Nonlinear quantum model for atomic Josephson junctions with one and two bosonic species

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Abstract

We study atomic Josephson junctions (AJJs) with one and two bosonic species confined by a double-well potential. Proceeding from the second quantized Hamiltonian, we show that it is possible to describe the zero-temperature AJJ microscopic dynamics by means of extended Bose–Hubbard (EBH) models, which include usually neglected nonlinear terms. Within the mean-field approximation, the Heisenberg equations derived from such two-mode models provide a description of AJJ macroscopic dynamics in terms of ordinary differential equations (ODEs). We discuss the possibility of distinguishing the Rabi, Josephson and Fock regimes in terms of the macroscopic parameters which appear in the EBH Hamiltonians, and then in the ODEs. We compare the predictions for the relative populations of the Bose gas atoms in the two wells obtained from the numerical solutions of the two-mode ODEs, with those deriving from the direct numerical integration of the Gross–Pitaevskii equations (GPEs). Our investigations show that the nonlinear terms of the ODEs are crucial to achieve a good agreement between the ODE and GPE approaches, and in particular to give quantitative predictions of the self-trapping regime.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The prediction \cite{1} of Bose–Einstein condensation (BEC) and the experimental achievement of BEC \cite{2} has played a crucial role for theoretical and experimental developments in the physics of ultracold atoms. The study of the atomic counterpart \cite{3–7} of the Josephson effect which occurs in superconductor–oxide–superconductor junctions \cite{8}—which is an example of macroscopic quantum coherence—represents one of these developments. Albiez \textit{et al} \cite{9} have provided the first experimental realization of the atomic Josephson junction (AJJ) previously analysed theoretically in a number of papers \cite{3–7}. In 2007, Gati \textit{et al} \cite{10} reviewed the experiment by Albiez \textit{et al} \cite{9} and compared the experimental data with the predictions of a many-body two-mode model \cite{11} and a mean-field description. In the above references the analysis of AJJ physics is carried out in the presence of a single bosonic component. The possibility of tuning intra- and inter-species interactions \cite{12, 13} by means of the Feshbach resonance technique makes it possible to study the AJJs with two bosonic species trapped together by double-well potentials and to use BEC mixtures as powerful instruments to investigate quantum coherence and nonlinear phenomena, with particular attention to the existence of self-trapped modes and intrinsically localized states.

In the superfluid regime, the dynamics of the relative populations and relative phases of the Bose condensed atoms can be described by Josephson’s two-mode equations, which are ordinary differential equations (ODEs), see for example \cite{5, 14–17}. This description is achieved in the presence of a confining double-well potential with a single bosonic component \cite{5} and also with bosonic mixtures \cite{14–18}. One of the most interesting aspects of AJJ analysis is to compare the predictions derived from the ODEs with the...
ones obtained from the Gross–Pitaevskii equations (GPEs). For single-component condensates, Salasnich et al [6] have shown that a good agreement exists between the results obtained from the GPE and those of the ODEs. Similar agreement was obtained in [7] for AJJs realized with weakly interacting solitons localized in two adjacent wells of an optical lattice. However, the situation may be quite different for multicomponent condensates due to the interplay of intra- and inter-species interactions which enlarges the number of achievable states (for instance, mixed symmetry states can exist only in the presence of the inter-species interaction) as well as their stability, giving to the system many more dynamical possibilities. Recently it was shown that for the two-component case, the integration of the ODEs allows us to predict the phenomenon analogous to the macroscopic quantum self-trapping phenomenon observed in AJJs with one bosonic component [15, 17]. This phenomenon has been discussed for a two-component nonlinear Schrödinger model with a double-well potential by Wang and co-workers [19]. More recently, a comparison between the reduced ODE system and the full GPE dynamics was performed, showing that, for various conditions, a good agreement exists between the two kinds of predictions [17].

The aim of the present work is to analyse how the accuracy of the two-mode approximation can be improved by taking into account the usually neglected nonlinear terms. These terms were derived from the overlaps between wavefunctions localized in different wells. Both for single-component and for two-component AJJs—introduced in section 2—we proceed from a full second quantized description of the system. In section 3, we describe the system by the extended Bose–Hubbard (EBH) Hamiltonian. In the single-component case, the EBH Hamiltonian is the two-site restriction of the Hamiltonian considered in [20, 21] to analyse bosons loaded in one-dimensional optical lattices. In the two-species case, the EBH Hamiltonian is the extended version of the one considered by Kuklov and Svidunov in [22] to study the countercflow superfluidity of two-species ultracold atoms. We note that the study of the two-component bosonic system proceeding from a pure quantum approach is a subject of wide interest. In fact, this topic is dealt with in certain regions of the phase space in [23] and in the case of hardcore bosons as discussed in [24].

The EBH Hamiltonian sustains the dynamics of the single-particle operators via the Heisenberg equations of motion [25, 26]. By performing the mean-field approximation on the single-particle operators of each component, the improved ODEs are achieved. In section 3, we also discuss how it is possible to distinguish the Rabi regime, the Josephson regime and the Fock regime. This analysis is carried out in terms of the macroscopic parameters involved in the EBH Hamiltonians, and then on the right-hand sides of the improved ODEs as discussed for single AJJs in [27]. In section 4, we write down the GPEs for the one- and the two-component AJJs. Here we compare the results obtained by numerically integrating the GPEs with the predictions obtained by numerically solving the improved ODEs. Also, in section 4, we plot the phase-plane portraits of the dynamical variables’ fractional imbalance-relative phase. Finally, in section 5, we draw our conclusions.

![Figure 1](image-url)

**Figure 1.** The double-well potential (2) as a function of \( z \) for \( z_0 = 3 \) and different values of \( b \). The dot-dashed line corresponds to \( b = 0.7 \), the continuous line corresponds to \( b = 1 \) and the dashed line corresponds to \( b = 1.3 \). Lengths are measured in units of \( a_{\perp,i} = \frac{\hbar}{m_i\omega_i} \) and energies in units of \( \hbar \omega \).

2. The system

We consider two interacting dilute and ultracold Bose gases denoted below by 1 and 2. We suppose that the two gases are confined in a double-well trap produced, for example, by a far off-resonance laser barrier that separates each trapped condensate into two parts, L (left) and R (right). We assume, moreover, that the two condensates interact with each other and that the trapping potential \( V_{\text{trap}}(\mathbf{r}) \) for both components is taken to be the superposition of a strong harmonic confinement in the radial \((r,y)\) plane and of a double-well (DW) potential in the axial \((z)\) direction. We model the trapping potential as

\[
V_{\text{trap}}(\mathbf{r}) = \frac{m_i\omega_i^2}{2}(x^2 + y^2) + V_{\text{DW}}(z),
\]

where \( m_i \) is the mass of the \( i \)th component. For simplicity, we take \( \omega_1 = \omega_2 \equiv \omega \). For symmetric configurations in the \( z \) direction, we take—for the \( i \)th species—the double-well potential in equation (1) as

\[
V_{\text{DW}}(z) = V_L(z) + V_R(z),
\]

\[
\begin{align*}
V_L(z) &= -V_0 \left[ \text{sech}^2 \left( \frac{z + z_0}{b} \right) \right], \\
V_R(z) &= -V_0 \left[ \text{sech}^2 \left( \frac{z - z_0}{b} \right) \right], \\
V_0 &= \hbar \omega_0 \left[ 1 + \text{sech}^2 \left( \frac{2z_0}{b} \right) \right]^{-1},
\end{align*}
\]

that is the combination of two Pöschl–Teller (PT) potentials, \( V_L(z) \) and \( V_R(z) \), centred at the points \(-z_0\) and \( z_0 \) and separated by a potential barrier which may be changed by varying \( b\) (see figure 1). We use PT potentials only for the benefit of improving accuracy in our numerical GPE calculations (see section 4), taking advantage of the integrability of the underlying linear system. We remark, however, that our results apply to a generic double-well potential. Eigenvalues and eigenfunctions of the PT potential for a single well are known analytically. The wavefunctions of the ground state of \( V_y(z) \) \((\alpha = L, R)\), centred around \(-z_0\) \((\pm z_0)\), are [28]

\[
\phi_{(\alpha,i,PT)}(z) = A \left[ 1 - \tanh^2 \left( \frac{z \pm z_0}{b} \right) \right]^{\beta_i/2},
\]

\[
B_i = -\frac{1}{2} + \sqrt{\frac{2m_iV_0b^2}{\hbar^2} + \frac{1}{4}}.
\]
The constant $A$, in equation (3), ensures the normalization of the wavefunction in each well.

### 3. The second quantization Hamiltonian

To describe our system at zero temperature, we proceed from the second quantized Hamiltonian, which reads

$$
\hat{H} = \sum_{i=1,2} \int d^3r \hat{\Psi}_i^\dagger (\mathbf{r}) \left( \frac{\hbar^2}{2m_i} \nabla^2 + V_{\text{trap}}(\mathbf{r}) \right) \hat{\Psi}_i (\mathbf{r}) + \sum_{i=1,2} \int d^3r \hat{\Psi}_i^\dagger (\mathbf{r}) \hat{\Psi}_i^\dagger (\mathbf{r}) \hat{\Psi}_i (\mathbf{r}) \hat{\Psi}_i (\mathbf{r})
$$

where $V_{\text{trap}}(\mathbf{r})$ is the potential (1). The coupling constants $g_i$ and $g_{12}$ are the intra- and inter-species atom–atom interaction strengths, respectively. These constants are given by

$$
g_i = \frac{4\pi\hbar^2a_i}{m_i}, \quad g_{12} = \frac{2\pi\hbar^2a_{12}}{m_r},
$$

where the reduced mass $m_r$ is equal to $m_1m_2/(m_1 + m_2)$. Equations (5) and (6) relate the two coupling constants to the respective s-wave scattering lengths, $a_i$ and $a_{12}$. In the following, we shall consider both $g_i$ and $g_{12}$ as free parameters due to the possibility of changing the s-wave scattering lengths $a_i$ and $a_{12}$ by the technique of Feshbach resonances. In the following, we will neglect the mass difference between the two bosonic components of the mixture, as for example in [13], and assume that $m_1 = m_2 \equiv m$. In equation (4), the field $\hat{\Psi}_i (\mathbf{r}) \ (\hat{\Psi}_i^\dagger (\mathbf{r})$ destroys (creates) a boson of the $i$th species at the point $\mathbf{r}$, and obeys the usual boson commutation relations.

We expand the field operator $\hat{\Psi}_i (\mathbf{r})$ in terms of the operators $\hat{a}_{\alpha,i}, (\hat{a}_{\alpha,i})^\dagger$—destroying (creating) a boson of the $i$th species in the well $\alpha = L, R$—according to

$$
\hat{\Psi}_i (\mathbf{r}) = \sum_{\alpha=L,R} \Phi_{\alpha,i} (\mathbf{r}) \hat{a}_{\alpha,i},
$$

where the $\hat{a}$ and $\hat{a}^\dagger$ satisfy the usual boson commutation relations, and the functions $\Phi_{\alpha,i} (\mathbf{r})$ can be decomposed as

$$
\Phi_{\alpha,i} (\mathbf{r}) = u_i (x) u_i (y) \phi_{\alpha,i} (z),
$$

where $u_i (x)$ and $u_i (y)$ are the ground state wavefunctions of the harmonic oscillator potentials $m_i\omega_i^2 x^2/2$ and $m_i\omega_i^2 y^2/2$, respectively. The functions $\phi_{L,i} (z)$ and $\phi_{R,i} (z)$ on the right-hand side of equation (8) are the two functions well localized in the left and right well, respectively. These functions are real and orthonormal. The functions $\phi_{\alpha,i} (z)$ and $\phi_{\beta,i} (z)$ can be determined following the same perturbative approach as in [17]. Under the same conditions, these functions may be written in terms of $\phi_{(L,i,PT)} (z)$ and $\phi_{(R,i,PT)} (z)$ of equation (3) as

$$
\phi_{L,i} (z) = \frac{1}{2} \left[ \left( \frac{1}{\sqrt{1+s}} + \frac{1}{\sqrt{1-s}} \right) \phi_{(L,i,PT)} (z) \right]
$$

and

$$
\phi_{R,i} (z) = \frac{1}{2} \left[ \left( \frac{1}{\sqrt{1+s}} - \frac{1}{\sqrt{1-s}} \right) \phi_{(L,i,PT)} (z) \right],
$$

where $s = \int_{-\infty}^{+\infty} dz \phi_{(L,i,PT)} (z)\phi_{(R,i,PT)} (z)$.

#### 3.1. AIs with a single bosonic species

Let us start our analysis by considering the presence of a single bosonic component. In this case, the inter-species coupling constant (6) is equal to zero. We use the field operator expansion (8) in the second quantized Hamiltonian (4). The AIJ microscopic dynamics is controlled by the EBH Hamiltonian [20, 25, 26]. The EBH model, by omitting the species index $i$, is described by the Hamiltonian

$$
\hat{H}_{\text{EBH}} = E_L^0 \hat{a}_L \hat{a}_L + E_R^0 \hat{a}_R \hat{a}_R + \frac{U_L}{2} \hat{a}_L \hat{a}_L \hat{a}_R \hat{a}_R - K (\hat{a}_L \hat{a}_R + \hat{a}_R \hat{a}_L)
$$

and

$$
+ K_0 (\hat{a}_L^2 \hat{a}_R \hat{a}_R + \hat{a}_R^2 \hat{a}_L \hat{a}_L + \hat{a}_R \hat{a}_L \hat{a}_R + \hat{a}_L \hat{a}_R \hat{a}_L + \hat{a}_R \hat{a}_L \hat{a}_R + \hat{a}_L \hat{a}_R \hat{a}_L).
$$

Here $\hat{a}_a = \hat{a}_L \hat{a}_R$ is the number of particles in the orth well. $E_0^0$ are the energies of the two wells, $U_0 > 0$ are the boson–boson repulsive interaction amplitudes and $K$ is the tunnel matrix element, which is the Rabi oscillation energy in the case of a model with $U_0$ equal to zero. The parameter $K_0$ is the induced collisional hopping amplitude, $V$ is the density–density bosonic interaction amplitude and $K_p$ describes the pair bosonic hopping [20]. By using the decomposition (8) and the explicit form of $w(x)$ and $w(y)$, the macroscopic parameters (10) may be shown to be related to the intra-species coupling constant (5) and to the other microscopic parameters (the mass and the frequency of the harmonic trap) by the formulæ

$$
E_0 = \int dz \left( \frac{\hbar^2}{2m} \left( \frac{d\phi}{dz} \right)^2 + \left( V_{\text{DWC}} + \frac{\hbar^2}{2ma^2} + \frac{m\omega^2a^4}{2} \right) (\phi^2)^2 \right)^2
$$

and

$$
K = \int dz \left( \frac{\hbar^2}{2m} \frac{d\phi}{dz} \frac{d\phi}{dz} + V_{\text{DWC}} (\phi L \phi R) \right)
$$

and

$$
K_e = \int dz \left( \frac{\hbar^2}{2m} \frac{d\phi}{dz} \frac{d\phi}{dz} + V_{\text{DWC}} (\phi L \phi R) \right)
$$

and

$$
V = 2\tilde{g} \int_{-\infty}^{+\infty} dz (\phi_L (z))^3 (\phi_R (z))^3
$$

and

$$
K_p = \frac{V}{4},
$$

where $\tilde{g} = \frac{g}{\pi a^2}$. We observe that the first two lines of Hamiltonian (10) involve only the overlaps between $\phi_a$.
localized in the same well, see [5]. The third and fourth lines of the Hamiltonian (10) also include the overlaps between \( \phi_a \) localized in different wells, see [27]. Proceeding from the Hamiltonian (10), we write down criteria to individuate different oscillation regimes sustained by the AJJ dynamics. To this end, as discussed in [4, 27], we express the Hamiltonian (10) in terms of the following operators:

\[
\begin{align*}
\hat{J}_x &= \frac{1}{2}(\hat{a}^\dagger_L\hat{a}_L - \hat{a}^\dagger_R\hat{a}_R) \\
\hat{J}_y &= \frac{1}{2}(\hat{a}^\dagger_L\hat{a}_R - \hat{a}^\dagger_R\hat{a}_L) \\
\hat{J}_z &= \frac{1}{2}(\hat{a}^\dagger_L\hat{a}_R + \hat{a}^\dagger_R\hat{a}_L),
\end{align*}
\]

and the SU(2) algebra invariant \( \mathcal{J}^2 = (\hat{N}/2)(\hat{N}/2 + 1) \), with \( \hat{N} \) being equal to \( \hat{n}_L + \hat{n}_R \).

We assume that the two potential wells are symmetric, \( E_L^0 = E_R^0 = E \) and \( U_L = U_R = U \). Neglecting constant terms and using the fact that \( N \gg 1 \), we obtain

\[
\hat{H} = (U - V)\mathcal{J}_z^2 - 2(K - K_z)\mathcal{J}_x + V\mathcal{J}_z^2.
\]

Here, if the condition \( (U - V) \gg V \) is verified, we can consider only the terms in \( \mathcal{J}_x^2 \) and \( \mathcal{J}_z^2 \). Then by defining the parameter \( R \) as

\[
R = \frac{(U - V)N}{(K - K_z)N},
\]

we are able (see [41]) to distinguish the following three regimes:

- **Rabi**: \( R \ll 1 \);
- **Josephson**: \( 1 < R \ll N^2 \);
- **Fock**: \( N^2 \ll R \).

In the Rabi regime, the bosons are in a coherent state and oscillate with a frequency given simply by the energy difference between the ground state and the first excited state associated with the double-well potential. In the Josephson regime, the bosons are in a coherent state and oscillate with a frequency which depends on the parameters \( U, K_z \) and \( V \). Moreover, if the interaction strength is sufficiently large, self-trapping takes place. In the Fock regime, the bosons are in a Fock state characterized by the suppression of number fluctuations. Now, we observe that the Hamiltonian (10) can be viewed as the two-site restriction of the Hamiltonian considered in [20, 21] within the study of bosons loaded in one-dimensional optical lattices. In particular, in [20] it is shown that within the Fock regime two regions open up. To this end, we denote by \( \Delta \) the energetic gap between the Fock state with \( N_0 \) bosons per well and the Fock state with \( (N_0 + 1) \) per well [20]:

\[
\Delta = 2(E + U N_0).
\]

Then, when

\[
|4\Delta - (2N_0 + 1)V| > V,
\]

we have a pure Mott insulating phase (PMI), driven by the density-density on-site interaction. When

\[
|4\Delta - (2N_0 + 1)V| < V,
\]

we have a density-wave Mott insulating (DWMI) regime, driven by the nearest-neighbour interaction [20]. Note that the DWMI phase is characterized by number fluctuations suppression as well.

At this point, we remark that we are interested in determining the fully coherent dynamical oscillations of the population of the Bose condensed atoms between the left and right wells. Then, we proceed from the Heisenberg equations of motion for the model Hamiltonian (10). These equations of motion control the temporal evolution of \( \hat{n}_a \). We observe that in the superfluid regime, the system is in a coherent state and the following mean-field approximation [25] can be performed:

\[
\langle \hat{n}_a \rangle = \sqrt{N_a}\exp(i\theta_a) \quad \langle \hat{n}_a \rangle = N_a.
\]

The averages involved in equation (18) are evaluated with respect to the coherent state. Under the assumption of symmetric wells and by inserting the mean-field approximation (18) into the aforementioned Heisenberg equations of motion, we obtain

\[
\begin{align*}
\dot{\theta}(t) &= \frac{N}{2\hbar}(1 - z^2(t)) \sin 2\theta(t) \\
\dot{z}(t) &= \frac{2(K - K_z)(N - N_L)}{h} z(t) \cos \theta(t)
\end{align*}
\]

where \( z = (N_L - N_R)/N \) and \( \theta = \theta_R - \theta_L \) are, respectively, the fractional imbalance and the relative phase.

3.2. **AJJs with two bosonic species**

In this subsection we shall consider AJJs in the presence of two interacting bosonic components. In this case, both the coupling constants (5) and (6) are finite, and the two-mode EBH model is described by the Hamiltonian

\[
\hat{H} = \sum_{i=1,2} \hat{H}_{(EBH,i)} + \hat{H}_{12}.
\]

The Hamiltonian \( \hat{H}_{(EBH,i)} \) is the single-component Hamiltonian (10) written in terms of the operators \( \hat{a}_{a,i} \) and \( \hat{a}^\dagger_{a,i} \). The parameters \( E^0_{a,i}, U_{a,i}, K_{C,i}, V, K_p \) and the function \( \phi_a \) read \( E^0_{a,i}, U_{a,i}, K_{C,i}, V, K_p \) and \( \phi_{a,i} \), respectively. The microscopic quantities referred to as a single bosonic component will be modified according to the same prescription. Under the hypothesis of symmetric wells, the coupling Hamiltonian \( \hat{H}_{12} \) reads

\[
\hat{H}_{12} = U_{12}(\hat{a}^\dagger_{L,1}\hat{a}^\dagger_{L,2}\hat{a}_{L,1}\hat{a}_{L,2} + \hat{a}^\dagger_{R,1}\hat{a}^\dagger_{R,2}\hat{a}_{R,1}\hat{a}_{R,2})
\]

\[
+ V_{12}(\hat{a}^\dagger_{L,1}\hat{a}^\dagger_{R,2}\hat{a}_{L,1}\hat{a}_{R,2} + \hat{a}^\dagger_{L,2}\hat{a}^\dagger_{R,1}\hat{a}_{L,2}\hat{a}_{R,1})
\]

\[
+ K_{p,12}(\hat{a}^\dagger_{L,1}\hat{a}^\dagger_{L,2}\hat{a}_{R,1}\hat{a}_{R,2} + \hat{a}^\dagger_{R,1}\hat{a}^\dagger_{R,2}\hat{a}_{L,1}\hat{a}_{L,2})
\]

\[
+ K_{C,12}(\hat{a}^\dagger_{L,1}\hat{a}_{L,2}\hat{a}_{R,1}\hat{a}_{R,2} + \hat{a}^\dagger_{L,2}\hat{a}_{L,1}\hat{a}_{R,1}\hat{a}_{R,2})
\]

\[
+ \hat{a}^\dagger_{L,1}\hat{a}_{L,2}\hat{a}_{R,1}\hat{a}_{R,2} + \hat{a}^\dagger_{R,1}\hat{a}_{R,2}\hat{a}_{L,1}\hat{a}_{L,2}
\]

\[
+ \hat{a}^\dagger_{L,2}\hat{a}_{L,1}\hat{a}_{R,1}\hat{a}_{R,2} + \hat{a}^\dagger_{R,2}\hat{a}_{R,1}\hat{a}_{L,1}\hat{a}_{L,2}
\]
In equation (21), $U_{12}$ is the inter-species interaction amplitude between the bosons localized in the same well and $V_{12}$ is the inter-species interaction amplitude between the bosons localized in different wells. The quantity $K_{p,12}$ is the inter-species pair hopping (hopping of particle–particle or hole–hole pairs made up of bosons of different species); $K_{c,12}$ is the amplitude of the inter-species collisionally induced hopping. By using the decomposition (8) and the explicit form of $w_i(x)$ and $w_j(y)$, the aforementioned parameters are shown to be related to the inter-species coupling constant (6) by

$$
\begin{align*}
U_{12} &= \bar{g}_{12} \int_{-\infty}^{+\infty} dz (\phi_{a,i}(z))^2 (\phi_{a,j}(z))^2 \\
V_{12} &= \bar{g}_{12} \int_{-\infty}^{+\infty} dz (\phi_{a,i}(z))^2 (\phi_{b,j}(z))^2 \\
K_{c,12} &= \bar{g}_{12} \int_{-\infty}^{+\infty} dz (\phi_{a,i}(z))^3 (\phi_{b,j}(z)) \\
K_{p,12} &= V_{12},
\end{align*}
$$

where $\bar{g}_{12} = \frac{\bar{g}_{12}}{\pi a_1 a_2}$. Note that we are considering both the overlaps between $\phi_a$ localized in the same well ($U_{a,i}$ and $U_{12}$)—that are the only terms taken into account in [17]—and the overlaps between $\phi_b$ localized in different wells ($V_{12}$, $K_{p,12}$, $K_{c,12}$). We observe that, in general, due to the presence of the parameters (22), the identification of different oscillation regimes proceeding from the Hamiltonian (20) is not immediate as for single-component AJJs. Nevertheless, under certain conditions, we are able to write down the criteria to select the different regimes sustained by the two-component AJJ dynamics. First, let us focus on the case in which only the overlaps between $\phi_a$ localized in the same well are considered. If certain relations exist between the intra- and the inter-species interaction amplitudes, we can recognize the two species corresponding to the Rabi, Josephson and Fock regimes discussed in the case of single-component AJJs. For each component $i$, we define the quantity $\gamma_i$ as

$$
\gamma_i = \frac{U_i N_i}{K_i}.
$$

We recognize the following 'weak-coupled' Rabi, Josephson, and Fock regimes

- **Rabi**: $\gamma_R \ll 1$, $|U_{12}| \approx |U|$;
- **Josephson**: $1 \ll \gamma_J \ll N^2$, $|U_{12}| \ll U$;
- **Fock**: $N^2 \ll \gamma_F$.

In the Josephson regime, even if the intra-species interaction is not strong enough to ensure self-trapping by itself, self-trapping occurs when the inter-species interaction strength exceeds a crossover value. In the Fock regime, the net number of atoms in the transport is suppressed. However, with repulsive inter-species interaction, the so-called counterflow survives [22]. This means that the currents of the two species are equal in absolute values and are in opposite directions. This conductive regime is named super(counter)fluid phase (SCF).

As discussed in [22], the system supports the SCF phase of the two components when

$$
U_1 + U_2 - 2U_{12} \gg 1.
$$

When the condition

$$
U_1 + U_2 = 2U_{12}
$$

is met, a phase separation (PS) is observed in the system, and the system can be viewed as composed of two totally independent Bose gases confined in the double-well potential. On a physical level, this phase separation means that one bosonic component will occupy the left well and the other the right well. If the inter-species interaction is attractive and the hypothesis $N_1 = N_2 = N$ is verified, then, when

$$
U_1 + U_2 - 2|U_{12}| \gg 1,
$$

a superfluid phase, in which the superfluid consists of pairs of bosons, is supported by the system. This phase is named the superfluid paired phase [30].

So far we have neglected the role played by the terms derived from the overlaps between $\phi_b$ localized in different wells. The presence of these terms makes the scenario more complicated. However, also in this situation, under certain conditions, it is possible to achieve a classification of the oscillation regimes. To this end, as discussed for the single-component case, we express the Hamiltonian (20) in terms of the operators $\hat{J}_{x,i}, \hat{J}_{y,i}, \hat{J}_{z,i}$ defined in equation (12) and the SU(2) algebra invariant $\hat{J}_{i}^2 = (\hat{N}_i/2)^2 + 1$, with $\hat{N}_i$ being equal to $\hat{n}_{L,i} + \hat{n}_{R,i}$. Since we are assuming symmetric potential wells, we can write that $E_{L,i}^i = E_{R,i}^i = E_i, U_{L,i} = U_{R,i} = U_i$. Neglecting the constant terms and using the fact that $\hat{N}_i \gg 1$, we obtain

$$
\hat{H} = (U_i - V_i) \hat{J}_{x,i}^2 - 2(K - K_{c,i}) \hat{N}_i - K_{c,12} \hat{N}_j \hat{J}_{z,j}
\begin{align*}
+ & V_j \hat{J}_{z,j}^2 + 4((U_i - V_i) \hat{J}_{x,i,j} \hat{J}_{x,j} + V_j \hat{J}_{x,j}^2)
+ U_{12} (\hat{n}_{L} \hat{\bar{\rho}}_{R,2} + \hat{n}_{R} \hat{\bar{\rho}}_{L,2}) + U_{12} (\hat{n}_{L} \hat{\bar{\rho}}_{L,2} + \hat{n}_{R} \hat{\bar{\rho}}_{R,2} + \hat{n}_{R} \hat{\bar{\rho}}_{L,2} + \hat{n}_{L} \hat{\bar{\rho}}_{R,2}).
\end{align*}
$$

Again, if $(U_i - V_i) \gg V_i, V_j, \text{ and } (U_{12} - V_{12}) \gg V_i, V_j$, we can consider only the terms in $\hat{J}_{x,i}^2, \hat{J}_{y,i}$ and $\hat{J}_{x,j} \hat{J}_{z,j}$. We will assume also that $N_i = N_2 \equiv N, U_1 = U_2 \equiv U, V_1 = V_2 \equiv V$ and $K_{c,i} = K_{c,12} \equiv K_c$, and that the initial conditions are the same for both the components. In analogy with the case of a single-component AJJ, we define the parameter $\tilde{R}$ as

$$
\tilde{R} = \frac{(U - V) + 4(U_{12} - V_{12})N}{(K - (K_c + K_{c,12})N).}
$$

Again, we are able to distinguish the three regimes.

- **Rabi**: $\tilde{R} \ll 1$;
- **Josephson**: $1 \ll \tilde{R} \ll N^2$;
- **Fock**: $N^2 \ll \tilde{R}$.

At this point, we remark that we are interested in determining the fully coherent dynamical oscillations of the population of the two bosonic components between the left and right wells. Then, we proceed from the Heinsenberg equations of motion for the model Hamiltonian (20). These equations of motion control the temporal evolution of $\hat{\bar{\rho}}_{a,i}$. Again, by inserting the mean-field approximation valid in the superfluid regime—$(\hat{\bar{\rho}}_{a,i}) = \sqrt{N_{a,i}} \exp(i\hat{\theta}_{a,i})$, $(\hat{\bar{\rho}}_{a,i}) = N_{a,i}$—into the
the aforementioned Heisenberg equations of motion, one obtains the coupled differential equations for the fractional imbalance \( z_i = (N_{L,i} - N_{R,i})/N_i \) and the relative phase \( \theta_i = \theta_{R,i} - \theta_{L,i} \) of the two species:

\[
\dot{z}_i(t) = \frac{2(K_i - K_{c,i}N_i)}{\hbar} \sqrt{1 - z_i^2(t)} \sin \theta_i(t) + \frac{V_iN_i}{2\hbar}(1 - z_i^2(t)) \sin 2\theta_i(t) + \frac{2}{\hbar}(V_{12} \sqrt{1 - z_i^2(t)} \cos \theta_i(t) + K_{c,12}) \\
\times N_i \sqrt{1 - z_i^2(t)} \sin \theta_i(t) \\
- \frac{V_i}{2\hbar} \frac{2}{\hbar} \sqrt{1 - z_i^2(t)} \cos \theta_i(t) + \frac{U_{12} - V_{12}}{\hbar} N_i z_i(t) \\
- \frac{2}{\hbar} (V_{12} \sqrt{1 - z_i^2(t)} \cos \theta_i(t) + K_{c,12}) \\
\times N_i \sqrt{1 - z_i^2(t)} \sin \theta_i(t).
\] (29)

4. Gross–Pitaevskii equation predictions: comparison with ordinary differential equation results

So far we have discussed how AJJ dynamics can be described by means of the ODEs, i.e. equations (19) and (29). We know that AJJ dynamics can be analysed, in the mean-field approximation, in terms of partial differential equations, i.e. the GPEs. This description can be achieved proceeding from the Heisenberg motion equations for the field operators \( \hat{\Psi}_i(\mathbf{r}, t) \) (\( i = 1, 2 \)) associated with the Hamiltonian (4), that is

\[
\hat{\mathcal{H}} \hat{\Psi}_i = [\hat{\Psi}_i, \hat{\mathcal{H}}].
\] (30)

The average—denoted by \( \langle \ldots \rangle \)—of both sides of equation (30) evaluated with respect to the coherent state, provides the two coupled GPEs

\[
\hat{\mathcal{H}} \hat{\Psi}_i = \hat{\mathcal{H}} \hat{\Psi}_i = \frac{\hbar^2}{2m_i} \nabla^2 \hat{\Psi}_i + \frac{\hbar}{2m_i} \dot{\theta}_i(t) \nabla^2 \hat{\Psi}_i + [V_{\text{trap}}(\mathbf{r}) + g_i |\hat{\Psi}_i|^2 + g_{ij} |\hat{\Psi}_j|^2] \hat{\Psi}_i.
\] (31)

The macroscopic wavefunctions \( \Psi_i(\mathbf{r}, t) = \langle \hat{\Psi}_i(\mathbf{r}, t) \rangle \) of interacting BECs in the trapping potential \( V_{\text{trap}}(\mathbf{r}) \) at zero temperature satisfy equation (31). The wavefunction \( \Psi_i(\mathbf{r}, t) \) is subject to the normalization condition

\[
\int d^3 \mathbf{r} |\Psi_i(\mathbf{r}, t)|^2 = N_i.
\] (32)

We are interested in studying the dynamical oscillations of the populations of each condensate between the left and right wells when the barrier is large enough so that the link is weak. To exploit the strong harmonic confinement in the \((x,y)\) plane and to get the effective one-dimensional (1D) equations describing the dynamics in the \(z\) directions, we write the Lagrangian associated with the GPE equations in (31)

\[
L = \int d^3 \mathbf{r} \left[ \sum_{i=1,2} \frac{\hbar^2}{2m_i} \frac{\partial^2 }{\partial t^2} \Psi_i - V_{\text{trap}}(\mathbf{r}) |\Psi_i|^2 - \frac{\hbar}{2} |\Psi_i|^4 \right] - g_{ij} |\Psi_i|^2 |\Psi_j|^2 + V_{\text{Dil}}(|\Psi_i|^2 - |\Psi_j|^2).
\] (33)

where \( \Psi_i^* \) denotes the complex conjugate of \( \Psi_i \), and \( i \neq j \); then, by following the decomposition (8) and the Gaussian approximation for the radial part of wavefunction, we adopt the ansatz

\[
\Psi_i(x, y, z, t) = \frac{1}{\sqrt{\pi a_{L,i} a_{R,i}}} \exp \left[ -\frac{x^2 + y^2}{2a_{L,i}^2} \right] f_i(z, t),
\] (34)

where the field \( f_i(z, t) \) obeys \( \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} 2 \pi d^2 z |f_i(z)|^2 = N_i \), so that the normalization condition given by equation (32) is satisfied. Note that the Gaussian ansatz with the transverse width simply given by \( a_{L,i} \) is reliable under very strong transverse confinements, namely when \( \sqrt{|g_i| f_i^2} \ll 2 \omega_0 \). By inserting the ansatz (34) in equation (33) and performing the integration in the radial plane, we obtain the effective 1D Lagrangian for the field \( f_i(z, t) \). Such an effective 1D Lagrangian reads

\[
\tilde{L} = \int dz \left[ \sum_{i=1,2} \frac{\hbar^2}{2m_i} \frac{\partial^2 f_i}{\partial z^2} + \hbar^2 \dot{\theta}_i^2 \frac{\partial^2 f_i}{\partial z^2} \right] - (\epsilon_i + V_{\text{Dil}}(z)) f_i^2 - \frac{\hbar^2}{2} |\tilde{f}_i|^2 - \tilde{g}_i |\tilde{f}_i|^2 |\tilde{f}_j|^2.
\] (35)

where \( \epsilon_i \) is given by \( \epsilon_i = \frac{\hbar^2}{2m_i} a_{L,i}^2 \). By varying \( \tilde{L} \) with respect to \( \tilde{f}_i \), we obtain the 1D GPE for the field \( \tilde{f}_i \):

\[
\frac{\hbar^2}{2m_i} \frac{\partial^2 f_i}{\partial z^2} = -\epsilon_i - V_{\text{Dil}}(z) - \tilde{g}_i |\tilde{f}_i|^2 - \tilde{g}_{ij} |\tilde{f}_j|^2 |\tilde{f}_i|^2.
\] (36)

In the presence of a single bosonic component, \( g_{12} = 0 \); then, the two coupled 1D GPEs (36), omitting the species index \( i \), reduce to

\[
\frac{\hbar}{2m_i} \frac{\partial^2 f_i}{\partial z^2} = -\epsilon_i + V_{\text{Dil}}(z) + \tilde{g}_i |\tilde{f}_i|^2 + \tilde{g}_{ij} |\tilde{f}_j|^2 |\tilde{f}_i|^2.
\] (37)

Now, we observe that it is possible to write the fields \( f_i (i = 1, 2) \) by using the two-mode approximation as done, for example, in [17]:

\[
f_i(z, t) = \psi_{L,i}(t) \phi_{L,i}(z) + \psi_{R,i}(t) \phi_{R,i}(z) \]

\[
\psi_{i,j}(t) = \sqrt{N_{i,j}}(t) \exp(\Theta_{i,j}(t))
\] (38)

with \( \phi_{i,j}(z) \) constructed as discussed in section 3, see equation (9). Then, one takes into account the overlaps both between \( \phi_{u} \) localized in the same well and between \( \phi_{u} \) localized in different wells. By following the same path as in [17], when the inter-species coupling constant \( g_{12} \) is finite, it is possible to recover equations (29) for binary AJJs, while for \( g_{12} \) equal to zero, one gets back the equations (19) for single-component AJJs.

At this point—both for single-component and for two-components AJJs—we may compare the predictions of the
Figure 2. Fractional imbalance $z(t)$ versus time for single-component atomic Josephson junctions. The parameters of the double-well potential (2) are chosen to be $b = 1$ and $z_0 = 3$. The dashed line represents data from the integration of GPE (37), the continuous line represents data from the integration of ODEs (19) and the dot-dashed one represents data from the integration of ODEs (19) with $K_e = V = 0$. We have set $N = 200$ and $K = 4.955 \times 10^{-3}$. We have used the initial conditions $z(0) = 0.6$ and $\theta(0) = 0$. In the top panels (from left to right): $U = 0.05 K$, $K_e = -1.842 \times 10^{-6}$ and $V = 2.268 \times 10^{-7}$; $U = 0.1 K$, $K_e = -3.684 \times 10^{-6}$ and $V = 4.535 \times 10^{-7}$. In the bottom panels (from left to right): $U = 0.2 K$, $K_e = -7.368 \times 10^{-6}$, $V = 9.070 \times 10^{-7}$; $U = 0.5 K$, $K_e = -1.842 \times 10^{-5}$ and $V = 2.268 \times 10^{-6}$. Time is measured in units of $\omega^{-1}$ and energies are measured in units of $\hbar\omega$.

Figure 3. Phase diagrams of the fractional imbalance $z(t)$ versus macroscopic phase $\theta(t)$ for single-component atomic Josephson junctions. The parameters of the double-well potential (2) are the same as in figure 2. In both the panels we have set $N = 200$ and $K = 4.955 \times 10^{-3}$. Left panel: the dashed line represents data from the ODE (19) with $U = 0.05 K$ and $K_e = V = 0$; the continuous line represents data from the ODE (19) with $U = 0.05 K$, $K_e = -1.842 \times 10^{-6}$ and $V = 2.268 \times 10^{-7}$. Right panel: the phase diagram for self-trapping. In this panel the dashed line represents data from the ODE (19) with $U = 0.2 K$ and $K_e = V = 0$; the continuous line represents data from the ODE (19) with $U = 0.2 K$, $K_e = -7.368 \times 10^{-6}$ and $V = 9.070 \times 10^{-7}$. Initial conditions are the same as in figure 2. Time is measured in units of $\omega^{-1}$ and energies are measured in units of $\hbar\omega$.

Figure 4. Fractional imbalance $z_i(t)$ of the two bosonic species versus time. The parameters of the double-well potential (2) are chosen to be $b = 1$ and $z_0 = 3$. Here, the dashed line represents data from the integration of GPEs (36), the continuous line represents data from the integration of ODEs (29) and the dot-dashed line represents data from the integration ODEs (29) with $K_{e,i} = V_i = K_{e,12} = V_{12} = 0$ (i.e. the ODEs analysed in [17]). We have fixed $N_1 = 200$ and $N_2 = 100$. Moreover, $K_1 = K_2 \equiv K = 4.955 \times 10^{-3}$, $U_1 = U_2 \equiv U = 0.1 K$, $K_{e,1} = K_{e,2} \equiv K_e = -3.684 \times 10^{-6}$ and $V_1 = V_2 = 2.268 \times 10^{-7}$. We used the initial conditions $z_i(0) = 0.5 = -z_i(0)$ and $\theta_i(0) = \theta_i(0) = 0$. In the top panels, we set $U_{12} = -U/20$, $K_{e,12} = -K_e/20$ and $V_{12} = -V/40$, in the middle panels $U_{12} = -U/2$, $K_{e,12} = -K_e/2$ and $V_{12} = -V/4$, and in the bottom panels $U_{12} = -U$, $K_{e,12} = -K_e$ and $V_{12} = -V/2$. Time is measured in units of $(\omega_i)^{-1} = (\omega_0)^{-1} \equiv \omega^{-1}$ and energies are measured in units of $\hbar\omega$.

ODEs, equations (19) and (29), and those of the GPEs, equations (37) and (36). The results of this analysis are reported in figure 2 for the single-component case, and in figures 4 and 6 for the two-component case. In obtaining figure 2, we have fixed the parameters $b$ and $z_0$ of the double-well potential (2). Then, by using the functions (9) into the third line of equations (11), we have obtained the tunnelling amplitude $K$. We have kept fixed $K$ and plotted the predictions of the ODEs (19) for $z(t)$ in correspondence with different intra-species interactions when both $K_e$ and $V$ are zero—dot-dashed lines—and in the presence of $K_e$ and $V$—continuous lines; the dashed lines represent $z(t)$ obtained by numerically integrating the GPE (37). In figures 4 and 6, we have fixed the tunnelling amplitude $K_e$—as done previously in the single-component case—and the intra-species interaction $U_i$, and we have plotted the predictions of the ODEs (29) for $z_i(t)$ in correspondence with different inter-species interactions both when $K_{e,ij}$, $V_i$, $K_{e,12}$, $V_{12}$ are all equal to zero—dot-dashed lines—and in the presence of $K_{e,ij}$, $V_i$, $K_{e,12}$, $V_{12}$—continuous lines; again, the dashed lines represent $z_i(t)$ obtained by numerically integrating the GPE (36). In the two top panels...
Figure 5. Phase diagrams of the fractional imbalance $z_i(t)$ versus macroscopic phase $\theta_i(t)$ of the two bosonic species. The parameters of the double-well potential (2) are the same as in figure 4. In both the panels we have set $N_1 = 200$, $N_2 = 100$, $K_1 = K_2 \equiv K = 4.955 \times 10^{-3}$ and $U_1 = U_2 \equiv U = 0.1 K$. In both the panels, the dashed line represents data from the ODEs (29) with $U_{12} = -U/2$ and $K_{c,i} = V_i = K_{c,12} = V_{12} = 0$, the continuous line represents data from the ODEs with $U_{12} = -U/2$, $K_{c,1} = K_{c,2} = K_c = -3.684 \times 10^{-6}$, $K_{c,12} = -K_{c,2}$ and $V_{12} = -V/4$. Initial conditions are the same as in figure 4. Time is measured in units of $(\omega_0)^{-1} = (\omega_2)^{-1} \equiv \omega^{-1}$ and energies are measured in units of $\hbar \omega$.

Figure 6. Fractional imbalance $z_i(t)$ of the two bosonic species versus time. In the double-well potential (2), we set $b = 1$ and $z_0 = 3$. In this figure, the dashed line represents data from the integration of GPEs (36), the continuous line represents data from the integration of ODEs (29) and the dotted line represents data from the integration ODEs (29) with $K_{c,i} = V_i = K_{c,12} = V_{12} = 0$ (i.e. the ODEs analysed in [17]). We have fixed $N_1 = 200$ and $N_2 = 100$. Moreover, $K_1 = K_2 \equiv K = 4.955 \times 10^{-3}$, $U_1 = U_2 \equiv U = 0.1 K$, $K_{c,1} = K_{c,2} = K_c = -3.684 \times 10^{-6}$, $V_i = V_2 \equiv V = 2.268 \times 10^{-7}$, $U_{12} = -2 U$ and $K_{c,12} = -2 K_c$. Initial conditions are the same as in figure 4. Time is measured in units of $(\omega_0)^{-1} = (\omega_2)^{-1} \equiv \omega^{-1}$ and energies are measured in units of $\hbar \omega$.

of figure 2 and in all the panels of figure 4, we have plotted the temporal evolution of the bosonic fractional imbalances $z_i$ when they oscillate around a zero time-averaged value, i.e. $(z_i(t)) = 0$. We see that the usually neglected nonlinear terms play a crucial role in order to improve the agreement between the OPE and ODE predictions. In fact, neglecting these terms, the solutions of ODEs and GPEs diverge rather rapidly, as shown by dot-dashed lines in figure 2 for single-component AJJs, and by dot-dashed lines in figure 4, for two-component AJJs. The bottom two panels of figure 2 show the results of our analysis when the intra-species interaction amplitude $U$ is sufficiently large to induce oscillations of $z(t)$ around a zero time-averaged value, that is, the self-trapping. We see that the inclusion, within the description of the system, of the usually neglected nonlinear terms produces an improvement in the agreement between the ODE and GPE predictions. In the two-component case, from figure 2 we can see that the nonlinearity associated with the intra-species interaction is not strong enough to induce oscillations of $z_i$ around a non-zero time-averaged value. Nevertheless, if the inter-species interaction is sufficiently large, oscillations of $z_i$ around $(z_i(t)) \neq 0$ are observed. We have shown this kind of behaviour for both the components in figure 6. From this figure we can see that, especially in the case of large inter-species interaction, the role played by the parameters describing the overlaps between $\theta_i$ localized in different wells becomes essential to improve the agreement between the ODE and the GPE predictions. Moreover, in figure 3 for single-component AJJs, and in figures 5 and 7 for two-component AJJs, we show the phase-plane portraits of the dynamical variables $z_i$ and $\theta_i$ for different values of the macroscopic parameters $(11)$ and $(22)$ (see figures 3, 5 and 7 for the details). These figures show the comparison between the trajectories in the phase space obtained by integrating the ODEs in the absence of the usually neglected nonlinear terms (dashed lines), and the trajectories obtained from the improved version of ODEs (continuous lines). In particular, the left and the right panels of figure 3 show the phase space trajectories for the Josephson and self-trapping regimes, respectively, for single-component AJJs. For two-component AJJs, in figure 5 we have plotted the phase space trajectories for the Josephson regime, and in figure 7 we have plotted the phase space trajectories when the system is self-trapped. From figures 3, 5 and 7, we can see that the trajectories predicted when the ODEs (19) and (29) are solved in the absence of the usually neglected nonlinear terms are sufficiently close to those predicted when these ODEs are solved in the presence of the aforementioned terms. Then, the dynamical evolution predicted by the standard ODEs reveals a good degree of reliability.
5. Conclusions

We have analysed atomic Josephson junctions for a single Bose gas and for binary mixtures of bosons in a double-well potential along the axial direction and a strong harmonic confinement in the transverse directions. We have shown that for both cases, the Hamiltonian belongs to the extended Bose–Hubbard model and besides the density–density interaction, it contains the pair hopping and collisionally induced hopping terms. These terms were derived from the overlaps between wavefunctions localized in different potential wells. We started from these Hamiltonian models and established connections with spin Hamiltonians. Proceeding from these, we have discussed the possibility of discriminating, under certain conditions, different dynamical regimes sustained by the bosonic juncions. From the mean-field analysis of the equations of motion for the single-particle operators involved in the extended Bose–Hubbard Hamiltonians, we have obtained the ordinary differential equations that control the macroscopic dynamics of the atomic Josephson junctions. Within the analysis of the atomic Josephson junctions’ macroscopic dynamics, we have plotted the phase-plane portraits of the dynamical variables (fractional imbalance-relative phase) showing that the inclusion of the aforementioned collisionally induced hopping and pair hopping terms are crucial to get good agreement between the dynamics of the Josephson model described by ordinary differential equations and the one of the time-dependent Gross–Pitaevskii equations, especially when the atom–atom interaction is strong.

Finally, it is important to remark that the obtained results are of general validity also for more confining (e.g. not saturating to zero at large distances) double-well potentials. Nevertheless, it is possible to design a model of pair hopping and collisionally induced hopping for bosonic atoms that is physically meaningful when optical lattices play the role of confining potentials. Physical effects related to pair hopping and collisionally induced hopping should be observable in generalizations of recent experiments to detect the superfluid and insulating phases [32].

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