

Density probabilities of a Bose-Fermi mixture in 1D double well potential

J Nisperuza, J P Rubio and R Avella

Fundación Universitaria los Libertadores, Faculty of Engineering and Basic Sciences, Department of Aeronautical Engineering, A. A. 75087 Bogotá, Colombia

E-mail: rgavellas@libertadores.edu.co

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Abstract

We use the two mode approximation for a interacting one-dimensional spinless soft core bosons and one half spin fermions in a double-well potential with a large central barrier. We include all the on-site boson-boson, fermion-fermion and boson-fermion repulsive contact potential represented by delta-function and considered bosonic and fermionic isotopes of ytterbium (Yb) $^{170}$Yb and $^{171}$Yb respectively. By means of this approximation, we find that in the regime $\lambda_{BF} > \lambda_{BB}$ give rise to an immiscible phase and in the regime $\lambda_{BB} \geq \lambda_{BF}$ give rise to a miscible phase, that is characterized by a temporal overlap of the bosonic and fermionic probability densities. We also report that due to the Bose-Fermi interaction, the system presents an apparent destruction of the collapse-revival oscillation of boson density probability at least in the ranges investigated.

1. Introduction

In the field of ultracold gases, there are perfectly controllable physical parameters [1] and many interesting quasi-one-dimension experiments have been realized in harmonic [2, 3], double-well [4, 5], periodic [6], and bichromatic [7] optical-lattice traps. The atoms in these experiments can be confined to different lattice sites and if two atomic species are considered, both the effective intra and inter component interactions can be tuned with great precision via the magnetic Feshbach resonance or confinement induced resonance [8–10].

Advances in laser technology allow experimental realization in one, two and three dimensions [11–13] of a single double-well and an array of many copies of the double well system, know as dimers. In these systems the tunneling between the local double-well potentials is negligible, compared to tunneling inside the double well potential and each site have a well-defined and almost identical quantum state [11, 14, 15]. These systems allow to study a very important concepts in quantum information theory, the notion of state as a linear superposition of classical' states [16], where the system can reside in a superposition of two or more degenerate states [17–19] and quantum tunneling, that have applications in solid-state devices, solar cells and microscopes [20].

Particular interesting phenomena that is present in systems of interacting atoms in double-well potentials are bosonic Josephson junction [4, 21, 22], squeezing and entanglement of matter waves [23, 24], matter wave interference [25, 26], and exact many-body quantum dynamic in one dimension. In quantum information processing, this systems has been used as a way to make quantum logic gates for ultracold neutral atoms confined in optical lattices [27].

One dimensional double well potential has been used to study both theoretically [28, 29] and experimentally [4, 30] the simplest case of Josephson effect using $^4$He and a superfluid Fermi gas with $^3$He [31–33], as well as the spontaneous symmetry breaking of a superfluid Bose–Fermi mixture [34].

The influence of fermions onto bosons has been investigated in different mixture, for example in a mixture of $^4$He $-$ $^3$He has been reported the observation of simultaneous quantum degeneracy [35, 36]. In mixture of $^{87}$Rb $-$ $^{40}$K [37, 38] has been found a pronounced asymmetry between strong repulsion and strong attraction [39]. Phase separation was found in a mixture of $^{41}$K $-$ $^6$Li [40]. A localized phase of ultracold bosonic quantum
gases of $^{87}$Rb induced by a small contribution of $^{40}$K fermionic atoms was observed in [41]. Attractive and repulsive Bose-Fermi interaction was study in a system composed by $^{170}$Yb $- 173$Yb (attractive) and $^{174}$Yb $- 171$Yb (Repulsive) [42]. Other Bose-Fermi mixtures that have been experimentally reported are $^7$Li $- ^6$Li [43], $^{39}$K $- ^{40}$K and $^{41}$K $- ^{40}$K [44].

Theoretically, numerous studies have been carried out to analyze the Bose-Fermi mixture (BFM). For example, the collapse in attractive mixtures has been studied numerically [45–48], semi-analytically [49, 50], or in the Thomas-Fermi approximation [51]. The Bose-Fermi interaction induce the pairing of fermions analogous to the formation of Cooper pairs in the BCS model [52–54] and the boson phase transition from the Mott insulator to super fluid [55–57]. Other studies indicate an asymmetry between the attraction and repulsion cases [58, 59], as well as phase separation, spatial modulation [60], supersolid phase and charge density wave [61].

There is a fine line separating properties of bosons and fermions, for example, in the Bose-Fermi mapping theorem for hard core particles [62] realized experimentally for first time in [63], the ground-state is highly degenerate in a limit of infinitely strong boson–fermion repulsions [64] due to the freedom of fixing the sign of many-body wave function under the exchange of a boson with a fermion [65–67]. To find a duality relation in systems composed by spin-1/2 fermions interacting with two-component bosons [68] was used the Cheon-Shigehara mapping.

The most general one-to-one mapping between bosons and fermions in one dimension was found by Valiente. This general mapping not restricted to pairwise forces, is valid for arbitrary single-particle dispersion, including non-relativistic, relativistic, continuum limits of lattice hamiltonians and can also be applied to any internal structure and spin [69].

This leaves the possibility of studying the transmutation of bosons into fermions and vice versa in a system of spinless bosons in the soft-core limit and spin one-half fermions, that is studied in this paper. In this work we focus on a repulsive interacting Bose-Fermi mixture of a few particles confined in a 1D double well potential at zero temperature and considering that both species have the same mass.

The paper is organized as follows. The model used to describe a mixture of bosonic and fermionic atoms is introduced in section 2. In section 3, we vary the inter and intra species interactions to study the temporal evolution of probability densities and finally in section 4 we make remarks.

2. Physical model

Due to the experimental possibility of confining quantum gases in an array of many copies of the double well system, where the tunneling between the local double-well potentials is negligible compared to tunneling inside the double well potential, we considered the study in one of these potentials. In our study we consider the experimental setup used in [70], where the radial separation of the potential wells is $d = 13 \mu$m, a trap depth of $h \times 4.7KHz$ and we considered the width of each well of $a = 6 \mu$m. This potential confines bosonic and fermionic isotopes of ytterbium(Yb) $^{170}$Yb and $^{171}$Yb respectively and we considered that the fermions isotopes have two internal degrees of freedom, allowing a density of fermions per site of $0 \leq \rho_F \leq 2$; the maximum number of scalar bosons on the ‘soft-core’ boundary per site, is $N_B^{\text{max}} = 2$. This value is due to the fact that in several reports has been found that the qualitative physical properties obtained for $N_B^{\text{max}} = 2$ do not change when $N_B^{\text{max}}$ is increased [71, 72].

The study of this system will be carried out by means of the two-mode model in a double well potential using the lowest symmetric and antisymmetric wavefunctions. This model produce the best agreement with experimental results and numerical solutions of the time-dependent Gross–Pitaevskii equation in 1D and 3D [73–75].

The general wave function in the basis of the two states that is noncommittal as to which particle is in which state and provide an accurate formulation [22, 29, 76] can be expressed as

$$\Psi^{BF}(x_1, x_2) = A [\psi_1^s(x_1) \psi_2^a(x_2) \pm \psi_1^a(x_1) \psi_2^s(x_2)],$$

where $A$ is the normalization constant, plus sign is for symmetric (Bosons) a minus sign is for antisymmetric (Fermions) functions. These wave functions are linear combinations of one particle states $\psi_i^s(x_i)$, where superscript $i$ indicate the first symmetric (s) or antisymmetric (a) state. The wave function $\psi$ satisfy the orthonormal condition

$$\int \psi_i(x) \psi_j(x) dx = \delta_{ij},$$
With this in mind we construct the two particles wave function for bosons at time $t$

$$
\Psi_{B,L}^B(x_1, x_2, t) = \frac{e^{-iE_1t/\hbar}}{\sqrt{2}} \left[ e^{i\Omega_1t} \psi_{1}^B(x_1) \psi_{1}^B(x_2) + \psi_{1}^B(x_1) \psi_{1}^B(x_2) \right] + \frac{e^{-iE_2t/\hbar}}{\sqrt{2}} \left[ e^{i\Omega_2t} \psi_{1}^B(x_1) \psi_{1}^B(x_2) - \psi_{1}^B(x_1) \psi_{1}^B(x_2) \right],
$$

(2)

where $\Omega_i = \frac{E_i - E_J}{\hbar}$ is the Bohr frequency and different one particle states were considered. It was also taken into account that at $t = 0$, the two particles are on right ($\Psi_{B,L}^B(x_1, x_2, t)$) or left ($\Psi_{B,L}^B(x_1, x_2, t)$) sides of double well potential.

The orbital wave function of two fermions with opposite spin in a double-well potential is decomposed into a singlet and three triplet states with respect to the pseudospin defined by the double-well potential at $t = 0$. Therefore for this study, we are going to choose singlet state as our initial state

$$
\Psi_{B,L}^F(x_1, x_2, t) = \pm \sqrt{\frac{1}{2}} \left[ \psi_{1}^F(x_1) \psi_{1}^F(x_2) + \psi_{1}^F(x_1) \psi_{1}^F(x_2) \right]
$$

(3)

From the two particles wave function 2 we get the probability density for a system of two bosonic particles

$$
|\Psi_{B,L}^B(x_1, x_2, t)|^2 = \left\{ \frac{1}{2} |\psi_{1}^B(x_1)|^2 \pm \frac{1}{2} |\psi_{1}^B(x_2)|^2 \pm \cos [\Omega_1 t \psi_{1}^B(x_1) \psi_{1}^B(x_2)] \right\}
$$

(4)

and from the two particle wave function 3 we get the probability density for fermions. From these equations we configure our system, considering that bosons and fermions are on the right side.

In this way the two-particle Hamiltonian for the system in one dimension is

$$
\hat{H}_{BF} = \hat{H}_{B}^{\text{iso}}(x_1, x_2) + \hat{H}_{F}^{\text{iso}}(x_1, x_2) + \lambda_{BF} \delta(x_1 - x_2),
$$

(5)

where

$$
\hat{H}_{B}^{\text{iso}}(x_1, x_2) = -\frac{\hbar^2}{2m_B} \frac{d^2}{dx_1^2} + V(x_1) - \frac{\hbar^2}{2m_B} \frac{d^2}{dx_2^2} + V(x_2) + \lambda_{BB} \delta(x_1 - x_2),
$$

(6)

and

$$
\hat{H}_{F}^{\text{iso}}(x_1, x_2) = -\frac{\hbar^2}{2m_F} \frac{d^2}{dx_1^2} + V(x_1) - \frac{\hbar^2}{2m_F} \frac{d^2}{dx_2^2} + V(x_2) + \lambda_{FF} \delta(x_1 - x_2),
$$

(7)

where $m_B$ is the mass of $^{170}$Yb ($^{171}$Yb), $V(x)$ is the external confinement potential that is the same for both species. The repulsive contact potential between bosons (fermions) is represented by delta-function potential $\lambda_{BB(BF)} \delta(x_1 - x_2)$, where $\lambda_{BB(BF)} > 0$ for a repulsive interaction and $\lambda_{BB} \delta(x_1 - x_2)$ is the repulsive interaction between two ultracold neutral atoms of different statistic. We consider that the perturbation is sufficiently small, therefore is considered that the amplitudes of other states do not mix [77], so we use the projection of the wave function onto two states that is used in the study of BEC in a double-well potential and in the investigation of Fermi super fluid [78]. The different contributions of these terms can be obtained in a general way from

$$
\lambda \left\langle \Psi_{j}(x_1, x_2) \right| \delta(x_1 - x_2) \left| \Psi_{k\lambda}(x_1, x_2) \right\rangle = \lambda \int \Psi_{j*}(x_1, x_2) \Psi_{k\lambda}(x_1, x_2) \delta(x_1 - x_2) dx_1 dx_2,
$$

(8)

where $\Psi_{j}(x_1, x_2)$ is the two particle wave function and $\Psi_{k\lambda}(x_1, x_2)$ is its complex conjugate. Because we are working on a two-mode approximation, the subscripts only run from 1 to 2 and to avoid possible repetitions, the ordering in the states of two particles is $i \geq j$ and $k \geq l$. Finally we adopt our units of length, $l = 1 \mu$, energy $E_k = E/\xi$ with $\xi = 10^{-31}$ and time $\tau = \hbar/\xi$ [79]. Henceforth, we will measure lengths, energies and time in these units.

3. Bose-Fermi probabilities

We consider that the initial state of our system is configured, with two spinless soft core bosons and two one half spin fermions in the right side of the double well potential. This configuration is mainly due to the fact that we want to explore the conditions for which is generated the transmutation of bosons into fermions and vice versa, for which the two species are had under the same initial configuration and we varied the boson-boson $\lambda_{BB}$ fermion-fermion $\lambda_{FF}$ and boson-fermion $\lambda_{BF}$ repulsive contact interaction terms. The immiscible and miscible phases for our system is found by means of the probability of finding each species at a point x, at time t. Therefore, an overlap of the probability density of each species indicates that both wave functions occupy the same spatial regions [80].
Since we are working with a two mode model, the inter and intra particle interaction, must be small enough to prevent the amplitudes of the two lower energy modes mixing with other states. With this consideration, a sweep was initially made through the interaction parameters and we found that for orders of magnitude smaller than $10^{-5}$ the two probability densities are the same until dimensionless time $\tau \approx 1363.97$.

Figure 1. Time evolution of Bose ($P_{BB}(\tau)$)–Fermi ($P_{FF}(\tau)$) density probabilities on the right side of the double well, as a function of the dimensionless parameter of time $\tau$.

(a) Bose (red squares) and Fermi (blue circles) density probabilities for: $\lambda_{BB} = 1 \times 10^{-5}$, $\lambda_{FF} = 1 \times 10^{-5}$ and $\lambda_{BF} = 1 \times 10^{-5}$. The two probability densities are the same until dimensionless time $\tau \approx 1363.97$.

(b) Bose (red squares) and Fermi (blue circles) density probabilities for: $\lambda_{BB} = 1 \times 10^{-5}$, $\lambda_{FF} = 3 \times 10^{-5}$ and $\lambda_{BF} = 1 \times 10^{-5}$. The two probability densities are the same until dimensionless time $\tau \approx 905.90$.

(c) Bose (red squares) and Fermi (blue circles) density probabilities for: $\lambda_{BB} = 7 \times 10^{-5}$, $\lambda_{FF} = 1 \times 10^{-5}$ and $\lambda_{BF} = 5 \times 10^{-5}$. The two probability densities are the same until dimensionless time $\tau \approx 4090.97$. 

Since we are working with a two mode model, the inter and intra particle interaction, must be small enough to prevent the amplitudes of the two lower energy modes mixing with other states. With this consideration, a sweep was initially made through the interaction parameters and we found that for orders of magnitude smaller than $10^{-5}$ the two probability densities are the same, producing a self-trapping because the particles do not have...
enough energy to cross the potential barrier resulting in complete miscibility of the bosonic and fermionic probability densities. For orders of magnitude of $10^{-5}$ we found that although the initial state of the two species is considered on the right side of the double potential well, the behavior of the probability density of bosons and fermions is completely different in the regime of $\lambda_{BF} > \lambda_{BB}$, where arise an immiscible phase characterized by almost perfectly separated fermionic and bosonic probability densities. In the regime of $\lambda_{BB} \geq \lambda_{BF}$ densities of bosons and fermions are overlapping as a function of time, as see in figure 1 where $P_{BB}^{BF}(\tau)$ represents the probability density of finding the two bosonic (fermionic) particles on the right side of the double well, as a function of the dimensionless parameter of time $\tau$. Theoretically the time independent miscible phase, was studied in [81, 82], considering a Bose Fermi mixture in an one-dimensional lattice with an imposed harmonic oscillator.

In our research we found a complete miscibility of bosons (red squares) and fermions (blue circles) probability densities until dimensionless time $\tau \approx 1363.97$ for $\lambda_{BB} = \lambda_{FF} = 1 \times 10^{-5}$ and $\lambda_{BF} = 1 \times 10^{-5}$ as show in figure 1(a). If fermion-fermion is greater than boson-fermion interaction, we found a miscibility of probabilities until $\tau \approx 905.90$ for $\lambda_{BB} = 1$, $\lambda_{FF} = 3 \times 10^{-5}$ and $\lambda_{BF} = 1 \times 10^{-5}$, which indicates that the interaction parameter $\lambda_{BF}$ induces a greater repulsive interaction in the bosons, forcing them to stay together for a shorter time and giving rise to immiscible phase more quickly, as illustrated in the figure 1(b).

It is interesting to note that by increasing the value of the interaction between bosons to $\lambda_{BB} = 7 \times 10^{-5}$ and considering that $\lambda_{BF} > \lambda_{BB}$ the two probabilities tend to be together until $\tau \approx 4090.97$ and the separation between the two probabilities tend to be closer than in the previous case. This is due to the fact that by increasing the interaction parameter between bosons, they tend to separate more quickly and due to the increase in $\lambda_{BF} = 5 \times 10^{-5}$, a repulsive potential is induced in the fermions that forces them to separate more quickly, as can be seen in figure 1(c). For these values, our study revealed that due to the small interaction between fermions, they tend to stay together on the right side of the double well (blue circles) in relation to the bosons (red squares), which separate more quickly for similar values, as seen in the figure 1.

By increasing the order of the interaction parameters, we found that in the regime of $\lambda_{BB} \geq \lambda_{BF}$, densities of bosons and fermions are overlapping when the two species begin their tunneling process on the left side of the double well in approximately the same time, again displaying a miscible phase for $\lambda_{BB} = 9 \times 10^{-4}$, $\lambda_{FF} = 1 \times 10^{-4}$ and $\lambda_{BF} = 1 \times 10^{-4}$ that is maintained until the two species peak again on the right side of the well. The amplitude of bosons and fermions probability densities is different after the first tunneling, which is evidence of the time dependence of the miscible phase; before reaching the second tunneling, the probability of the two species ceases to be the same, giving rise to an immiscible phase as show in figure 2(a). We found a transitive process from correlated Rabi oscillation of the boson particles to the apparent uncorrelated collapse-revival oscillation of $P_{BB}^{BF}(\tau)$ [79, 83] due to an increasing temporary decay of the bosons oscillation amplitude (red squares) as show in figure 2(a). However when we increase the adimensional time, we found a apparent destruction of the uncorrelated collapse-revival oscillation as seen in the figure 2(b), which indicates that the bosons tunnel through the central barrier in correlated state at least in the ranges investigated. This phenomenon indicates that due to the boson-fermion interaction, an attractive boson-boson interaction is induced and that forces the bosons to tunnel in a correlated state.

Another interesting result that emerges from this research, is related to the sensitivity of the system to change in the magnitude order of the interaction parameters, thus when comparing figure 1(a) with figure 2(a), we find that in the latter, the repulsive interaction inter and intra particles allows a richer dynamics of the system, in which the particles move from one side of the double well to the other, with widely varying probability densities.

4. Summary and conclusion

We have investigated the ground state properties of a two-component model where boson-boson, fermion-fermion and boson-fermion interaction is a weak repulsive contact potential and the two species are confined in the same one dimensional double well potential. Tuning the ratio between the inter and intraspecies interaction strengths we found that for orders of magnitude smaller than $10^{-5}$ the particles do not have enough energy to cross the potential barrier producing a complete miscibility of the wave functions of bosons and fermions. On the other hand for orders of magnitude $\geq 10^{-5}$, although in the initial state both species are considered to the right side of the confinement potential, the probability densities of both species are completely different, in the regime $\lambda_{BF} > \lambda_{BB}$ giving rise to a immiscible phase. This phase occurs because fermions, despite their repulsive interaction, tend to stay longer in the initial state, while bosons tend to separate more quickly due to the fact that in addition to the repulsive contact potential between bosons, a repulsive potential is induced in them, for fermion-fermion and boson-fermion interaction
In the regime $\lambda_{BB} \geqslant \lambda_{BF}$ probability densities of bosons and fermions are overlapping, giving rise to a miscibility phase that disappears as a function of time. These results indicate that the immiscible and miscible phases depend on the competition between the inter and intra species interaction strength and are characterized by negligible and complete overlap of the density probabilities, respectively.

As a final attempt we increase the order of the interaction parameters, and found that the miscible phase is a time function again and as a result of the interaction between bosons and fermions the system presents an apparent destruction of the uncorrelated collapse-revival oscillation of boson density probability at least in the ranges investigated.

Our findings can help interpret experimental results in bosonic Josephson junction, squeezing, entanglement of matter waves, matter wave interference and in quantum information processing.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).
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