Binary mixture of a BEC and a Fermi Gas: dependence on effective s-wave interaction and number of particles. Stability conditions.

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We study the behaviour of a two component mixture of bosons and fermions at zero temperature. We use the Thomas-Fermi approximation and an effective s-wave contact interaction to calculate the density profiles of both species and investigate the dependence on the scattering lengths. We observe that the bosons are concentrated in the center of the trap, while the fermions are pushed out of the center, as the repulsive interaction is increased. We also analyze the dependence on the particle number and find that the bosons are squeezed in the center more and more, as the number of fermions or the strength of the repulsive boson-fermion interaction is increased. Finally, we discuss the collapse of the system induced by attractive interactions.

1 Introduction.

The mixtures of bosons and fermions trapped at ultralow temperatures have been studied by a series of experiments [1, 2], achieving very interesting results for the behaviour of the system.

We intend here to study the behaviour of the simplest mixture, where one component consists of bosons and the other of fermions, taking into account the boson-fermion interaction and the number of particles in the system. Our starting point is the theoretical model, discussed in section 2. There, we sketch the model, discuss the various approximations made, and explain how to work with the energy density functional.

The third section deals with our results about the behaviour of the mixture depending on the different physical parameters.

In section 4, we report on the stability of the system, give stability conditions and discuss their meaning.

Finally, we state our conclusions in section 5.

2 Energy functional of a binary boson-fermion mixture.

As we are dealing with a many-body system, some approximations are required to make the problem solvable. We use the mean-field approximation, where the total wave function is just the direct product of the single particle wave functions, symmetrizing the product for bosons and antisymmetrizing the product for fermions. The original interactions between the atoms cannot be used in the hamiltonian of the mean-field approximation, so we take an Effective Contact Interaction (ECI) based on the two-body system. We suppose that our system is dilute.

2.1 *Effective Contact Interaction and hamiltonian.*

The ECI is an effective interaction of zero range that replaces the original interaction in the hamiltonian so that it is suited for a mean-field calculation. It is written as a sum over all partial waves. For our purpose the first term, called s-wave contribution, is enough [3]:

$$\mathbf{v}^{eff} = \frac{4\pi}{2\mu} a_0 \, \delta^{(3)}(\vec{\mathbf{r}}). \qquad (1)$$

Here μ is the reduced mass of the two-body system. The strength of the interaction is given by the scattering length, a_0.

We investigate the ground state of a mixture of bosons and fermions, trapped in an external potential at T=0K. The hamiltonian contains the operators of the kinetic energy, the interaction between bosons, between fermions and between bosons and fermions, and an external potential, $\mathbf{U}$:

$$\mathbf{H} = \mathbf{U} + \mathbf{H_{int}}, \tag{2}$$

where

$$\begin{aligned}\mathbf{H_{int}} &= \frac{1}{2m}\sum_i \vec{\mathbf{p}}^2 \\ &+ \frac{4\pi}{m}\Bigg(a_b \sum_{i,j>i} \delta^{(3)}\left(\vec{\mathbf{r}}_{ij}\right)\ \Pi_{bi}\Pi_{bj} \\ &+ a_f \sum_{i,j>i} \delta^{(3)}\left(\vec{\mathbf{r}}_{ij}\right)\ \Pi_{fi}\Pi_{fj} \\ &+ a_{bf} \sum_{i,j>i} \delta^{(3)}(\vec{\mathbf{r}}_{ij})(\Pi_{bi}\Pi_{fj} + \Pi_{fi}\Pi_{bj})\Bigg).\end{aligned} \tag{3}$$

We sum both indices over the total number of particles. We use just the first order of the partial wave expansion, i.e. s-wave interaction. The projector Π_{bi} extracts the particle i only when it is a boson and Π_{fi} when it is a fermion. Note that each interaction has its scattering length, labeled with b for boson-boson, f for fermion-fermion and bf for boson-fermion.

For the trapping potential, with the same notation,

$$\mathbf{U} = \sum_i \left(U_b\left(\vec{x}_i\right)\Pi_{bi} + U_f\left(\vec{x}_i\right)\Pi_{fi}\right), \tag{4}$$

where, to make it simple, we assume a harmonic oscillator with spherical symmetry

$$U(\vec{x}) = \frac{m\omega^2}{2}\vec{x}^2 = \frac{1}{2m\ell^4}\vec{x}^2. \tag{5}$$

2.2 Energy density of the homogeneus gas.

The next step is to calculate the energy density. First we need it for a simple case: homogeneous gas in a volume V.

We start by defining the state, and then we can evaluate the energy with it. The total state is the direct product of the boson and the fermion states,

$$|\Psi\rangle = |\Psi_b\rangle \otimes |\Psi_f\rangle. \tag{6}$$

The boson state is the direct product of the single particle states, one for each boson. We suppose the bosons to be in a Bose-Einstein Condensate (BEC), so all of them are in the same state (and we do not need to symmetrize because it is already symmetric):

$$|\Psi_b\rangle = |\phi\rangle \otimes \cdots \otimes |\phi\rangle, \tag{7}$$

$$\langle\vec{x}|\phi\rangle = \frac{1}{\sqrt{V}}, \tag{8}$$

The fermions cannot be in the same state, and we need to antisymmetrize. For a homogeneous gas, we use plane waves of momentum $\vec{k}_i$:

$$|\Psi_f\rangle = \mathcal{A}\prod_{i}^{N_f}{}_{\otimes} |\vec{k}_i\rangle, \tag{9}$$

$$\langle\vec{x}|\vec{k}_i\rangle = \frac{1}{\sqrt{V}}e^{i\vec{k}_i\cdot\vec{x}}. \tag{10}$$

Where $\mathcal{A}$ is the operator that makes the antisymmetrization. With this state, we can calculate the expectation value of the energy density of the homogeneous system

$$\mathcal{E}_{hom} = \frac{\langle\Psi|\mathbf{H}_{int}|\Psi\rangle}{V}. \tag{11}$$

By doing so, we obtain contributions from (in the order they appear in the equation): the kinetic energy for fermions, the boson-boson interaction and the boson-fermion interaction:

$$\mathcal{E}_{hom} = \frac{3^{5/3}\pi^{4/3}}{5 2^{1/3} m}n_f^{5/3} + \frac{2\pi}{m}a_b n_b^2 + \frac{4\pi}{m}a_{bf}n_b n_f, \tag{12}$$

where n_b and n_f are the boson and fermion densities respectively.

Note that kinetic energy for bosons is zero due to the constant wave function (8) and s-wave fermion-fermion interaction is also zero, due to the Pauli Principle.

2.3 Thomas-Fermi approximation for trapped gas.

The problem with the inhomogeneous system is that for a potential $\mathbf{U}(\vec{x})$ that depends on the position, the single particle states are no longer plane waves, and a Schrödinger equation including $\mathbf{U}(\vec{x})$ and the mean field created by the two body interaction has to be solved. Therefore, we use an approximation.

In the Thomas-Fermi approximation one calculates the energy density of the homogeneous system, and then assumes that the energy density for the inhomogeneous case is locally the same as in the homogeneous one. Two more terms, the interaction of the bosons and the interaction of the fermions with the trap, are added. Now n_b and n_f are functions of $\vec{x}$:

$$\begin{aligned}\mathcal{E}[n_b, n_f] = & \frac{3^{5/3}\pi^{4/3}}{52^{1/3}m} n_f^{5/3}(\vec{x}) \\ & + \frac{2\pi}{m} a_b n_b^2(\vec{x}) \\ & + \frac{4\pi}{m} a_{bf} n_b(\vec{x}) n_f(\vec{x}) \\ & + \frac{m\omega^2}{2} x^2 n_b(\vec{x}) + \frac{m\omega^2}{2} x^2 n_f(\vec{x}).\end{aligned} \tag{13}$$

This is a very useful method, but restricts our study only to repulsive boson-boson interactions. It cannot be used for vanishing or negative a_b, because we neglet the kinetic energy of the bosons in this approximation, so it cannot balance a possible attraction between bosons.

2.4 Functional variation: searching for extremums. Lagrange multipliers.

We want to find the ground state with the constraint that the number of particles in the trap is fixed. We can do that by using the Lagrange multipliers μ_b and μ_f (well known as chemical potentials), i.e., defining the Legendre transformed functional

$$\mathcal{F}[n_b, n_f] = \mathcal{E}[n_b, n_f] - \mu_b n_b(\vec{x}) - \mu_f n_f(\vec{x}), \tag{14}$$

and minimize the total energy

$$F[n_b, n_f] = \int d^3x \; \mathcal{F}[n_b, n_f]. \tag{15}$$

It is well known (from the Euler-Lagrange equations) that it is enough to require the first derivative of $\mathcal{F}[n_b, n_f]$ to be equal to zero for finding an extremum:

$$\frac{\partial \mathcal{F}[n_b, n_f]}{\partial n_b} = 0, \quad \frac{\partial \mathcal{F}[n_b, n_f]}{\partial n_f} = 0. \tag{16}$$

This gives us two equations

$$\begin{aligned}&\frac{4\pi}{m} a_b n_b(\vec{x}) + \frac{4\pi}{m} a_{bf} n_f(\vec{x}) + m\omega^2 \frac{x^2}{2} - \mu_b = 0 \\ &\frac{4\pi}{m} a_{bf} n_b(\vec{x}) + \frac{3^{\frac{2}{3}}\pi^{\frac{4}{3}}}{m} n_f^{\frac{2}{3}}(\vec{x}) + m\omega^2 \frac{x^2}{2} - \mu_f = 0.\end{aligned} \tag{17}$$

From these two conditions, we find certain values for the densities (one at each position $\vec{x}$ in the trap). Note that we have to check whether it is a minumum, maximum or saddle point.

3 Influence of scattering lengths and number of particles.

Using our results, we can determine the density for bosons and fermions at each point of the trap. We assume spherical symmetry, so we work with the radial coordinate only, and obtain the density profiles for different values of the scattering length and of the number of particles, bosons as well as fermions. We cannot plot here all the results, so we report the behaviour of the profiles as a function of the boson-fermion scattering length, and the dependence on the number of particles.

We can see three different behaviours depending on a_{bf} (see figure 1):

- $a_{bf} < 0$: For attractive interactions between bosons and fermions, the fermion density profile shows a significant increase in the overlap region.
- $a_{bf} = 0$: In this case, as we would expect, since bosons and fermions cannot interact with each other, they just show the density profile as if each one of them were alone.
- $a_{bf} > 0$: As we make the repulsive interaction stronger, we can see that the bosons form a core, and the fermions are expelled out of the center, surrounding the core.
- $a_{bf} = a_b$: This is a very special case, because we can see that the bosons show their usual behaviour, but fermions show a constant profile until the boson density is almost zero, going then to zero. This happens independently of the number of particles.

The dependence on a_b is not relevant at all, because it only causes little differences that do not change the generic behaviour of the system.

About the dependence on the number of particles, there is one interesting fact: as the ratio of boson and fermion number is decreased, we can see that the bosons are a little bit more concentrated in the center, for the same scattering lenghts. As we increase the repulsive interaction between bosons and fermions, they are even more confined in the center of the trap,

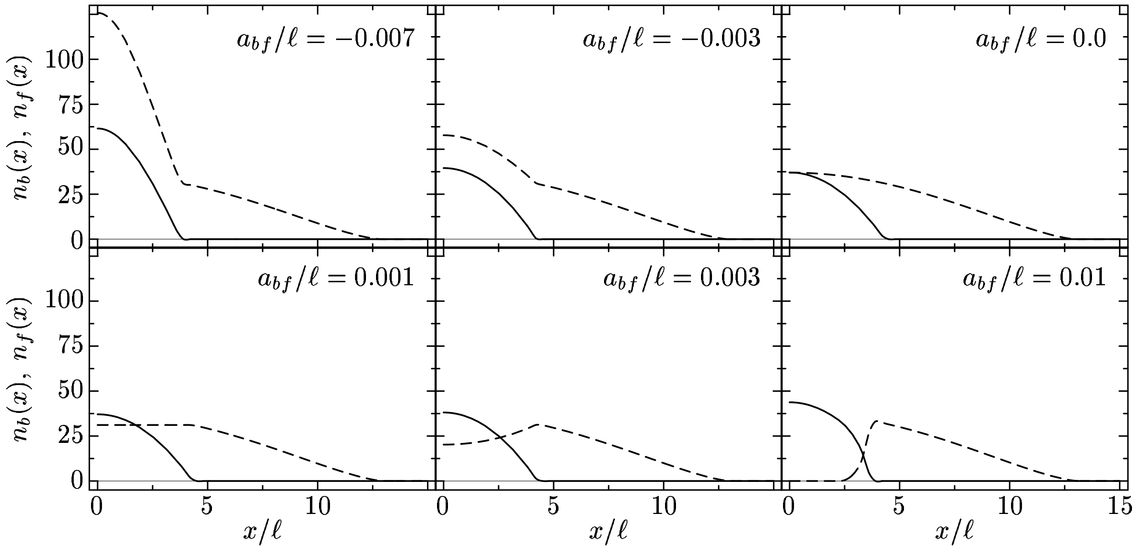

Fig. 1: *Radial density profiles of a trapped boson-fermion mixture with* $N_f = N_b = 10^5$ *particles and* $a_b/\ell = 0.001$ *for different strength* a_{bf}/ℓ *of the boson-fermion interaction. Solid lines depict* $n_b(x)$ *scaled down by a factor* $1/20$*, dashed lines show* $n_f(x)$*.*

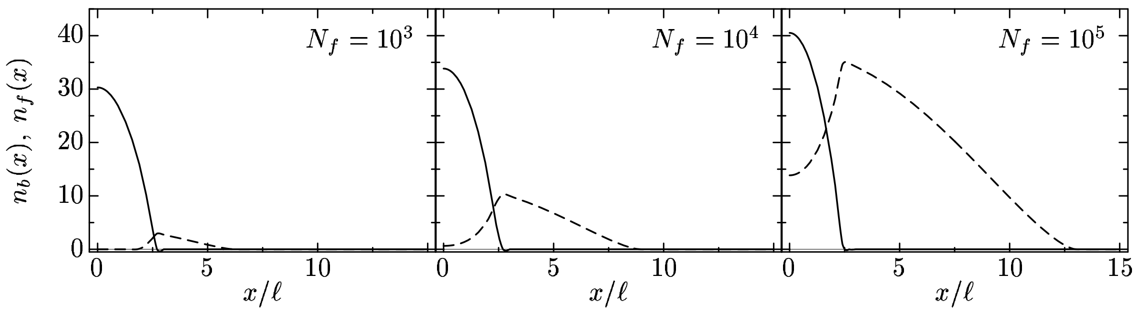

Fig. 2: *Radial density profiles of a trapped boson-fermion mixture with* $N_b = 10^4$ *particles,* $a_b/\ell = 0.001$ *and* $a_{bf}/\ell = 0.008$*, for different fermion particle number* N_f*. Solid lines depict* $n_b(x)$*, dashed lines show* $n_f(x)$ *scaled by a factor* 10*.*

being squeezed. This growth continues until a certain maximal density is reached. These two behaviours can be seen in figures 1 and 2.

4 Mean-Field Collapse.

Once we have seen how the system behaves, it is interesting to investigate its stability. As usual, the stability condition is given by the second derivatives, taken at the equilibrium values for the densities. Since we are dealing with a two variable function, we need to construct the hessian matrix:

$$D(n_b, n_f) = \begin{pmatrix} \frac{\partial^2 \mathcal{F}[n_b,n_f]}{\partial n_b^2} & \frac{\partial^2 \mathcal{F}[n_b,n_f]}{\partial n_b \partial n_f} \\ \frac{\partial^2 \mathcal{F}[n_b,n_f]}{\partial n_f \partial n_b} & \frac{\partial^2 \mathcal{F}[n_b,n_f]}{\partial n_f^2} \end{pmatrix}. \quad (18)$$

Looking at the determinant of the hessian matrix, we can find out the stability against the separation of the two components, as well as the stability against collapse. We are dealing with the second one.

A positive value of the hessian determinant is associated with a minimum or maximum, while the saddle points are characterized by a negative value of it. If we inspect the determinant equal zero, we can determine the point where the system starts to be unstable. We solve

$$det\,(D(n_b, n_f)) = -4\pi^2 a_{bf}^2 + \frac{2^{2/3} a_b \pi^{7/3}}{3^{1/3} n_f^{1/3}} = 0, \quad (19)$$

and we achieve the condition

$$n_f^{lim} = \frac{\pi\ a_b^3}{48\ a_{bf}^6}. \quad (20)$$

Notice that we cannot have negative boson-boson interaction, because it would give a negative value for the fermion density. For $a_b < 0$ we must include the positive kinetic energy of the bosons that is neglected in the simple Thomas-Fermi approximation.

The maximum density of fermions n_f^{lim} depends strongly on the boson-fermion interaction, but not on the chemical potentials or the boson density. It only depends on the scattering lengths.

For negative a_{bf} the system collapses, if the fermion density is larger than n_f^{lim} in the center of the trap, where the maximum is located. In the presence of a strong enough attractive interaction between bosons and fermions, the system undergoes a collective collapse towards a high density configuration. This is due to the attractive mean field generated by the interaction: at low densities, the kinetic contribution can compensate this attraction, but there exists a critical density, due to the fermions, as we see in equation (20). Then, if we overcome this critical density, the kinetic contribution cannot compensate the attraction, and the system collapses.

This behaviour has been observed before in a Bose gas and also for fermionic gases [3, 4], and now we report also the collapse in boson-fermion mixtures [5].

5 Conclusions.

We have studied the behaviour of a binary mixture of bosons and fermions in a parabolic trap, with spherical symmetry. We have used the mean field approximation for the trapped mixture and the Thomas-Fermi approximation for the density functional. The ground state was found by minimization of the energy.

We have studied the dependence on the strengths of the boson-boson and the boson-fermion interaction. It turned out that the boson-fermion scattering length is decisive for the behaviour of the system, and there is a little dependence on the boson scattering length. Different density profiles have been calculated, depending on a_b and a_{bf}, and on the number of particles.

Finally, we have also presented a condition for the stability of the system against mean-field collapse, and discussed its meaning.

This theoretical work can be taken as a starting point for later and deeper studies of the stability of the system, or to add the kinetic energy of the bosons or the next contribution in the partial wave expansion of the interaction.

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