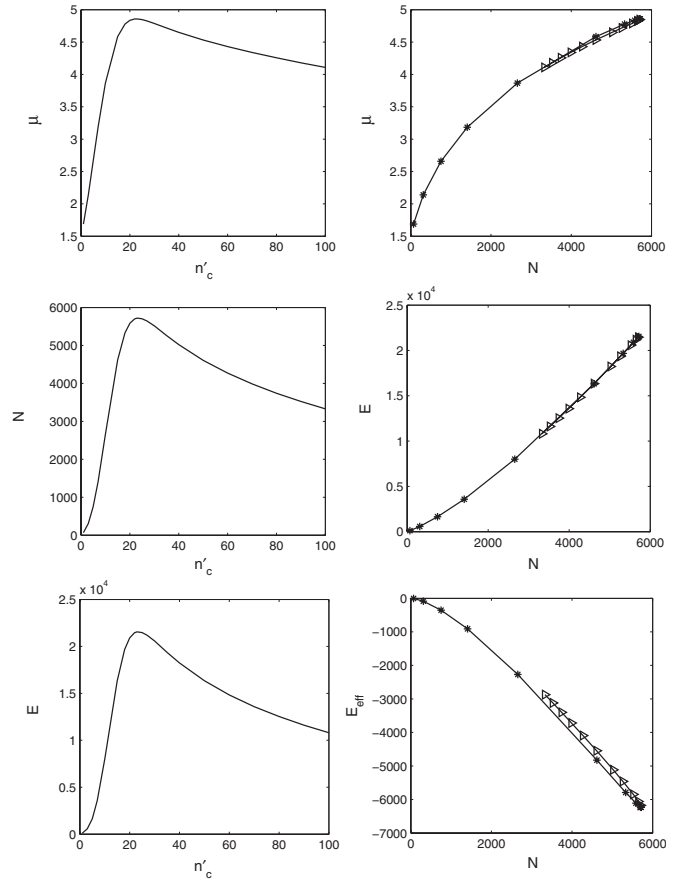


FIG. 4. BF mixture behavior. The left and right panels are the same as in Fig. 3.

mation up to $n'_c \sim 20$. In this region the positive zero-point energy and boson-boson repulsion energy [the first two terms in Eq. (1)] stabilize the system. However, if the central density grows too much, the kinetic energy and the boson-boson repulsion are no longer able to prevent the collapse of the gas. We see similar behavior of the system with attraction [25–27] and the BF mixture at $n'_c \geq 23$. The collapse is expected to occur when the number of particles in the condensate exceeds the critical value N_{Bc} . For the BF mixture, the curves $\mu(N)$, $E(N)$, and $E_{\text{eff}}(N)$ have a point of termination which corresponds to the maximum number of particles $N_{cr} \sim 6000$ (symmetric trap). Taking into account the asymmetry parameter $\lambda \approx 0.076$ we obtain $N_{Bc} \sim 10^5$, which is in good agreement with the experiment [28]. However, there is a controversy about the measurements of the critical number of bosons and the s -wave boson-fermion scattering length a_{BF} (see, for example, [9]). It should be noted that this controversy does not have any qualitative influence on the collapse scenario described in this paper and can change only the concrete values of the collapse parameters.

It is interesting to compare the behavior of μ , E , and E_{eff} for the ${}^7\text{Li}$ and BF systems as functions of N (see right panels of Figs. 3 and 4). One can see that the differences between the effective energies E_{eff} corresponding to the stable and unstable branches are large for the ${}^7\text{Li}$ and BF systems as functions of N system and very small for the BF system. A small difference in E_{eff} for the stable and unstable branches

arises solely from a very small difference in chemical potentials of these states and is not connected with computational accuracy. To understand this difference let us consider qualitatively the difference in the nature of the collapse transition in these systems. In the case of the ${}^7\text{Li}$ system where the interaction is attractive ($g_B < 0$), the gas tends to increase its density in the center of the trap in order to lower the interaction energy. This tendency is counteracted by the zero-point kinetic energy, which can stabilize the system. However, if the central density grows too much, the kinetic energy is no longer able to prevent the collapse of the gas. The collapse is expected to occur when the number of particles in the condensate exceeds some critical value. A similar picture holds for the BF mixture; however, in this case the effective two-particle interaction is repulsive [$g_{eff} > 0$ in (1)]. The collapse occurs due to the attractive three-particle interaction [last term in (1)] which is small in comparison with the two-particle one. It should be noted that this is a reason for the large difference between the critical numbers of bosons in these two systems: the critical number of Bose atoms in the Bose-Fermi mixture is about two orders larger than the critical number for the condensate with a purely attractive interaction, ${}^7\text{Li}$.

To find the disappearance of the local minimum of the functional E_{eff} which suggests an instability of the system, we explore the second-order variation $\delta^2 E_{eff}$. $\delta^2 E_{eff}$ changes sign from positive to negative at the point of instability. In terms of the steepest descent method, the absence of a local minimum implies that the convergence toward the local minimum falls through. The second-order variation $\delta^2 E_{eff}$ is given by the quadratic form of $\delta\phi$ and $\nabla\delta\phi$ and for the functional (2) has the form (for our purposes it is sufficient to consider only real $\delta\phi$)

$$\delta^2 E_{eff} = \int [(r^2 - 2\mu + 3u\phi^2 + 5v\phi^4)(\delta\phi)^2 + (\nabla\delta\phi)^2] d^3r.$$

Numerical calculations show that $\delta^2 E_{eff} > 0$ for the solution $\phi = \phi(r, n_c)$ if we take $\delta\phi(r)$ as a Gaussian, satisfying condition (7). This implies that the extremum of the Hamiltonian is a local minimum. In the case of the Bose condensate with attraction, the existence of a barrier around the metastable state was confirmed in Ref. [32] by extensive variational studies of the nearby wave function.

On the stable branch ($n'_c < n'_{c0}$) the value of $d\mu/dN$ is negative for the ${}^7\text{Li}$ system and is positive for the BF mixture. In a homogeneous one-component system ($N/V = \text{const}$) $d\mu/dN$ is proportional to $\partial\mu/\partial\rho = 1/(\rho^2\kappa_T)$ ($\rho = m|\phi|^2$ is the mass density and κ_T is the isothermal compressibility of the system) and the criterion of thermodynamic stability $\kappa_T > 0$ reduces to the requirement that $d\mu/dN$ should be positive. It is easily generalized for an inhomogeneous system which can be treated in the framework of the local density approximation. In the local density approximation the density profile $n(r) = |\phi|^2$ depends on N as a parameter and monotonically expands with increasing particle number. So the density $n(r, N)$ undergoes a steady increase: $dn(r, N)/dN > 0$ at any point r within a radius of external

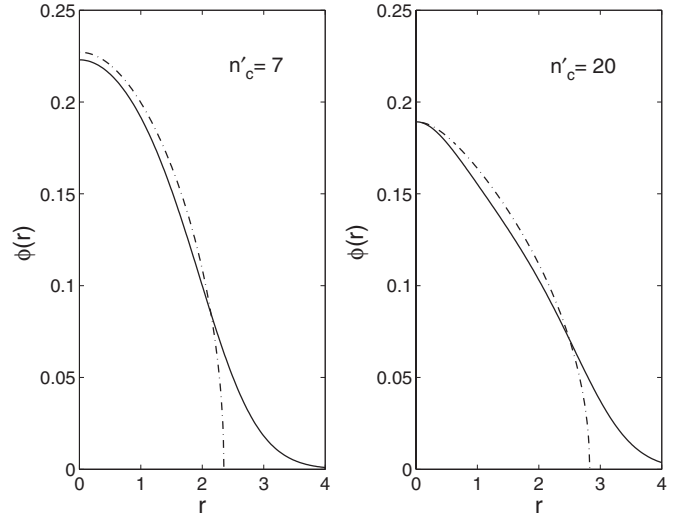


FIG. 5. Profile of the condensate wave function $\phi(r)$ found from the numeric solution of Eq. (4) (solid line) and the TF approximation Eq. (12) (dash-dotted line). The radius r is in units of a_{\perp} . Normalization of $\phi(r)$ is the same as in Fig. 1.

potential $V_{ext}(r)$. A density profile is determined from the equation

$$\mu_{loc}(n(r, N)) + V_{ext}(r) = \mu(N).$$

So in the local density approximation the criterion of local stability $\partial\mu_{loc}/\partial n > 0$ through the relation $d\mu/dN = (\partial\mu_{loc}/\partial n)(\partial n/\partial N)$ gives the stability condition $d\mu/dN > 0$ for an inhomogeneous system in an external potential.

The BF mixture at $7 \lesssim n'_c \lesssim 20$ safely can be considered in the TF approximation (Fig. 5) [31]. In this case the density profile has the form

$$\phi_{TF}^2(r) = n_{cr} \left(1 - \sqrt{1 - \frac{R^2 - r^2}{R_{cr}^2}} \right), \quad R^2 = 2\mu, \quad (12)$$

where $R_{cr}^2 = u^2/(4|v|)$, $n_{cr} = u/(2|v|)$, $R \leq R_{cr}$, and the profile is considered in the interval $0 \leq r \leq R$. The evolution of the profile corresponds to a monotonic expansion of the boson cloud with increasing number of bosons. That is why the stable branch of the BF mixture corresponds to the positive value of $d\mu/dN$.

In contrast, the TF approximation is not applicable for a ${}^7\text{Li}$ system for which the sign of $dn(r, N)/dN$ depends on r . At $r \lesssim a_{\perp}$ one observes a rapid growth of the condensate density, while at $r > a_{\perp}$ a strong depletion of the condensate density occurs. The negative value of $d\mu/dN < 0$ in this case can be explained by the following. Using Eq. (11), the derivative $d\mu/dN$ in terms of the central density can be rewritten in the form $d\mu/dN = (d\mu/dn_c)(dn_c/dN) = \delta^2 E_{eff}(n_c)/(dN/dn_c)^2$. So the value of $d\mu/dN$ gives, at most, information about a particular class of variations (8) of the functional (2), which do not satisfy (7). For variations satisfying condition (7) we have $\delta^2 E_{eff} > 0$. So the solution $\phi(r, n_c)$ provides the local minimum of E_{eff} on those functions which preserve the normalization. The stability of the system is explained by the dynamics, namely, for collapse of

the system to occur, fluctuations with $\delta N \neq 0$ should exist, which energetically are not favorable at the temperatures under discussion.

In conclusion, our analysis of the stability of a K-Rb Fermi-Bose mixture on the basis of an effective Bose Hamiltonian shows clear resemblance to the behavior of the ^7Li system. There is a value of the central density at which small variations of density profile conserve the number of particles $\delta N=0$ and the second variation $\delta^2 E_{eff}$ changes sign. The value we determined for N_{Bc} is in good accordance with experiment. The points of extremum of the functions $\mu(n_c)$ and $N(n_c)$ are related to the first and second derivatives of functions $E(n_c)$ and $E_{eff}(n_c)$. On the other hand, as discussed above, the collapse in the BF mixture occurs due to the attractive three-particle interaction, and the magnitude of the coefficient of this interaction is small in comparison with that of the two-particle one. As a result, the critical number of Bose atoms in a Bose-Fermi mixture is about two orders

larger than the critical number for the condensate with a purely attractive interaction, ^7Li .

We note that the investigation of the actual dynamics after the system has been driven into the unstable region would require a description that goes beyond the stationary scenario of Eq. (4), in similar fashion to what happens during the collapse of a single Bose-Einstein condensate with attractive interaction [26,27]. Here we will not discuss these aspects, since we are concerned with the determination of the critical values for the onset of instability. Another interesting issue concerns the relevance of finite-temperature effects, which are not included in the present treatment.

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